

Dierk Raabe, Publikationen

- Abdellaoui, L., Chen, Z., Yu, Y., Luo, T., Hanus, R., Schwarz, T., Bueno Villoro, R., Cojocar-Mirédin, O., Snyder, G. J., & Raabe, D. (2021). Parallel Dislocation Networks and Cottrell Atmospheres Reduce Thermal Conductivity of PbTe Thermoelectrics. *Advanced Functional Materials*, 31(20), 2101214.
- Abdellaoui, L., Zhang, S., Zaefferer, S., Bueno-Villoro, R., Baranovskiy, A., Cojocar-Mirédin, O., Yu, Y., Amouyal, Y., Raabe, D., Snyder, G. J., & Scheu, C. (2019). Density, distribution and nature of planar faults in silver antimony telluride for thermoelectric applications. *Acta Materialia*, 178, 135–145. <https://doi.org/10.1016/j.actamat.2019.07.031>
- Aboufadi, H., Deges, J., Choi, P., & Raabe, D. (2015). Dynamic strain aging studied at the atomic scale. *Acta Materialia*, 86, 34–42. <https://doi.org/10.1016/j.actamat.2014.12.028>
- Alankar, A., Eisenlohr, P., & Raabe, D. (2011). A dislocation density-based crystal plasticity constitutive model for prismatic slip in α -titanium. *Acta Materialia*, 59(18), 7003–7009. <https://doi.org/10.1016/j.actamat.2011.07.053>
- Alankar, A., Field, D. P., & Raabe, D. (2014). Plastic anisotropy of electro-deposited pure α -iron with sharp crystallographic $\langle 111 \rangle$ texture in normal direction: Analysis by an explicitly dislocation-based crystal plasticity model. *International Journal of Plasticity*, 52, 18–32. <https://doi.org/10.1016/j.ijplas.2013.03.006>
- Al-Sawalmih, A., Li, C., Siegel, S., Fabritius, H., Yi, S., Raabe, D., Fratzl, P., Paris, O., Al-Sawalmih, A., Li, C., Siegel, S., Fabritius, H., Yi, S., Raabe, D., Fratzl, P., & Paris, O. (2008). Microtexture and chitin/calcite orientation relationship in the mineralized exoskeleton of the American lobster. *Advanced Functional Materials*, 18(20), 3307–3314. <https://doi.org/10.1002/adfm.200800520>
- Aparicio-Fernández, R., Springer, H., Szczepaniak, A., Zhang, H., & Raabe, D. (2016). In-situ metal matrix composite steels: Effect of alloying and annealing on morphology, structure and mechanical properties of TiB₂ particle containing high modulus steels. *Acta Materialia*, 107, 38–48. <https://doi.org/10.1016/j.actamat.2016.01.048>
- Aparicio-Fernández, R., Szczepaniak, A., Springer, H., & Raabe, D. (2017). Crystallisation of amorphous Fe – Ti – B alloys as a design pathway for nano-structured high modulus steels. *Journal of Alloys and Compounds*, 704, 565–573. <https://doi.org/10.1016/j.jallcom.2017.02.077>
- Ayodele, S. G., Raabe, D., & Varnik, F. (2013). Lattice boltzmann modeling of advection-diffusion-reaction equations: Pattern formation under uniform differential advection. *Communications in Computational Physics*, 13(3), 741–756. <https://doi.org/10.4208/cicp.441011.270112s>
- Ayodele, S. G., Raabe, D., & Varnik, F. (2015). Shear-flow-controlled mode selection in a nonlinear autocatalytic medium. *Physical Review E*, 91(2), 22913. <https://doi.org/10.1103/PhysRevE.91.022913>
- Ayodele, S. G., Varnik, F., & Raabe, D. (2009). Effect of aspect ratio on transverse diffusive broadening: A lattice Boltzmann study. *Physical Review E*, 80(1), 16304. <https://doi.org/10.1103/PhysRevE.80.016304>

- Ayodele, S. G., Varnik, F., & Raabe, D. (2011). Lattice Boltzmann study of pattern formation in reaction-diffusion systems. *Physical Review E*, 83(1), 16702. <https://doi.org/10.1103/PhysRevE.83.016702>
- Bai, Y., Mianroodi, J., Ma, Y., da Silva, A. K., Svendsen, B., & Raabe, D. (2021). Chemo-Mechanical Phase-Field Modeling of Iron Oxide Reduction with Hydrogen. *Acta Materialia*, 231(6), 117899. <https://doi.org/10.1016/j.actamat.2022.117899>
- Bajaj, P., Hariharan, A., Kini, A., Kürnsteiner, P., Raabe, D., & Jägle, E. A. E. A. A. (2020). Steels in additive manufacturing: A review of their microstructure and properties. *Materials Science and Engineering A*, 772(November 2019), 138633. <https://doi.org/10.1016/j.msea.2019.138633>
- Balachandran, S., Orava, J., Köhler, M., Breen, A. J., Kaban, I., Raabe, D., & Herbig, M. (2019). Elemental re-distribution inside shear bands revealed by correlative atom-probe tomography and electron microscopy in a deformed metallic glass. *Scripta Materialia*, 168, 14–18. <https://doi.org/10.1016/j.scriptamat.2019.04.014>
- Balachandran, S., Zachariah, Z., Fischer, A., Mayweg, D., Wimmer, M. A., Raabe, D., & Herbig, M. (2020). Atomic Scale Origin of Metal Ion Release from Hip Implant Taper Junctions. *Advanced Science*, 7(5), 1–10. <https://doi.org/10.1002/advs.201903008>
- Barani, A. A., Li, F., Romano, P., Ponge, D., & Raabe, D. (2007). Design of high-strength steels by microalloying and thermomechanical treatment. *Materials Science and Engineering A*, 463(1–2), 138–146. <https://doi.org/10.1016/j.msea.2006.08.124>
- Barani, A. A., Ponge, D., & Raabe, D. (2006). Strong and Ductile Martensitic Steels for Automotive Applications. *Steel Research International*, 77(9–10), 704–711. <https://doi.org/10.1002/srin.200606451>
- Barani, A. A., Ponge, D., Raabe, D., Ardehali Barani, A., Ponge, D., & Raabe, D. (2006). Refinement of grain boundary carbides in a Si–Cr spring steel by thermomechanical treatment. *Materials Science and Engineering: A*, 426(1–2), 194–201. <https://doi.org/10.1016/j.msea.2006.04.002>
- Baron, C., Springer, H., & Raabe, D. (2016). Combinatorial screening of the microstructure–property relationships for Fe–B–X stiff, light, strong and ductile steels. *Materials and Design*, 112, 131–139. <https://doi.org/10.1016/j.matdes.2016.09.065>
- Baron, C., Springer, H., & Raabe, D. (2016). Effects of Mn additions on microstructure and properties of Fe–TiB₂ based high modulus steels. *Materials & Design*, 111, 185–191. <https://doi.org/10.1016/j.matdes.2016.09.003>
- Baron, C., Springer, H., & Raabe, D. (2016). Efficient liquid metallurgy synthesis of Fe–TiB₂ high modulus steels via in-situ reduction of titanium oxides. *Materials and Design*, 97, 357–363. <https://doi.org/10.1016/j.matdes.2016.02.076>
- Baron, C., Springer, H., & Raabe, D. (2018). Development of high modulus steels based on the Fe–Cr–B system. *Materials Science and Engineering: A*, 724, 142–147.
- Baron, C., Springer, H., & Raabe, D. (2018). Development of high modulus steels based on the Fe – Cr – B system. *Materials Science and Engineering A*, 724(February), 142–147. <https://doi.org/10.1016/j.msea.2018.03.082>

- Bartels, C., Raabe, D., Gottstein, G., & Huber, U. (1997). Investigation of the precipitation kinetics in an A16061/TiB₂ metal matrix composite. *Materials Science and Engineering: A*, 237(1), 12–23. [https://doi.org/10.1016/S0921-5093\(97\)00104-4](https://doi.org/10.1016/S0921-5093(97)00104-4)
- Bastos, A., Zaefferer, S., & Raabe, D. (2008). Three-dimensional EBSD study on the relationship between triple junctions and columnar grains in electrodeposited Co-Ni films. *Journal of Microscopy*, 230(3), 487–498. <https://doi.org/10.1111/j.1365-2818.2008.02008.x>
- Bastos, A., Zaefferer, S., & Raabe, D. (2008). Three-dimensional EBSD study on the relationship between triple junctions and columnar grains in electrodeposited Co–Ni films. *Journal of Microscopy*, 230(3), 487–498.
- Bastos, A., Zaefferer, S., Raabe, D., & Schuh, C. (2006). Characterization of the microstructure and texture of nanostructured electrodeposited NiCo using electron backscatter diffraction (EBSD). *Acta Materialia*, 54(9), 2451–2462. <https://doi.org/10.1016/j.actamat.2006.01.033>
- Belde, M., Springer, H., & Raabe, D. (2016). Vessel microstructure design: A new approach for site-specific core-shell micromechanical tailoring of TRIP-assisted ultra-high strength steels. *Acta Materialia*, 113, 19–31. <https://doi.org/10.1016/j.actamat.2016.04.051>
- Belde, M., Springer, H., Inden, G., & Raabe, D. (2015). Multiphase microstructures via confined precipitation and dissolution of vessel phases: Example of austenite in martensitic steel. *Acta Materialia*, 86, 1–14. <https://doi.org/10.1016/j.actamat.2014.11.025>
- Benzing, J. T. T., Liu, Y., Zhang, X., Luecke, W. E. E., Ponge, D., Dutta, A., Oskay, C., Raabe, D., & Wittig, J. E. E. (2019). Experimental and numerical study of mechanical properties of multi-phase medium-Mn TWIP-TRIP steel: Influences of strain rate and phase constituents. *Acta Materialia*, 177, 250–265. <https://doi.org/10.1016/j.actamat.2019.07.036>
- Benzing, J. T., Bentley, J., McBride, J. R., Ponge, D., Han, J., Raabe, D., & Wittig, J. E. (2017). Characterization of Partitioning in a Medium-Mn Third-Generation AHSS. *Microscopy and Microanalysis*, 23(S1), 402–403. <https://doi.org/10.1017/s1431927617002690>
- Benzing, J. T., Kwiatkowski da Silva, A., Morsdorf, L., Bentley, J., Ponge, D., Dutta, A., Han, J., McBride, J. R., Van Leer, B., Gault, B., Raabe, D., & Wittig, J. E. (2019). Multi-scale characterization of austenite reversion and martensite recovery in a cold-rolled medium-Mn steel. *Acta Materialia*, 166, 512–530. <https://doi.org/10.1016/j.actamat.2019.01.003>
- Benzing, J. T., Poling, W. A., Pierce, D. T., Bentley, J., Findley, K. O., Raabe, D., & Wittig, J. E. (2018). Effects of strain rate on mechanical properties and deformation behavior of an austenitic Fe-25Mn-3Al-3Si TWIP-TRIP steel. *Materials Science and Engineering A*, 711(November 2017), 78–92. <https://doi.org/10.1016/j.msea.2017.11.017>
- Bieler, T. R., Eisenlohr, P., Roters, F., Kumar, D., Mason, D. E., Crimp, M. A., & Raabe, D. (2009). The role of heterogeneous deformation on damage nucleation at grain boundaries in single phase metals. *International Journal of Plasticity*, 25(9), 1655–1683. <https://doi.org/10.1016/j.ijplas.2008.09.002>
- Bong, H. J., Kirchlechner, C., Raabe, D., Choi, W. S., Pang, E. L., Ko, W.-S., Jun, H., Bong, H. J., Kirchlechner, C., Raabe, D., & Choi, P.-P. (2021). Orientation-dependent plastic deformation

- mechanisms and competition with stress-induced phase transformation in microscale NiTi. *Acta Materialia*, 208, 116731. <https://doi.org/10.1016/j.actamat.2021.116731>
- Boßelmann, F., Romano, P., Fabritius, H., Raabe, D., & Epple, M. (2007). The composition of the exoskeleton of two crustacea: The American lobster *Homarus americanus* and the edible crab *Cancer pagurus*. *Thermochimica Acta*, 463(1–2), 65–68. <https://doi.org/10.1016/j.tca.2007.07.018>
- Brahme, A., Winning, M., & Raabe, D. (2009). Prediction of cold rolling texture of steels using an Artificial Neural Network. *Computational Materials Science*, 46(4), 800–804. <https://doi.org/10.1016/j.commatsci.2009.04.014>
- Brands, D., Balzani, D., Scheunemann, L., Schröder, J., Richter, H., & Raabe, D. (2016). Computational modeling of dual-phase steels based on representative three-dimensional microstructures obtained from EBSD data. *Archive of Applied Mechanics*, 86(3), 575–598. <https://doi.org/10.1007/s00419-015-1044-1>
- Brands, D., Schröder, J., Balzani, D., Dmitrieva, O., & Raabe, D. (2011). On the Reconstruction and Computation of Dual-Phase Steel Microstructures Based on 3D EBSD Data. *PAMM*, 11(1), 503–504. <https://doi.org/10.1002/pamm.201110243>
- Breen, A. J., Mouton, I., Lu, W., Wang, S., Szczepaniak, A., Kontis, P., Stephenson, L. T. T., Chang, Y., da Silva, A. K., Liebscher, C. H., Raabe, D., Britton, T. B., Herbig, M., & Gault, B. (2018). Atomic scale analysis of grain boundary deuteride growth front in Zircaloy-4. *Scripta Materialia*, 156, 42–46. <https://doi.org/10.1016/j.scriptamat.2018.06.044>
- Breitbarth, E., Zaefferer, S., Archie, F., Besel, M., Raabe, D., & Requena, G. (2018). Evolution of dislocation patterns inside the plastic zone introduced by fatigue in an aged aluminium alloy AA2024-T3. *Materials Science and Engineering: A*, 718(January), 345–349. <https://doi.org/10.1016/j.msea.2018.01.068>
- Bu, Y., Li, Z., Liu, J., Wang, H., Raabe, D., & Yang, W. (2019). Nonbasal slip systems enable a strong and ductile hexagonal-close-packed high-entropy phase. *Physical Review Letters*, 122(7), 75502. <https://doi.org/10.1103/PhysRevLett.122.075502>
- Calcagnotto, M., Adachi, Y., Ponge, D., & Raabe, D. (2011). Deformation and fracture mechanisms in fine- and ultrafine-grained ferrite/martensite dual-phase steels and the effect of aging. *Acta Materialia*, 59(2), 658–670. <https://doi.org/10.1016/j.actamat.2010.10.002>
- Calcagnotto, M., Ponge, D., & Raabe, D. (2008). Ultrafine grained ferrite/martensite dual phase steel fabricated by large strain warm deformation and subsequent intercritical annealing. *ISIJ International*, 48(8), 1096–1101. <https://doi.org/10.2355/isijinternational.48.1096>
- Calcagnotto, M., Ponge, D., & Raabe, D. (2010). Effect of grain refinement to 1 μ m on strength and toughness of dual-phase steels. *Materials Science and Engineering A*, 527(29–30), 7832–7840. <https://doi.org/10.1016/j.msea.2010.08.062>
- Calcagnotto, M., Ponge, D., & Raabe, D. (2012). Microstructure control during fabrication of ultrafine grained dual-phase steel: characterization and effect of intercritical annealing parameters. *ISIJ International*, 52(5), 874–883. <https://doi.org/10.2355/isijinternational.52.874>

- Calcagnotto, M., Ponge, D., & Raabe, D. (2012). On the effect of manganese on grain size stability and hardenability in ultrafine-grained ferrite/martensite dual-phase steels. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 43(1), 37–46. <https://doi.org/10.1007/s11661-011-0828-3>
- Calcagnotto, M., Ponge, D., Demir, E., & Raabe, D. (2010). Orientation gradients and geometrically necessary dislocations in ultrafine grained dual-phase steels studied by 2D and 3D EBSD. *Materials Science and Engineering A*, 527(10–11), 2738–2746. <https://doi.org/10.1016/j.msea.2010.01.004>
- Cao, Y., Ma, D., & Raabe, D. (2009). The use of flat punch indentation to determine the viscoelastic properties in the time and frequency domains of a soft layer bonded to a rigid substrate. *Acta Biomaterialia*, 5(1), 240–248. <https://doi.org/10.1016/j.actbio.2008.07.020>
- Cao, Y., Xue, Z., Chen, X., & Raabe, D. (2008). Correlation between the flow stress and the nominal indentation hardness of soft metals. *Scripta Materialia*, 59(5), 518–521. <https://doi.org/10.1016/j.scriptamat.2008.04.039>
- Cédat, D., Fandeur, O., Rey, C., & Raabe, D. (2012). Polycrystal model of the mechanical behavior of a Mo–TiC30 vol.% metal–ceramic composite using a three-dimensional microstructure map obtained by dual beam focused ion beam scanning electron microscopy. *Acta Materialia*, 60(4), 1623–1632. <https://doi.org/10.1016/j.actamat.2011.11.055>
- Cereceda, D., Diehl, M., Roters, F., Raabe, D., Perlado, J. M., & Marian, J. (2016). Unraveling the temperature dependence of the yield strength in single-crystal tungsten using atomistically-informed crystal plasticity calculations. *International Journal of Plasticity*, 78, 242–265. <https://doi.org/10.1016/j.ijplas.2015.09.002>
- Cereceda, D., Diehl, M., Roters, F., Shanthraj, P., Raabe, D., Perlado, J. M., & Marian, J. (2015). Linking atomistic, kinetic Monte Carlo and crystal plasticity simulations of single-crystal tungsten strength. *GAMM Mitteilungen*, 38(2), 213–227. <https://doi.org/10.1002/gamm.201510012>
- Chang, Y. H., Mouton, I., Stephenson, L., Ashton, M., Zhang, G. K., Szczepaniak, A., Lu, W. J., Ponge, D., Raabe, D., & Gault, B. (2019). Quantification of solute deuterium in titanium deuteride by atom probe tomography with both laser pulsing and high-voltage pulsing: influence of the surface electric field. *New Journal of Physics*, 21(5), 53025. <https://doi.org/10.1088/1367-2630/ab1c3b>
- Chang, Y., Breen, A. J. J., Tarzimoghdam, Z., Kürsteiner, P., Gardner, H., Ackerman, A., Radecka, A., Bagot, P. A. J. A. J., Lu, W., Li, T., Jäggle, E. A. A., Herbig, M., Stephenson, L. T. T., Moody, M. P. P., Rugg, D., Dye, D., Ponge, D., Raabe, D., & Gault, B. (2018). Characterizing solute hydrogen and hydrides in pure and alloyed titanium at the atomic scale. *Acta Materialia*, 150, 273–280. <https://doi.org/10.1016/j.actamat.2018.02.064>
- Chang, Y., Lu, W., Guérolé, J., Stephenson, L. T., Szczepaniak, A., Kontis, P., Ackerman, A. K., Dear, F. F., Mouton, I., Zhong, X., Zhang, S., Dye, D., Liebscher, C. H., Ponge, D., Korte-Kerzel, S., Raabe, D., & Gault, B. (2019). Ti and its alloys as examples of cryogenic focused ion beam milling of environmentally-sensitive materials. *Nature Communications*, 10(1). <https://doi.org/10.1038/s41467-019-08752-7>

- Chang, Y., Zhang, S., Liebscher, C. H., Dye, D., Ponge, D., Scheu, C., Dehm, G., Raabe, D., Gault, B., & Lu, W. (2020). Could face-centered cubic titanium in cold-rolled commercially-pure titanium only be a Ti-hydride? *Scripta Materialia*, *178*, 39–43.
- Chauvet, E., Kontis, P., Jäggle, E. A., Gault, B., Raabe, D., Tassin, C., Blandin, J.-J. J., Dendievel, R., Vayre, B., Abed, S., & Martin, G. (2018). Hot cracking mechanism affecting a non-weldable Ni-based superalloy produced by selective electron Beam Melting. *Acta Materialia*, *142*, 82–94. <https://doi.org/10.1016/j.actamat.2017.09.047>
- Chen, N., Zaefferer, S., Lahn, L., Günther, K., & Raabe, D. (2003). Effects of topology on abnormal grain growth in silicon steel. *Acta Materialia*, *51*(6), 1755–1765. [https://doi.org/10.1016/S1359-6454\(02\)00574-8](https://doi.org/10.1016/S1359-6454(02)00574-8)
- Chen, R., Sandlöbes, S., Zehnder, C., Zeng, X., Korte-Kerzel, S., & Raabe, D. (2018). Deformation mechanisms, activated slip systems and critical resolved shear stresses in an Mg-LPSO alloy studied by micro-pillar compression. *Materials and Design*, *154*, 203–216. <https://doi.org/10.1016/j.matdes.2018.05.037>
- Chen, R., Sandlöbes, S., Zeng, X., Li, D., Korte-Kerzel, S., & Raabe, D. (2017). Room temperature deformation of LPSO structures by non-basal slip. *Materials Science and Engineering: A*, *682*(November 2016), 354–358. <https://doi.org/10.1016/j.msea.2016.11.056>
- Chen, Y. Z., Herz, A., Li, Y. J., Borchers, C., Choi, P., Raabe, D., & Kirchheim, R. (2013). Nanocrystalline Fe-C alloys produced by ball milling of iron and graphite. *Acta Materialia*, *61*(9), 3172–3185. <https://doi.org/10.1016/j.actamat.2013.02.006>
- Chikkadi, V., Mandal, S., Nienhuis, B., Raabe, D., Varnik, F., & Schall, P. (2012). Shear-induced anisotropic decay of correlations in hard-sphere colloidal glasses. *EPL (Europhysics Letters)*, *100*(5), 56001. <https://doi.org/10.1209/0295-5075/100/56001>
- Choi, P. P., Povstugar, I., Ahn, J. P., Kostka, A., & Raabe, D. (2011). Thermal stability of TiAlN/CrN multilayer coatings studied by atom probe tomography. *Ultramicroscopy*, *111*(6), 518–523. <https://doi.org/10.1016/j.ultramic.2010.11.012>
- Choi, P., Li, Y. J., Kirchheim, R., & Raabe, D. (2011). Deformation-induced cementite decomposition in pearlitic steel wires studied by atom probe tomography. *ICCM International Conferences on Composite Materials*.
- Choi, P., Wuerz, R., & Raabe, D. (2012). *Exploring the p-n junction region in Cu (In, Ga) Se 2 thin-film solar cells at the. 181603*, 1–5.
- Choi, P.-P. P., Cojocar-Mirédin, O., Wuerz, R., & Raabe, D. (2011). Comparative atom probe study of Cu (In, Ga) Se₂ thin-film solar cells deposited on soda-lime glass and mild steel substrates. *Journal of Applied Physics*, *110*(12), 124513. <https://doi.org/10.1063/1.3665723>
- Choi, P.-P., Cojocar-Mirédin, O., Abou-Ras, D., Caballero, R., Raabe, D., Smentkowski, V. S., Park, C. G., Gu, G. H., Mazumder, B., Wong, M. H., Hu, Y.-L., Melo, T. P., & Speck, J. S. (2012). Atom probe tomography of compound semiconductors for photovoltaic and light-emitting device applications. *Microscopy Today*, *20*(3), 18–24. <https://doi.org/10.1017/s1551929512000235>

- Choi, W. S., De Cooman, B. C., Sandlöbes, S., & Raabe, D. (2015). Size and orientation effects in partial dislocation-mediated deformation of twinning-induced plasticity steel micro-pillars. *Acta Materialia*, *98*, 391–404. <https://doi.org/10.1016/j.actamat.2015.06.065>
- Choi, W. S., Sandlöbes, S., Malyar, N. V., Kirchlechner, C., Korte-Kerzel, S., Dehm, G., Choi, P. P., & Raabe, D. (2018). On the nature of twin boundary-associated strengthening in Fe-Mn-C steel. *Scripta Materialia*, *156*, 27–31. <https://doi.org/10.1016/j.scriptamat.2018.07.009>
- Choi, W. S., Sandlöbes, S., Malyar, N. V., Kirchlechner, C., Korte-Kerzel, S., Dehm, G., De Cooman, B. C., & Raabe, D. (2017). Dislocation interaction and twinning-induced plasticity in face-centered cubic Fe-Mn-C micro-pillars. *Acta Materialia*, *132*, 162–173. <https://doi.org/10.1016/j.actamat.2017.04.043>
- Choisez, L., van Rooij, N., Hessels, C., da Silva, A. K., Ma, Y., Souza Filho, I., de Goey, P., Springer, H., & Raabe, D. (2022). Phase Transformations and Microstructure Evolution During Combustion of Iron Powder. *Acta Materialia*, *239*, 118261. <https://doi.org/10.2139/ssrn.4080963>
- Cojocar-Mirédin, O., Abdellaoui, L., Nagli, M., Zhang, S., Yu, Y., Scheu, C., Raabe, D., Wuttig, M., & Amouyal, Y. (2017). Role of Nanostructuring and Microstructuring in Silver Antimony Telluride Compounds for Thermoelectric Applications. *ACS Applied Materials and Interfaces*, *9*(17), 14779–14790. <https://doi.org/10.1021/acsami.7b00689>
- Cojocar-Mirédin, O., Choi, P. P., Abou-Ras, D., Schmidt, S. S., Caballero, R., & Raabe, D. (2011). Characterization of grain boundaries in Cu(In,Ga)Se₂ films using atom-probe tomography. *IEEE Journal of Photovoltaics*, *1*(2), 207–212. <https://doi.org/10.1109/JPHOTOV.2011.2170447>
- Cojocar-Mirédin, O., Choi, P., Wuerz, R., & Raabe, D. (2011). Atomic-scale characterization of the CdS/CuInSe₂ interface in thin-film solar cells. *Applied Physics Letters*, *98*(10), 103504.
- Cojocar-Mirédin, O., Choi, P., Wuerz, R., & Raabe, D. (2012). Exploring the p-n junction region in Cu(In,Ga)Se₂ thin-film solar cells at the nanometer-scale. *Applied Physics Letters*, *101*(18). <https://doi.org/10.1063/1.4764527>
- Cojocar-Mirédin, O., Choi, P., Wuerz, R., Raabe, D., Cojocar-Mirédin, O., Choi, P., Wuerz, R., & Raabe, D. (2011). Atomic-scale distribution of impurities in CuInSe₂-based thin-film solar cells. *Ultramicroscopy*, *111*(6), 552–556. <https://doi.org/10.1016/j.ultramic.2010.12.034>
- Cojocar-Mirédin, O., Fu, Y., Kostka, A., Sáez-Araoz, R., Beyer, A., Knaub, N., Volz, K., Fischer, C., & Raabe, D. (2015). Interface engineering and characterization at the atomic-scale of pure and mixed ion layer gas reaction buffer layers in chalcopyrite thin-film solar cells. *Progress in Photovoltaics: Research and Applications*, *23*(6), 705–716.
- Cojocar-Mirédin, O., Schwarz, T., Choi, P. P., Herbig, M., Wuerz, R., & Raabe, D. (2013). Atom probe tomography studies on the Cu(In,g)Se₂ grain boundaries. *Journal of Visualized Experiments : JoVE*, *74*, 1–8. <https://doi.org/10.3791/50376>
- Cojocar-Mirédin, O., Schwarz, T., Choi, P.-P., Herbig, M., Wuerz, R., & Raabe, D. (2013). Atom probe tomography studies on the Cu (In, Ga) Se₂ grain boundaries. *Journal of Visualized Experiments: JoVE*, *74*.

- Colombara, D., Elanzeery, H., Nicoara, N., Sharma, D., Claro, M., Schwarz, T., Koprek, A., Wolter, M. H., Melchiorre, M., Sood, M., Valle, N., Bondarchuk, O., Babbe, F., Spindler, C., Cojocaru-Miredin, O., Raabe, D., Dale, P. J., Sadewasser, S., & Siebentritt, S. (2020). Chemical instability at chalcogenide surfaces impacts chalcopyrite devices well beyond the surface. *Nature Communications*, *11*(1), 1–14. <https://doi.org/10.1038/s41467-020-17434-8>
- Colombara, D., Werner, F., Schwarz, T., Infante, I. C., Fleming, Y., Valle, N., Spindler, C., Vacchieri, E., Rey, G., Guennou, M., Cañero Infante, I., Fleming, Y., Valle, N., Spindler, C., Vacchieri, E., Rey, G., Guennou, M., Bouttemy, M., Manjón, A. G., ... Siebentritt, S. (2018). Sodium enhances indium-gallium interdiffusion in copper indium gallium diselenide photovoltaic absorbers. *Nature Communications*, *9*(1), 1–12. <https://doi.org/10.1038/s41467-018-03115-0>
- Counts, W. A., Friák, M., Battaile, C. C., Raabe, D., & Neugebauer, J. (2008). A comparison of polycrystalline elastic properties computed by analytic homogenization schemes and FEM. *Physica Status Solidi (B)*, *245*(12), 2630–2635. <https://doi.org/10.1002/pssb.200844226>
- Counts, W. A., Friak, M., Raabe, D., & Neugebauer, J. (2009). Using ab initio calculations in designing bcc Mg–Li alloys for ultra-lightweight applications. *Acta Materialia*, *57*(1), 69–76.
- Counts, W. A., Friak, M., Raabe, D., & Neugebauer, J. (2010). Ab Initio Guided Design of bcc Ternary Mg–Li–X (X= Ca, Al, Si, Zn, Cu) Alloys for Ultra-Lightweight Applications. *Advanced Engineering Materials*, *12*(7), 572–576.
- Darvishi Kamachali, R., Kwiatkowski da Silva, A., McEniry, E., Ponge, D., Gault, B., Neugebauer, J., & Raabe, D. (2020). Segregation-assisted spinodal and transient spinodal phase separation at grain boundaries. *Npj Computational Materials*, *6*(1), 1–13. <https://doi.org/10.1038/s41524-020-00456-7>
- Darvishi Kamachali, R., Schwarze, C., Lin, M., Diehl, M., Shanthraj, P., Prahl, U., Steinbach, I., Raabe, D., Kamachali, R. D., Schwarze, C., Lin, M., Diehl, M., Shanthraj, P., Prahl, U., Steinbach, I., Raabe, D., Darvishi Kamachali, R., Schwarze, C., Lin, M., ... Raabe, D. (2018). Numerical Benchmark of Phase-Field Simulations with Elastic Strains: Precipitation in the Presence of Chemo-Mechanical Coupling. *Computational Materials Science*, *155*(September), 541–553. <https://doi.org/10.1016/j.commatsci.2018.09.011>
- De Siqueira, R. P., Sandim, H. R. Z., & Raabe, D. (2013). Particle stimulated nucleation in coarse-grained ferritic stainless steel. *Metallurgical and Materials Transactions A*, *44*(1), 469–478. <https://doi.org/10.1007/s11661-012-1408-x>
- Demir, E., & Raabe, D. (2010). Mechanical and microstructural single-crystal Bauschinger effects: Observation of reversible plasticity in copper during bending. *Acta Materialia*, *58*(18), 6055–6063. <https://doi.org/10.1016/j.actamat.2010.07.023>
- Demir, E., Raabe, D., & Roters, F. (2010). The mechanical size effect as a mean-field breakdown phenomenon: Example of microscale single crystal beam bending. *Acta Materialia*, *58*(5), 1876–1886. <https://doi.org/10.1016/j.actamat.2009.11.031>
- Demir, E., Raabe, D., Zaafarani, N., & Zaefferer, S. (2009). Experimental investigation of geometrically necessary dislocations beneath small indents of different depths using EBSD tomography. *Acta Materialia*, *57*, 559–569.

- Demir, E., Raabe, D., Zaafarani, N., & Zaefferer, S. (2009). Investigation of the indentation size effect through the measurement of the geometrically necessary dislocations beneath small indents of different depths using EBSD tomography. *Acta Materialia*, *57*(2), 559–569. <https://doi.org/10.1016/j.actamat.2008.09.039>
- Demir, E., Roters, F., & Raabe, D. (2010). Bending of single crystal microcantilever beams of cube orientation: Finite element model and experiments. *Journal of the Mechanics and Physics of Solids*, *58*(10), 1599–1612. <https://doi.org/10.1016/j.jmps.2010.07.007>
- Deng, Y., Tasan, C. C., Pradeep, K. G., Springer, H., Kostka, A., & Raabe, D. (2015). Design of a twinning-induced plasticity high entropy alloy. *Acta Materialia*, *94*, 124–133. <https://doi.org/10.1016/j.actamat.2015.04.014>
- Dey, P., Nazarov, R., Dutta, B., Yao, M., Herbig, M., Friák, M., Hickel, T., Raabe, D., & Neugebauer, J. (2017). Ab initio explanation of disorder and off-stoichiometry in Fe-Mn-Al-C κ carbides. *Physical Review B*, *95*(10), 104108. <https://doi.org/10.1103/PhysRevB.95.104108>
- Diehl, M., An, D., Shanthraj, P., Zaefferer, S., Roters, F., & Raabe, D. (2017). Crystal plasticity study on stress and strain partitioning in a measured 3D dual phase steel microstructure. *Physical Mesomechanics*, *20*(3), 311–323. <https://doi.org/10.1134/S1029959917030079>
- Diehl, M., Groeber, M., Haase, C., Molodov, D. A., Roters, F., & Raabe, D. (2017). Identifying Structure–Property Relationships Through DREAM.3D Representative Volume Elements and DAMASK Crystal Plasticity Simulations: An Integrated Computational Materials Engineering Approach. *JOM*, *69*(5), 848–855. <https://doi.org/10.1007/s11837-017-2303-0>
- Diehl, M., Kertsch, L., Traka, K., Helm, D., & Raabe, D. (2019). Site-specific quasi in situ investigation of primary static recrystallization in a low carbon steel. *Materials Science and Engineering: A*, *755*, 295–306.
- Diehl, M., Wicke, M., Shanthraj, P., Roters, F., Brueckner-Foit, A., & Raabe, D. (2017). Coupled Crystal Plasticity–Phase Field Fracture Simulation Study on Damage Evolution Around a Void: Pore Shape Versus Crystallographic Orientation. *JOM*, *69*(5), 872–878. <https://doi.org/10.1007/s11837-017-2308-8>
- Ding, R., Yao, Y., Sun, B., Liu, G., He, J., Li, T., Wan, X., Dai, Z., Ponge, D., Raabe, D., Zhang, C., Godfrey, A., Miyamoto, G., Furuhashi, T., Yang, Z., van der Zwaag, S., & Chen, H. (2020). Chemical boundary engineering: A new route toward lean, ultrastrong yet ductile steels. *Science Advances*, *6*(13), eaay1430. <https://doi.org/10.1126/sciadv.aay1430>
- Djaziri, S., Li, Y., Nematollahi, G. A., Grabowski, B., Goto, S., Kirchlechner, C., Kostka, A., Doyle, S., Neugebauer, J., Raabe, D., & Dehm, G. (2016). Deformation-induced martensite: a new paradigm for exceptional steels. *Advanced Materials*, *28*(35), 7753–7757. <https://doi.org/10.1002/adma.201601526>
- Dmitrieva, O., Choi, P., Gerstl, S. S. A., Ponge, D., & Raabe, D. (2011). Pulsed-laser atom probe studies of a precipitation hardened maraging TRIP steel. *Ultramicroscopy*, *111*(6), 623–627. <https://doi.org/10.1016/j.ultramic.2010.12.007>

- Dmitrieva, O., Dondl, P. W., Müller, S., & Raabe, D. (2009). Lamination microstructure in shear deformed copper single crystals. *Acta Materialia*, *57*(12), 3439–3449. <https://doi.org/10.1016/j.actamat.2009.03.035>
- Dmitrieva, O., Ponge, D., Inden, G., Millán, J., Choi, P., Sietsma, J., & Raabe, D. (2011). Chemical gradients across phase boundaries between martensite and austenite in steel studied by atom probe tomography and simulation. *Acta Materialia*, *59*(1), 364–374. <https://doi.org/10.1016/j.actamat.2010.09.042>
- Dmitrieva, O., Svirina, J. V., Demir, E., & Raabe, D. (2010). Investigation of the internal substructure of microbands in a deformed copper single crystal: experiments and dislocation dynamics simulation. *Modelling and Simulation in Materials Science and Engineering*, *18*(8), 85011. <https://doi.org/10.1088/0965-0393/18/8/085011>
- Dorner, D., Zaefferer, S., & Raabe, D. (2007). Retention of the Goss orientation between microbands during cold rolling of an Fe3%Si single crystal. *Acta Materialia*, *55*(7), 2519–2530. <https://doi.org/10.1016/j.actamat.2006.11.048>
- Dorner, D., Zaefferer, S., Lahn, L., & Raabe, D. (2006). Overview of microstructure and microtexture development in grain-oriented silicon steel. *Journal of Magnetism and Magnetic Materials*, *304*(2), 183–186. <https://doi.org/10.1016/j.jmmm.2006.02.116>
- Duarte, M. J., Klemm, J., Klemm, S. O., Mayrhofer, K. J. J., Stratmann, M., Borodin, S., Romero, A. H., Madinehei, M., Crespo, D., Serrano, J., Gerstl, S. S. A., Choi, P. P., Raabe, D., & Renner, F. U. (2013). Element-resolved corrosion analysis of stainless-type glass-forming steels. *Science*, *341*(6144), 372–376. <https://doi.org/10.1126/science.1230081>
- Duarte, M. J., Kostka, A., Jimenez, J. A., Choi, P., Klemm, J., Crespo, D., Raabe, D., & Renner, F. U. (2014). Crystallization, phase evolution and corrosion of Fe-based metallic glasses: An atomic-scale structural and chemical characterization study. *Acta Materialia*, *71*, 20–30. <https://doi.org/10.1016/j.actamat.2014.02.027>
- Dutta, A., Ponge, D., Sandlöbes, S., & Raabe, D. (2019). Strain partitioning and strain localization in medium manganese steels measured by in situ microscopic digital image correlation. *Materialia*, *5*(February), 100252. <https://doi.org/10.1016/j.mtla.2019.100252>
- Eiselt, C. C., Klimenkov, M., Lindau, R., Möslang, A., Sandim, H. R. Z. Z., Padilha, A. F., & Raabe, D. (2009). High-resolution transmission electron microscopy and electron backscatter diffraction in nanoscaled ferritic and ferritic–martensitic oxide dispersion strengthened–steels. *Journal of Nuclear Materials*, *385*(2), 231–235. <https://doi.org/10.1016/j.jnucmat.2008.11.029>
- Eisenlohr, A., Gutierrez-Urrutia, I., & Raabe, D. (2012). Adiabatic temperature increase associated with deformation twinning and dislocation plasticity. *Acta Materialia*, *60*(9), 3994–4004. <https://doi.org/10.1016/j.actamat.2012.03.008>
- Eisenlohr, P., Tjahjanto, D. D., Hochrainer, T., Roters, F., & Raabe, D. (2009). Texture prediction from a novel grain cluster-based homogenization scheme. *International Journal of Material Forming*, *2*(1), 523–526.

- Eisenlohr, P., Tjahjanto, D. D., Hochrainer, T., Roters, F., & Raabe, D. (2009). Comparison of texture evolution in fcc metals predicted by various grain cluster homogenization schemes. *International Journal of Materials Research*, *100*(4), 500–509. <https://doi.org/10.3139/146.110071>
- Elkot, M. N., Sun, B., Zhou, X., Ponge, D., & Raabe, D. (2022). Hydrogen-assisted decohesion associated with nanosized grain boundary κ -carbides in a high-Mn lightweight steel. *Acta Materialia*, *241*, 118392. <https://doi.org/10.1016/J.ACTAMAT.2022.118392>
- Elstnerová, P., Friák, M., Fabritius, H. O., Lymperakis, L., Hickel, T., Petrov, M., Nikolov, S., Raabe, D., Ziegler, A., Hild, S., & Neugebauer, J. (2010). Ab initio study of thermodynamic, structural, and elastic properties of Mg-substituted crystalline calcite. *Acta Biomaterialia*, *6*(12), 4506–4512. <https://doi.org/10.1016/j.actbio.2010.07.015>
- El-Zoka, A. A., Stephenson, L. T., Kim, S. H., Gault, B., & Raabe, D. (2023). The Fate of Water in Hydrogen-Based Iron Oxide Reduction. *Advanced Science*, *2300626*, 1–8. <https://doi.org/10.1002/advs.202300626>
- Enax, J., Fabritius, H.-O. O., Rack, A., Prymak, O., Raabe, D., & Epple, M. (2013). Characterization of crocodile teeth: correlation of composition, microstructure, and hardness. *Journal of Structural Biology*, *184*(2), 155–163. <https://doi.org/10.1016/j.jsb.2013.09.018>
- Enax, J., Janus, A. M., Raabe, D., Epple, M., & Fabritius, H.-O. O. (2014). Ultrastructural organization and micromechanical properties of shark tooth enameloid. *Acta Biomaterialia*, *10*(9), 3959–3968. <https://doi.org/10.1016/j.actbio.2014.04.028>
- Enax, J., Prymak, O., Raabe, D., & Epple, M. (2012). Structure, composition, and mechanical properties of shark teeth. *Journal of Structural Biology*, *178*(3), 290–299.
- Ener, S., Skokov, K. P., Palanisamy, D., Devillers, T., Fischbacher, J., Eslava, G. G., Maccari, F., Schäfer, L., Diop, L. V. B., & Radulov, I. (2021). Twins—A weak link in the magnetic hardening of ThMn12-type permanent magnets. *Acta Materialia*, *214*, 116968.
- Eswarappa Prameela, S., Pollock, T. M., Raabe, D., Meyers, M. A., Aitkaliyeva, A., Chintersingh, K.-L., Cordero, Z. C., & Graham-Brady, L. (2022). Materials for extreme environments. *Nature Reviews Materials*, 1–8. <https://doi.org/10.1038/s41578-022-00496-z>
- Evertz, S., Kirchlechner, I., Soler, R., Kirchlechner, C., Kontis, P., Bednarcik, J., Gault, B., Dehm, G., Raabe, D., & Schneider, J. M. (2020). Electronic structure based design of thin film metallic glasses with superior fracture toughness. *Materials & Design*, *186*, 108327.
- Evertz, S., Schnabel, V., Köhler, M., Kirchlechner, I., Kontis, P., Chen, Y.-T. T., Soler, R., Jaya, B. N., Kirchlechner, C., Music, D., Gault, B., Schneider, J. M., Raabe, D., & Dehm, G. (2020). Review on quantum mechanically guided design of ultra-strong metallic glasses. *Frontiers in Materials*, *7*(April), 89. <https://doi.org/10.3389/fmats.2020.00089>
- Fabritius, H. O., Sachs, C., Triguero, P. R., & Raabe, D. (2009). Influence of structural principles on the mechanics of a biological fiber-based composite material with hierarchical organization: the exoskeleton of the lobster *Homarus americanus*. *Advanced Materials*, *21*(4), 391–400. <https://doi.org/10.1002/adma.200801219>

- Fabritius, H.-O. O., Karsten, E. S., Balasundaram, K., Hild, S., Huemer, K., & Raabe, D. (2012). Correlation of structure, composition and local mechanical properties in the dorsal carapace of the edible crab *Cancer pagurus*. *Zeitschrift Für Kristallographie-Crystalline Materials*, *227*(11), 766–776. <https://doi.org/10.1524/zkri.2012.1532>
- Fabritius, H.-O. O., Ziegler, A., Friák, M., Nikolov, S., Huber, J., Seidl, B. H. M. M., Ruangchai, S., Alagboso, F. I., Karsten, S., Lu, J., Janus, A. M., Petrov, M., Zhu, L. F., Hemzalová, P., Hild, S., Raabe, D., & Neugebauer, J. (2016). Functional adaptation of crustacean exoskeletal elements through structural and compositional diversity: a combined experimental and theoretical study. *Bioinspiration & Biomimetics*, *11*(5), 55006. <https://doi.org/10.1088/1748-3190/11/5/055006>
- Fabritius-Vilpoux, K., Enax, J., Herbig, M., Raabe, D., & Fabritius, H.-O. O. (2019). Quantitative affinity parameters of synthetic hydroxyapatite and enamel surfaces in vitro. *Bioinspired, Biomimetic and Nanobiomaterials*, *8*(2), 141–153. <https://doi.org/10.1680/jbibn.18.00035>
- Fan, H., Wang, Q., El-Awady, J. A., Raabe, D., & Zaiser, M. (2021). Strain rate dependency of dislocation plasticity. *Nature Communications*, *12*(1), 1–11.
- Fan, H., Zhu, Y., El-Awady, J. A., & Raabe, D. (2018). Precipitation hardening effects on extension twinning in magnesium alloys. *International Journal of Plasticity*, *106*(November 2017), 186–202. <https://doi.org/10.1016/j.ijplas.2018.03.008>
- Fedosseev, A. I., & Raabe, D. (1994). Application of the method of superposition of harmonic currents for the simulation of inhomogeneous deformation during hot rolling of FeCr. *Scripta Metallurgica et Materiala*, *30*(1), 1–6. [https://doi.org/10.1016/0956-716X\(94\)90348-4](https://doi.org/10.1016/0956-716X(94)90348-4)
- Fischle, A., Neff, P., & Raabe, D. (2017). The relaxed-polar mechanism of locally optimal Cosserat rotations for an idealized nanoindentation and comparison with 3D-EBSD experiments. *Zeitschrift Für Angewandte Mathematik Und Physik*, *68*(4), 1–30.
- Friák, M., Counts, W. A., Ma, D., Sander, B., Holec, D., Raabe, D., & Neugebauer, J. (2012). Theory-guided materials design of multi-phase Ti-Nb alloys with bone-matching elastic properties. *Materials*, *5*(10), 1853–1872. <https://doi.org/10.3390/ma5101853>
- Friák, M., Counts, W. A., Raabe, D., Neugebauer, J., Friák, M., Counts, W. A., Raabe, D., & Neugebauer, J. (2008). Error propagation in multiscale approaches to the elasticity of polycrystals. *Physica Status Solidi (B)*, *245*(12), 2636–2641. <https://doi.org/10.1002/pssb.200844240>
- Friák, M., Hickel, T., Grabowski, B., Lymperakis, L., Udyansky, A., Dick, A., Ma, D., Roters, F., Zhu, L. F., Schlieter, A., Kühn, U., Ebrahimi, Z., Lebensohn, R. A., Holec, D., Eckert, J., Emmerich, H., Raabe, D., & Neugebauer, J. (2011). Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. *European Physical Journal Plus*, *126*(10), 1–22. <https://doi.org/10.1140/epjp/i2011-11101-2>
- Friák, M., Hickel, T., Körmann, F., Udyansky, A., Dick, A., Von Pezold, J., Ma, D., Kim, O., Counts, W. A., Šob, M., Gebhardt, T., Music, D., Schneider, J., Raabe, D., & Neugebauer, J. (2011). Determining the elasticity of materials employing quantum-mechanical approaches from the electronic ground state to the limits of materials stability. *Steel Research International*, *82*(2), 86–100. <https://doi.org/10.1002/srin.201000264>

- Friak, M., Nikolov, S., Petrov, M., Elstnerova, P., Sachs, C., Fabritius, H., Ma, D., Lymperakis, L., Raabe, D., & Neugebauer, J. (2010). Ab initio based study of multiscale elastic properties of hierarchical biocomposites. *Advanced Materials*, *22*, 519.
- Friak, M., Sander, B., Raabe, D., & Neugebauer, J. (2008). Theory-guided design of Ti-based binaries for human implants. *Journal of Physics: Condensed Matter*, *20*(6), 64221.
- Friák, M., Tytko, D., Holec, D., Choi, P. P., Eisenlohr, P., Raabe, D., & Neugebauer, J. (2015). Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases. *New Journal of Physics*, *17*(9), 13–16. <https://doi.org/10.1088/1367-2630/17/9/093004>
- Frommert, M., Zobrist, C., Lahn, L., Böttcher, A., Raabe, D., & Zaefferer, S. (2008). Texture measurement of grain-oriented electrical steels after secondary recrystallization. *Journal of Magnetism and Magnetic Materials*, *320*(20), 657–660. <https://doi.org/10.1016/j.jmmm.2008.04.102>
- Fujita, N., Igi, S., Diehl, M., Roters, F., & Raabe, D. (2019). The through-process texture analysis of plate rolling by coupling finite element and fast Fourier transform crystal plasticity analysis. *Modelling and Simulation in Materials Science and Engineering*, *27*(8), 85005.
- Fujita, N., Ishikawa, N., Roters, F., Tasan, C. C., & Raabe, D. (2018). Experimental-numerical study on strain and stress partitioning in bainitic steels with martensite-austenite constituents. *International Journal of Plasticity*, *104*(August 2017), 39–53. <https://doi.org/10.1016/j.ijplas.2018.01.012>
- Garbe, S., Juul Jensen, D., Poulsen, H. F., Krieger Lassen, N. C., & Raabe, D. (1998). Through-thickness texture variations determined non-destructively by high energy synchrotron radiation. *Materials Science Forum*, *273*, 271–276.
- Gault, B., Breen, A. J., Chang, Y., He, J., Jäggle, E. A., Kontis, P., Kürnsteiner, P., Kwiatkowski Da Silva, A., Makineni, S. K., Mouton, I., Peng, Z., Ponge, D., Schwarz, T., Stephenson, L. T., Szczepaniak, A., Zhao, H., & Raabe, D. (2018). Interfaces and defect composition at the near-atomic scale through atom probe tomography investigations. *Journal of Materials Research*, *33*(23), 4018–4030. <https://doi.org/10.1557/jmr.2018.375>
- George, E. P., Raabe, D., & Ritchie, R. O. (2019). High-entropy alloys. *Nature Reviews Materials*, *4*(8), 515–534. <https://doi.org/10.1038/s41578-019-0121-4>
- Godara, A., & Raabe, D. (2007). Influence of fiber orientation on global mechanical behavior and mesoscale strain localization in a short glass-fiber-reinforced epoxy polymer composite during tensile deformation investigated using digital image correlation. *Composites Science and Technology*, *67*(11–12), 2417–2427. <https://doi.org/10.1016/j.compscitech.2007.01.005>
- Godara, A., Raabe, D., & Green, S. (2007). The influence of sterilization processes on the micromechanical properties of carbon fiber-reinforced PEEK composites for bone implant applications. *Acta Biomaterialia*, *3*(2), 209–220. <https://doi.org/10.1016/j.actbio.2006.11.005>
- Godara, A., Raabe, D., Bergmann, I., Putz, R., & Müller, U. (2009). Influence of additives on the global mechanical behavior and the microscopic strain localization in wood reinforced polypropylene

- composites during tensile deformation investigated using digital image correlation. *Composites Science and Technology*, 69(2), 139–146. <https://doi.org/10.1016/j.compscitech.2008.08.031>
- Godara, A., Raabe, D., Van Puyvelde, P., & Moldenaers, P. (2006). Influence of flow on the global crystallization kinetics of iso-tactic polypropylene. *Polymer Testing*, 25(4), 460–469. <https://doi.org/10.1016/j.polymertesting.2006.01.010>
- Goetz, A. J., Steinmetz, D. R., Griesshaber, E., Zaefferer, S., Raabe, D., Kelm, K., Irsen, S., Sehrbrock, A., & Schmahl, W. W. (2011). Interdigitating biocalcite dendrites form a 3-D jigsaw structure in brachiopod shells. *Acta Biomaterialia*, 7(5), 2237–2243. <https://doi.org/10.1016/j.actbio.2011.01.035>
- Gottstein, G., & Raabe, D. (1998). Integral modeling of metallic materials. *Current Opinion in Solid State and Materials Science*, 3(3), 264–268. [https://doi.org/10.1016/S1359-0286\(98\)80101-0](https://doi.org/10.1016/S1359-0286(98)80101-0)
- Grilli, N., Janssens, K. G. F. F., Nellessen, J., Sandlöbes, S., & Raabe, D. (2018). Multiple slip dislocation patterning in a dislocation-based crystal plasticity finite element method. *International Journal of Plasticity*, 100, 104–121. <https://doi.org/10.1016/j.ijplas.2017.09.015>
- Gross, M., Steinbach, I., Raabe, D., & Varnik, F. (2013). Viscous coalescence of droplets: A lattice Boltzmann study. *Physics of Fluids*, 25(5), 52101. <https://doi.org/10.1063/1.4803178>
- Gross, M., Varnik, F., & Raabe, D. (2009). Fall and rise of small droplets on rough hydrophobic substrates. *Europhysics Letters*, 88(2), 1–6. <https://doi.org/10.1209/0295-5075/88/26002>
- Gross, M., Varnik, F., Raabe, D., & Steinbach, I. (2010). Small droplets on superhydrophobic substrates. *Physical Review E*, 81(5), 51606. <https://doi.org/10.1103/PhysRevE.81.051606>
- Guillon, O., Elsässer, C., Gutfleisch, O., Janek, J., Korte-Kerzel, S., Raabe, D., & Volkert, C. A. (2018). Manipulation of matter by electric and magnetic fields: Toward novel synthesis and processing routes of inorganic materials. *Materials Today*, 21(5), 527–536. <https://doi.org/10.1016/j.mattod.2018.03.026>
- Guo, W., Gan, B., Molina-Aldareguia, J. M., Poplawsky, J. D., & Raabe, D. (2016). Structure and dynamics of shear bands in amorphous–crystalline nanolaminates. *Scripta Materialia*, 110, 28–32.
- Guo, W., Jäggle, E. A., Choi, P. P., Yao, J., Kostka, A., Schneider, J. M., & Raabe, D. (2014). Erratum: Shear-induced mixing governs codeformation of crystalline- amorphous nanolaminates (Physical Review Letters (2014) 113 (035501)). *Physical Review Letters*, 113(6), 69903. <https://doi.org/10.1103/PhysRevLett.113.069903>
- Guo, W., Jäggle, E. A., Choi, P.-P. P., Yao, J., Kostka, A., Schneider, J. M., & Raabe, D. (2014). Shear-induced mixing governs codeformation of crystalline-amorphous nanolaminates. *Physical Review Letters*, 113(3), 35501. <https://doi.org/10.1103/PhysRevLett.113.035501>
- Guo, W., Jäggle, E., Yao, J., Maier, V., Korte-Kerzel, S., Schneider, J. M., & Raabe, D. (2014). Intrinsic and extrinsic size effects in the deformation of amorphous CuZr/nanocrystalline Cu nanolaminates. *Acta Materialia*, 80, 94–106. <https://doi.org/10.1016/j.actamat.2014.07.027>

- Guo, W., Pei, Z., Sang, X., Poplawsky, J. D., Bruschi, S., Qu, J., Raabe, D., & Bei, H. (2019). Shape-preserving machining produces gradient nanolaminate medium entropy alloys with high strain hardening capability. *Acta Materialia*, *170*, 176–186. <https://doi.org/10.1016/j.actamat.2019.03.024>
- Guo, W., Yao, J., Jäggle, E. A., Choi, P. P., Herbig, M., Schneider, J. M., & Raabe, D. (2015). Deformation induced alloying in crystalline - metallic glass nano-composites. *Materials Science and Engineering A*, *628*, 269–280. <https://doi.org/10.1016/j.msea.2015.01.062>
- Gutierrez-Urrutia, I., & Raabe, D. (2011). Dislocation and twin substructure evolution during strain hardening of an Fe-22 wt.% Mn-0.6 wt.% C TWIP steel observed by electron channeling contrast imaging. *Acta Materialia*, *59*(16), 6449–6462. <https://doi.org/10.1016/j.actamat.2011.07.009>
- Gutierrez-Urrutia, I., & Raabe, D. (2012). Dislocation density measurement by electron channeling contrast imaging in a scanning electron microscope. *Scripta Materialia*, *66*(6), 343–346. <https://doi.org/10.1016/j.scriptamat.2011.11.027>
- Gutierrez-Urrutia, I., & Raabe, D. (2012). Grain size effect on strain hardening in twinning-induced plasticity steels. *Scripta Materialia*, *66*(12), 992–996. <https://doi.org/10.1016/j.scriptamat.2012.01.037>
- Gutierrez-Urrutia, I., & Raabe, D. (2012). Study of deformation twinning and planar slip in a TWIP steel by electron channeling contrast imaging in a SEM. *Materials Science Forum*, *702–703*, 523–529. <https://doi.org/10.4028/www.scientific.net/MSF.702-703.523>
- Gutierrez-Urrutia, I., & Raabe, D. (2013). Influence of Al content and precipitation state on the mechanical behavior of austenitic high-Mn low-density steels. *Scripta Materialia*, *68*(6), 343–347. <https://doi.org/10.1016/j.scriptamat.2012.08.038>
- Gutierrez-Urrutia, I., & Raabe, D. (2013). Microbanding mechanism in an Fe-Mn-C high-Mn twinning-induced plasticity steel. *Scripta Materialia*, *69*(1), 53–56. <https://doi.org/10.1016/j.scriptamat.2013.03.010>
- Gutiérrez-Urrutia, I., & Raabe, D. (2013). Microbanding mechanism in an Fe–Mn–C high-Mn twinning-induced plasticity steel. *Scripta Materialia*, *69*(1), 53–56.
- Gutierrez-Urrutia, I., & Raabe, D. (2014). High strength and ductile low density austenitic FeMnAlC steels: Simplex and alloys strengthened by nanoscale ordered carbides. *Materials Science and Technology (United Kingdom)*, *30*(9), 1099–1104. <https://doi.org/10.1179/1743284714Y.00000000515>
- Gutierrez-Urrutia, I., Böttcher, A., Lahn, L., Raabe, D., Gutiérrez-Urrutia, I., Böttcher, A., Lahn, L., & Raabe, D. (2014). Microstructure–magnetic property relations in grain-oriented electrical steels: quantitative analysis of the sharpness of the Goss orientation. *Journal of Materials Science*, *49*(1), 269–276. <https://doi.org/10.1007/s10853-013-7701-2>
- Gutierrez-Urrutia, I., Del Valle, J. A., Zaefferer, S., & Raabe, D. (2010). Study of internal stresses in a TWIP steel analyzing transient and permanent softening during reverse shear tests. *Journal of Materials Science*, *45*(24), 6604–6610. <https://doi.org/10.1007/s10853-010-4750-7>

- Gutierrez-Urrutia, I., Raabe, D., Gutiérrez-Urrutia, I., & Raabe, D. (2012). Multistage strain hardening through dislocation substructure and twinning in a high strength and ductile weight-reduced Fe–Mn–Al–C steel. *Acta Materialia*, *60*(16), 5791–5802. <https://doi.org/10.1016/j.actamat.2012.07.018>
- Gutierrez-Urrutia, I., Zaefferer, S., & Raabe, D. (2009). Electron channeling contrast imaging of twins and dislocations in twinning-induced plasticity steels under controlled diffraction conditions in a scanning electron microscope. *Scripta Materialia*, *61*(7), 737–740. <https://doi.org/10.1016/j.scriptamat.2009.06.018>
- Gutierrez-Urrutia, I., Zaefferer, S., & Raabe, D. (2010). The effect of grain size and grain orientation on deformation twinning in a Fe-22wt.% Mn-0.6wt.% C TWIP steel. *Materials Science and Engineering A*, *527*(15), 3552–3560. <https://doi.org/10.1016/j.msea.2010.02.041>
- Gutierrez-Urrutia, I., Zaefferer, S., & Raabe, D. (2013). Coupling of electron channeling with EBSD: Toward the quantitative characterization of deformation structures in the sem. *JOM*, *65*(9), 1229–1236. <https://doi.org/10.1007/s11837-013-0678-0>
- Hafez Haghghat, S. M., Eggeler, G., Raabe, D., Hafez, S. M., Haghghat, G. E., Raabe, D., Haghghat, S. M. H., Eggeler, G., & Raabe, D. (2013). Effect of climb on dislocation mechanisms and creep rates in γ' -strengthened Ni base superalloy single crystals: A discrete dislocation dynamics study. *Acta Materialia*, *61*(10), 3709–3723. <https://doi.org/10.1016/j.actamat.2013.03.003>
- Haghghat, S. M. H., Schäublin, R., Raabe, D., Hafez Haghghat, S. M., Schäublin, R., & Raabe, D. (2014). Atomistic simulation of the $a_0 \langle 1\ 0\ 0 \rangle$ binary junction formation and its unzipping in body-centered cubic iron. *Acta Materialia*, *64*, 24–32. <https://doi.org/10.1016/j.actamat.2013.11.037>
- Haghghat, S. M. H., von Pezold, J., Race, C. P., Körmann, F., Friák, M., Neugebauer, J., Raabe, D., Hafez Haghghat, S. M., von Pezold, J., Race, C. P., Körmann, F., Friák, M., Neugebauer, J., & Raabe, D. (2014). Influence of the dislocation core on the glide of the $\frac{1}{2} \langle 1\ 1\ 1 \rangle \{1\ 1\ 0\}$ edge dislocation in bcc-iron: An embedded atom method study. *Computational Materials Science*, *87*, 274–282. <https://doi.org/10.1016/j.commatsci.2014.02.031>
- Haley, D., Choi, P., & Raabe, D. (2015). Guided mass spectrum labelling in atom probe tomography. *Ultramicroscopy*, *159*, 338–345. <https://doi.org/10.1016/j.ultramic.2015.03.005>
- Haley, D., Merzlikin, S. V., Choi, P., & Raabe, D. (2014). Atom probe tomography observation of hydrogen in high-Mn steel and silver charged via an electrolytic route. *International Journal of Hydrogen Energy*, *39*(23), 12221–12229. <https://doi.org/10.1016/j.ijhydene.2014.05.169>
- Han, C. S., Ma, A., Roters, F., & Raabe, D. (2007). A Finite Element approach with patch projection for strain gradient plasticity formulations. *International Journal of Plasticity*, *23*(4), 690–710. <https://doi.org/10.1016/j.ijplas.2006.08.003>
- Han, F., Diehl, M., Roters, F., & Raabe, D. (2020). Using spectral-based representative volume element crystal plasticity simulations to predict yield surface evolution during large scale forming simulations. *Journal of Materials Processing Technology*, *277*(September 2019), 116449. <https://doi.org/10.1016/j.jmatprotec.2019.116449>
- Han, F., Roters, F., & Raabe, D. (2020). Microstructure-based multiscale modeling of large strain plastic deformation by coupling a full-field crystal plasticity-spectral solver with an implicit finite

- element solver. *International Journal of Plasticity*, 125(September 2019), 97–117. <https://doi.org/10.1016/j.ijplas.2019.09.004>
- Han, J., da Silva, A. K., Ponge, D., Raabe, D., Lee, S. M., Lee, Y. K., Lee, S. I., & Hwang, B. (2017). The effects of prior austenite grain boundaries and microstructural morphology on the impact toughness of intercritically annealed medium Mn steel. *Acta Materialia*, 122, 199–206. <https://doi.org/10.1016/j.actamat.2016.09.048>
- Han, J., Kang, S. H., Lee, S. J., Kawasaki, M., Lee, H. J., Ponge, D., Raabe, D., & Lee, Y. K. (2017). Superplasticity in a lean Fe-Mn-Al steel. *Nature Communications*, 8(1), 8–13. <https://doi.org/10.1038/s41467-017-00814-y>
- Han, J., Kang, S.-H., Lee, S.-J., Kawasaki, M., Lee, H.-J., Ponge, D., Raabe, D., & Lee, Y.-K. (2018). Superplasticity in a lean Fe-Mn-Al steel (vol 8, 2017). *Nature Communications*, 9(1).
- Hangen, U., & Raabe, D. (1995). Experimental Investigation and Simulation of the Normal Conducting Properties of a Heavily Cold Rolled Cu-20 mass%Nb in Situ Composite. *Physica Status Solidi (A)*, 147(2), 515–527. <https://doi.org/10.1002/pssa.2211470222>
- Hangen, U., & Raabe, D. (1995). Modelling of the yield strength of a heavily wire drawn Cu-20%Nb composite by use of a modified linear rule of mixtures. *Acta Metallurgica Et Materialia*, 43(11), 4075–4082. [https://doi.org/10.1016/0956-7151\(95\)00079-B](https://doi.org/10.1016/0956-7151(95)00079-B)
- Harding, I., Mouton, I., Gault, B., Raabe, D., & Kumar, K. S. (2019). Carbon partitioning and microstructure evolution during tempering of an Fe-Ni-C steel. *Scripta Materialia*, 172, 38–42.
- Hariharan, A., Lu, L., Risse, J., Kostka, A., Gault, B., Jäggle, E. A., & Raabe, D. (2019). Misorientation-dependent solute enrichment at interfaces and its contribution to defect formation mechanisms during laser additive manufacturing of superalloys. *Physical Review Materials*, 3(12), 123602.
- Hassani, M., Engels, P., Raabe, D., & Varnik, F. (2016). Localized plastic deformation in a model metallic glass: A survey of free volume and local force distributions. *Journal of Statistical Mechanics: Theory and Experiment*, 2016(8), 84006. <https://doi.org/10.1088/1742-5468/2016/08/084006>
- Haubrich, J., Gussone, J., Barriobero-Vila, P., Kürnstener, P., Jäggle, E. A., Raabe, D., Schell, N., & Requena, G. (2019). The role of lattice defects, element partitioning and intrinsic heat effects on the microstructure in selective laser melted Ti-6Al-4V. *Acta Materialia*, 167, 136–148. <https://doi.org/10.1016/j.actamat.2019.01.039>
- He, D., Zhu, J. C., Zaefferer, S., Raabe, D., Liu, Y., Lai, Z. L., & Yang, X. W. (2012). Influences of deformation strain, strain rate and cooling rate on the Burgers orientation relationship and variants morphology during $\beta \rightarrow \alpha$ phase transformation in a near α titanium alloy. *Materials Science and Engineering: A*, 549, 20–29. <https://doi.org/10.1016/j.msea.2012.03.110>
- He, D., Zhu, J., Zaefferer, S., & Raabe, D. (2014). Effect of retained beta layer on slip transmission in Ti-6Al-2Zr-1Mo-1V near alpha titanium alloy during tensile deformation at room temperature. *Materials & Design (1980-2015)*, 56, 937–942. <https://doi.org/10.1016/j.matdes.2013.12.018>

- He, J., Zenk, C. H., Zhou, X., Neumeier, S., Raabe, D., Gault, B., & Mäkinen, S. K. (2020). On the atomic solute diffusional mechanisms during compressive creep deformation of a Co-Al-W-Ta single crystal superalloy. *Acta Materialia*, *184*, 86–99. <https://doi.org/10.1016/j.actamat.2019.11.035>
- He, Z. F., Jia, N., Ma, D., Yan, H.-L., Li, Z. M., & Raabe, D. (2019). Joint contribution of transformation and twinning to the high strength-ductility combination of a FeMnCoCr high entropy alloy at cryogenic temperatures. *Materials Science and Engineering: A*, *759*, 437–447.
- Helm, D., Butz, A., Raabe, D., & Gumbsch, P. (2011). Microstructure-based description of the deformation of metals: theory and application. *JOM: Journal of The Minerals, Metals & Materials Society*, *63*(4), 26–33. <https://doi.org/10.1007/s11837-011-0056-8>
- Hemzalová, P., Friák, M., Šob, M., Ma, D., Udyansky, A., Raabe, D., & Neugebauer, J. (2013). Ab initio study of thermodynamic, electronic, magnetic, structural, and elastic properties of Ni 4 N allotropes. *Physical Review B*, *88*(17), 174103.
- Herbig, M., Choi, P., & Raabe, D. (2015). Combining structural and chemical information at the nanometer scale by correlative transmission electron microscopy and atom probe tomography. *Ultramicroscopy*, *153*, 32–39. <https://doi.org/10.1016/j.ultramic.2015.02.003>
- Herbig, M., Choi, P.-P. P.-P., & Raabe, D. (2013). Combining structural and chemical information on the nanometer scale by correlative TEM and APT. *Microscopy and Microanalysis*, *19*(S2), 948–949. <https://doi.org/10.1017/s1431927613006739>
- Herbig, M., Kuzmina, M., Haase, C., Marceau, R. K. W., Gutierrez-Urrutia, I., Haley, D., Molodov, D. A., Choi, P., & Raabe, D. (2015). Grain boundary segregation in Fe-Mn-C twinning-induced plasticity steels studied by correlative electron backscatter diffraction and atom probe tomography. *Acta Materialia*, *83*, 37–47. <https://doi.org/10.1016/j.actamat.2014.09.041>
- Herbig, M., Raabe, D., Li, Y. J., Choi, P., Zaeferrer, S., & Goto, S. (2014). Atomic-scale quantification of grain boundary segregation in nanocrystalline material. *Physical Review Letters*, *112*(12), 126103. <https://doi.org/10.1103/PhysRevLett.112.126103>
- Heringhaus, F., Raabe, D., & Gottstein, G. (1995). On the correlation of microstructure and electromagnetic properties of heavily cold worked Cu-20 wt% Nb wires. *Acta Metallurgica Et Materialia*, *43*(4), 1467–1476. [https://doi.org/10.1016/0956-7151\(94\)00378-U](https://doi.org/10.1016/0956-7151(94)00378-U)
- Herrera, C., Ponge, D., & Raabe, D. (2008). Characterization of the Microstructure, Crystallographic Texture and Segregation of an As-cast Duplex Stainless Steel Slab. *Steel Research International*, *79*(6), 482–488. <https://doi.org/10.1002/srin.200806156>
- Herrera, C., Ponge, D., & Raabe, D. (2008). Microstructure and texture of hot-rolled duplex stainless steel. *3rd International Conference on Thermomechanical Processing of Steels, TMP 2008*.
- Herrera, C., Ponge, D., & Raabe, D. (2011). Design of a novel Mn-based 1 GPa duplex stainless TRIP steel with 60% ductility by a reduction of austenite stability. *Acta Materialia*, *59*(11), 4653–4664. <https://doi.org/10.1016/j.actamat.2011.04.011>
- Hickel, T., Sandlöbes, S., Marceau, R. K. W., Dick, A., Bleskov, I., Neugebauer, J., & Raabe, D. (2014). Impact of nanodiffusion on the stacking fault energy in high-strength steels. *Acta Materialia*, *75*, 147–155. <https://doi.org/10.1016/j.actamat.2014.04.062>

- Hohenwarter, A., Völker, B., Kapp, M. W., Li, Y., Goto, S., Raabe, D., & Pippan, R. (2016). Ultra-strong and damage tolerant metallic bulk materials: a lesson from nanostructured pearlitic steel wires. *Scientific Reports*, 6(1), 1–10. <https://doi.org/10.1038/srep33228>
- Hölscher, M., Raabe, D., & Lücke, K. (1991). Overview textures steels. *Steel Research*, 62, 567–575. <https://doi.org/10.1155/TSM.14-18.585>
- Hölscher, M., Raabe, D., & Lücke, K. (1991). Rolling and recrystallization textures of bcc steels. *Steel Research-Dusseldorf*, 62(12), 567–575.
- Hölscher, M., Raabe, D., & Lücke, K. (1994). Relation and Texture.Pdf. *Acta Metallurgica*, 42(3), 879–886.
- Hölscher, M., Raabe, D., & Lücke, K. (1994). Relationship between rolling textures and shear textures in f.c.c. and b.c.c. metals. *Acta Metallurgica Et Materialia*, 42(3), 879–886. [https://doi.org/10.1016/0956-7151\(94\)90283-6](https://doi.org/10.1016/0956-7151(94)90283-6)
- Hono, K., Raabe, D., Ringer, S. P., & Seidman, D. N. (2016). Atom probe tomography of metallic nanostructures. *MRS Bulletin*, 41(1), 23–29. <https://doi.org/10.1557/mrs.2015.314>
- Huang, L. F., Grabowski, B., Zhang, J., Lai, M. J., Tasan, C. C., Sandlöbes, S., Raabe, D., & Neugebauer, J. (2016). From electronic structure to phase diagrams: A bottom-up approach to understand the stability of titanium–transition metal alloys. *Acta Materialia*, 113, 311–319. <https://doi.org/10.1016/j.actamat.2016.04.059>
- Huang, L., Chen, D., Xie, D., Li, S., Zhang, Y., Zhu, T., Raabe, D., Ma, E., Li, J., & Shan, Z. (2023). Quantitative tests revealing hydrogen-enhanced dislocation motion in α -iron. *Nature Materials*, 22(6), 710–716. <https://doi.org/10.1038/s41563-023-01537-w>
- Huh, M. Y., Lee, J. H., Park, S. H., Engler, O., & Raabe, D. (2005). Effect of through-thickness macro and micro-texture gradients on ridging of 17%Cr ferritic stainless steel sheet. *Steel Research International*, 76(11), 797–806. <https://doi.org/10.1002/srin.200506098>
- Huh, M., Raabe, D., & Engler, O. (1995). Influence of solution treatment on the microstructure and crystallographic texture of cold rolled and recrystallised low carbon steel. *Steel Research*, 66(8), 353–359.
- Im, H. J., Lee, S., Choi, W. S., Makineni, S. K., Raabe, D., Ko, W. S., & Choi, P. P. (2020). Effects of Mo on the mechanical behavior of γ/γ' -strengthened Co-Ti-based alloys. *Acta Materialia*, 197, 69–80. <https://doi.org/10.1016/j.actamat.2020.07.037>
- Im, H. J., Lee, S., Choi, W. S., Makineni, S. K., Raabe, D., Ko, W.-S., & Choi, P.-P. (2020). Effects of Mo on the mechanical behavior of γ/γ' -strengthened Co-Ti-based alloys. *Acta Materialia*, 197, 69–80.
- Im, H. J., Makineni, S. K., Gault, B., Stein, F., Raabe, D., & Choi, P. P. (2018). Elemental partitioning and site-occupancy in γ/γ' forming Co-Ti-Mo and Co-Ti-Cr alloys. *Scripta Materialia*, 154, 159–162. <https://doi.org/10.1016/j.scriptamat.2018.05.041>
- Isik, M. I., Kostka, A., & Yardley, V. A. (2016). Microstructural stability and short-term creep properties of 12Cr-W-Mo-Co steel. *Materials Science and Engineering A*. <https://doi.org/10.1016/j.msea.2014.11.024>

- Isik, M. I., Kostka, A., Yardley, V. A., Pradeep, K. G., Duarte, M. J., Choi, P. P., Raabe, D., & Eggeler, G. (2015). The nucleation of Mo-rich Laves phase particles adjacent to M23C6 micrograin boundary carbides in 12% Cr tempered martensite ferritic steels. *Acta Materialia*, *90*, 94–104. <https://doi.org/10.1016/j.actamat.2015.01.027>
- Jafari, M., Jamshidian, M., Ziaei-Rad, S., Raabe, D., & Roters, F. (2017). Constitutive modeling of strain induced grain boundary migration via coupling crystal plasticity and phase-field methods. *International Journal of Plasticity*, *99*(September), 19–42. <https://doi.org/10.1016/j.ijplas.2017.08.004>
- Jäggle, E. A., Choi, P. P., Van Humbeeck, J., & Raabe, D. (2014). Precipitation and austenite reversion behavior of a maraging steel produced by selective laser melting. *Journal of Materials Research*, *29*(17), 2072–2079. <https://doi.org/10.1557/jmr.2014.204>
- Jäggle, E. A., Choi, P.-P. P., & Raabe, D. (2014). The maximum separation cluster analysis algorithm for atom-probe tomography: Parameter determination and accuracy. *Microscopy and Microanalysis*, *20*(6), 1662–1671. <https://doi.org/10.1017/S1431927614013294>
- Jäggle, E. A., Sheng, Z., Kürnsteiner, P., Ocylok, S., Weisheit, A., & Raabe, D. (2017). Comparison of maraging steel micro- and nanostructure produced conventionally and by laser additive manufacturing. *Materials*, *10*(1), 1–15. <https://doi.org/10.3390/ma10010008>
- Jäggle, E. A., Sheng, Z., Wu, L., Lu, L., Risse, J., Weisheit, A., & Raabe, D. (2016). Precipitation reactions in age-hardenable alloys during laser additive manufacturing. *Jom*, *68*(3), 943–949. <https://doi.org/10.1007/s11837-015-1764-2>
- Janssens, K., Raabe, D., Nestler, B., Kozeschnik, E., & Miodownik, M. (2007). Cellular automata. *Computational Materials Engineering: An Introduction to Microstructure Evolution*, 109–150.
- Jia, N., Eisenlohr, P., Roters, F., Raabe, D., Zhao, X., & Jia, N. (2012). Orientation dependence of shear banding in face-centered-cubic single crystals. *Acta Materialia*, *60*(8), 3415–3434. <https://doi.org/10.1016/j.actamat.2012.03.005>
- Jia, N., Raabe, D., & Zhao, X. (2014). Texture and microstructure evolution during non-crystallographic shear banding in a plane strain compressed Cu-Ag metal matrix composite. *Acta Materialia*, *76*, 238–251. <https://doi.org/10.1016/j.actamat.2014.05.036>
- Jia, N., Raabe, D., & Zhao, X. (2016). Crystal plasticity modeling of size effects in rolled multilayered Cu-Nb composites. *Acta Materialia*, *111*, 116–128. <https://doi.org/10.1016/j.actamat.2016.03.055>
- Jia, N., Roters, F., Eisenlohr, P., Kords, C., & Raabe, D. (2012). Non-crystallographic shear banding in crystal plasticity FEM simulations: Example of texture evolution in α -brass. *Acta Materialia*, *60*(3), 1099–1115. <https://doi.org/10.1016/j.actamat.2011.10.047>
- Jia, N., Roters, F., Eisenlohr, P., Raabe, D., & Zhao, X. (2013). Simulation of shear banding in heterophase co-deformation: Example of plane strain compressed Cu-Ag and Cu-Nb metal matrix composites. *Acta Materialia*, *61*(12), 4591–4606. <https://doi.org/10.1016/j.actamat.2013.04.029>

- Jiang, S., Wang, H., Wu, Y., Liu, X., Chen, H., Yao, M., Gault, B., Ponge, D., Raabe, D., Hirata, A., Chen, M., Wang, Y., & Lu, Z. (2017). Ultrastrong steel via minimal lattice misfit and high-density nanoprecipitation. *Nature*, *544*(7651), 460–464. <https://doi.org/10.1038/nature22032>
- Joseph, S., Kontis, P., Chang, Y., Shi, Y., Raabe, D., Gault, B., & Dye, D. (2022). A cracking oxygen story: A new view of stress corrosion cracking in titanium alloys. *Acta Materialia*, *227*. <https://doi.org/10.1016/j.actamat.2022.117687>
- Juntunen, P., Karjalainen, P., Raabe, D., Bolle, G., & Kopio, T. (2001). Optimizing continuous annealing of interstitial-free steels for improving deep drawability. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, *32*(8), 1989–1995. <https://doi.org/10.1007/s11661-001-0011-3>
- Kadkhodapour, J., Schmauder, S., Raabe, D., Ziaei-Rad, S., Weber, U., & Calcagnotto, M. (2011). Experimental and numerical study on geometrically necessary dislocations and non-homogeneous mechanical properties of the ferrite phase in dual phase steels. *Acta Materialia*, *59*(11), 4387–4394. <https://doi.org/10.1016/j.actamat.2011.03.062>
- Kapoor, R., Sarkar, A., Singh, J., Samajdar, I., & Raabe, D. (2014). Effect of strain rate on twinning in a Zr alloy. *Scripta Materialia*, *74*, 72–75. <https://doi.org/10.1016/j.scriptamat.2013.10.025>
- Kasian, O., Geiger, S., Li, T., Grote, J.-P., Schweinar, K., Zhang, S., Scheu, C., Raabe, D., Cherevko, S., & Gault, B. (2019). Degradation of iridium oxides via oxygen evolution from the lattice: correlating atomic scale structure with reaction mechanisms. *Energy & Environmental Science*, *12*(12), 3548–3555.
- Katnagallu, S., Dagan, M., Parviainen, S., Nematollahi, A., Grabowski, B., Bagot, P. A. J. J., Rolland, N., Neugebauer, J., Raabe, D., Vurpillot, F., Moody, M. P., & Gault, B. (2018). Impact of local electrostatic field rearrangement on field ionization. *Journal of Physics D: Applied Physics*, *51*(10), 105601. <https://doi.org/10.1088/1361-6463/aaaba6>
- Katnagallu, S., Gault, B., Grabowski, B., Neugebauer, J., Raabe, D., & Nematollahi, A. (2018). Advanced data mining in field ion microscopy. *Materials Characterization*, *146*, 307–318. <https://doi.org/10.1016/j.matchar.2018.02.040>
- Katnagallu, S., Nematollahi, A., Dagan, M., Moody, M., Grabowski, B., Gault, B., Raabe, D., & Neugebauer, J. (2017). High Fidelity Reconstruction of Experimental Field Ion Microscopy Data by Atomic Relaxation Simulations. *Microscopy and Microanalysis*, *23*(S1), 642–643. <https://doi.org/10.1017/s1431927617003877>
- Katnagallu, S., Wu, G., Singh, S. P., Nandam, S. H., Xia, W., Stephenson, L. T., Gleiter, H., Schwaiger, R., Hahn, H., & Herbig, M. (2020). Nanoglass–Nanocrystal Composite—a Novel Material Class for Enhanced Strength–Plasticity Synergy. *Small*, *16*(39), 2004400.
- Keerthika, B., Cao, Y. P., & Raabe, D. (2009). Mechanical characterization of viscoelastic-plastic soft matter using spherical indentation. *Cmc-Computers Materials & Continua*, *10*(3), 243–258.
- Khanchandani, H., El-Zoka, A. A., Kim, S. H., Tezins, U., Vogel, D., Sturm, A., Raabe, D., Gault, B., & Stephenson, L. T. (2022). Laser-equipped gas reaction chamber for probing environmentally sensitive materials at near atomic scale. *PLoS ONE*, *17*(2 February), e0262543. <https://doi.org/10.1371/journal.pone.0262543>

- Khorashadizadeh, A., Raabe, D., Winning, M., & Pippan, R. (2011). Recrystallization and Grain Growth in Ultrafine-Grained Materials Produced by High Pressure Torsion. *Advanced Engineering Materials*, *13*(4), 245–250. <https://doi.org/10.1002/adem.201000253>
- Khorashadizadeh, A., Raabe, D., Zaefferer, S., Rohrer, G. S., Rollett, A. D., & Winning, M. (2011). Five-parameter grain boundary analysis by 3D EBSD of an ultra fine grained CuZr alloy processed by equal channel angular pressing. *Advanced Engineering Materials*, *13*(4), 237–244. <https://doi.org/10.1002/adem.201000259>
- Khorrami, M. S., Mianroodi, J. R., Siboni, N. H., Goyal, P., Svendsen, B., Benner, P., & Raabe, D. (2023). An artificial neural network for surrogate modeling of stress fields in viscoplastic polycrystalline materials. *Npj Computational Materials*, *9*(1). <https://doi.org/10.1038/s41524-023-00991-z>
- Kim, J. K., Guo, W., Choi, P. P., & Raabe, D. (2018). Compositional evolution of long-period stacking ordered structures in magnesium studied by atom probe tomography. *Scripta Materialia*, *156*, 55–59. <https://doi.org/10.1016/j.scriptamat.2018.07.017>
- Kim, J. K., Jin, L., Sandlöbes, S., & Raabe, D. (2017). Diffusional-displacive transformation enables formation of long-period stacking order in magnesium. *Scientific Reports*, *7*(1), 1–8. <https://doi.org/10.1038/s41598-017-04343-y>
- Kim, J. K., Sandlöbes, S., & Raabe, D. (2015). On the room temperature deformation mechanisms of a Mg-Y-Zn alloy with long-period-stacking-ordered structures. *Acta Materialia*, *82*, 414–423. <https://doi.org/10.1016/j.actamat.2014.09.036>
- Kim, J., Oh, H. S., Kim, W., Choi, P.-P. P., Raabe, D., & Park, E. S. (2017). Modulation of plastic flow in metallic glasses via nanoscale networks of chemical heterogeneities. *Acta Materialia*, *140*, 116–129. <https://doi.org/10.1016/j.actamat.2017.08.002>
- Kim, J.-H. H., Kim, B. K., Kim, D.-I. I., Choi, P.-P. P., Raabe, D., & Yi, K.-W. W. (2015). The role of grain boundaries in the initial oxidation behavior of austenitic stainless steel containing alloyed Cu at 700 C for advanced thermal power plant applications. *Corrosion Science*, *96*, 52–66. <https://doi.org/10.1016/j.corsci.2015.03.014>
- Kim, J.-K. K., Ko, W.-S. S., Sandlöbes, S., Heidelmann, M., Grabowski, B., & Raabe, D. (2016). The role of metastable LPSO building block clusters in phase transformations of an Mg-Y-Zn alloy. *Acta Materialia*, *112*, 171–183. <https://doi.org/10.1016/j.actamat.2016.04.016>
- Kim, S. H., Zhang, X., Ma, Y., Souza Filho, I. R., Schweinar, K., Angenendt, K., Vogel, D., Stephenson, L. T., El-Zoka, A. A., Mianroodi, J. R., Rohwerder, M., Gault, B., & Raabe, D. (2021). Influence of microstructure and atomic-scale chemistry on the direct reduction of iron ore with hydrogen at 700°C. *Acta Materialia*, *212*, 116933. <https://doi.org/10.1016/j.actamat.2021.116933>
- Kim, S.-H., Antonov, S., Zhou, X., Stephenson, L. T., Jung, C., El-Zoka, A. A., Schreiber, D. K., Conroy, M., & Gault, B. (2022). Atom probe analysis of electrode materials for Li-ion batteries: challenges and ways forward. *Journal of Materials Chemistry A*, *10*(9), 4926–4935. <https://doi.org/10.1039/d1ta10050e>
- Kini, A. R., Maischner, D., Weisheit, A., Ponge, D., Gault, B., Jäggle, E. A., & Raabe, D. (2020). In-situ synthesis via laser metal deposition of a lean Cu–3.4 Cr–0.6 Nb (at%) conductive alloy hardened by Cr nano-scale precipitates and by Laves phase micro-particles. *Acta Materialia*, *197*, 330–340.

- Kishida, K., Okutani, M., Suzuki, H., Inui, H., Heilmaier, M., & Raabe, D. (2023). Room-temperature deformation of single crystals of the sigma-phase compound FeCr with the tetragonal D8b structure investigated by micropillar compression. *Acta Materialia*, 249(February), 118829. <https://doi.org/10.1016/j.actamat.2023.118829>
- Klinkenberg, C., Raabe, D., & Lücke, K. (1992). cementite on the cold-rolling textures of low-carbon steel. *Steel Research*, 63(6).
- Klinkenberg, C., Raabe, D., & Lücke, K. (1992). Effects of volume fraction and dispersion rate of grain boundary cementite on the recrystallization textures of low carbon steel. *Scripta Metallurgica et Materiala*, 26(7), 1137–1141. [https://doi.org/10.1016/0956-716X\(92\)90243-8](https://doi.org/10.1016/0956-716X(92)90243-8)
- Klinkenberg, C., Raabe, D., & Lucke, K. (1992). Influence of volume fraction and dispersion rate of grain-boundary cementite on the cold-rolling textures of low-carbon steel. *Steel Research*, 63(6), 263–269. <https://doi.org/10.1002/srin.199200512>
- Klinkenberg, C., Raabe, D., & Lucke, K. (1993). Influence of intercritical annealing on the texture formation in low-carbon steel strips. *Steel Research(Germany)*, 64(5), 262–266.
- Klinkenberg, C., Raabe, D., & Lücke, K. (1994). Modelling of the anisotropy of Young's modulus in polycrystals. *Steel Research*, 65(7), 291–297.
- Knoll, H., Ocylok, S., Weisheit, A., Springer, H., Jäggle, E., & Raabe, D. (2017). Combinatorial Alloy Design by Laser Additive Manufacturing. *Steel Research International*, 88(8), 1–11. <https://doi.org/10.1002/srin.201600416>
- Kobayashi, S., Schneider, A., Zaefferer, S., Frommeyer, G., & Raabe, D. (2005). Phase equilibria among α -Fe (Al, Cr, Ti), liquid and TiC and the formation of TiC in Fe₃Al-based alloys. *Acta Materialia*, 53(14), 3961–3970. <https://doi.org/10.1016/j.actamat.2005.04.044>
- Kobayashi, S., Zaefferer, S., Schneider, A., Raabe, D., & Frommeyer, G. (2005). Optimisation of precipitation for controlling recrystallisation of wrought Fe₃Al based alloys. *Intermetallics*, 13(12), 1296–1303. <https://doi.org/10.1016/j.intermet.2004.10.016>
- Kobayashi, S., Zaefferer, S., Schneider, A., Raabe, D., & Frommeyer, G. (2004). Slip system determination by rolling texture measurements around the strength peak temperature in a Fe₃Al-based alloy. *Materials Science and Engineering A*, 387–389(1-2 SPEC. ISS.), 950–954. <https://doi.org/10.1016/j.msea.2004.02.086>
- Kobayashi, S., Zambaldi, C., & Raabe, D. (2010). Orientation dependence of local lattice rotations at precipitates: Example of κ -Fe₃AlC carbides in a Fe₃Al-based alloy. *Acta Materialia*, 58(20), 6672–6684. <https://doi.org/10.1016/j.actamat.2010.08.030>
- Kolb, M., Freund, L. P., Fischer, F., Povstugar, I., Makineni, S. K., Gault, B., Raabe, D., Müller, J., Spiecker, E., Neumeier, S., & Göken, M. (2018). On the grain boundary strengthening effect of boron in γ/γ' Cobalt-base superalloys. *Acta Materialia*, 145, 247–254. <https://doi.org/10.1016/j.actamat.2017.12.020>
- Kolb, M., Zenk, C. H., Kirzinger, A., Povstugar, I., Raabe, D., Neumeier, S., & Göken, M. (2017). Influence of rhenium on γ' -strengthened cobalt-base superalloys. *Journal of Materials Research*, 32(13), 2551–2559.

- Konijnenberg, P. J., Zaefferer, S., & Raabe, D. (2015). Assessment of geometrically necessary dislocation levels derived by 3D EBSD. *Acta Materialia*, *99*, 402–414. <https://doi.org/10.1016/j.actamat.2015.06.051>
- Konijnenberg, P., Khorashadizadeh, A., Zaefferer, S., & Raabe, D. (2013). Analysis of 3D-EBSD Datasets Obtained by FIB Tomography. *Microscopy and Microanalysis*, *19*(S2), 846–847.
- Konrad, J., Zaefferer, S., & Raabe, D. (2006). Investigation of orientation gradients around a hard Laves particle in a warm-rolled Fe₃Al-based alloy using a 3D EBSD-FIB technique. *Acta Materialia*, *54*(5), 1369–1380. <https://doi.org/10.1016/j.actamat.2005.11.015>
- Konrad, J., Zaefferer, S., Schneider, A., Raabe, D., & Frommeyer, G. (2005). Hot deformation behavior of a Fe₃Al-binary alloy in the A2 and B2-order regimes. *Intermetallics*, *13*(12), 1304–1312. <https://doi.org/10.1016/j.intermet.2004.10.017>
- Kontis, P., Chauvet, E., Peng, Z., He, J., da Silva, A. K., Raabe, D., Tassin, C., Blandin, J.-J., Abed, S., Dendievel, R., Gault, B., & Martin, G. (2019). Atomic-scale grain boundary engineering to overcome hot-cracking in additively-manufactured superalloys. *Acta Materialia*, *177*, 209–221. <https://doi.org/10.1016/j.actamat.2019.07.041>
- Kontis, P., Collins, D. M., Wilkinson, A. J., Reed, R. C., Raabe, D., & Gault, B. (2018). Microstructural degradation of polycrystalline superalloys from oxidized carbides and implications on crack initiation. *Scripta Materialia*, *147*, 59–63. <https://doi.org/10.1016/j.scriptamat.2017.12.028>
- Kontis, P., Köhler, M., Evertz, S., Chen, Y.-T. T., Schnabel, V., Soler, R., Bednarick, J., Kirchlechner, C., Dehm, G., Raabe, D., Schneider, J. M., & Gault, B. (2018). Nano-laminated thin film metallic glass design for outstanding mechanical properties. *Scripta Materialia*, *155*, 73–77. <https://doi.org/10.1016/j.scriptamat.2018.06.015>
- Kontis, P., Kostka, A., Raabe, D., & Gault, B. (2019). Influence of composition and precipitation evolution on damage at grain boundaries in a crept polycrystalline Ni-based superalloy. *Acta Materialia*, *166*, 158–167. <https://doi.org/10.1016/j.actamat.2018.12.039>
- Kontis, P., Li, Z., Collins, D. M., Cormier, J., Raabe, D., & Gault, B. (2018). The effect of chromium and cobalt segregation at dislocations on nickel-based superalloys. *Scripta Materialia*, *145*, 76–80. <https://doi.org/10.1016/j.scriptamat.2017.10.005>
- Kontis, P., Li, Z., Segersäll, M., Moverare, J. J., Reed, R. C., Raabe, D., & Gault, B. (2018). The role of oxidized carbides on thermal-mechanical performance of polycrystalline superalloys. *Metallurgical and Materials Transactions A*, *49*(9), 4236–4245. <https://doi.org/10.1007/s11661-018-4709-x>
- Koprek, A., Cojocar-Mirédin, O., Wuerz, R., Freysoldt, C., & Raabe, D. (2015). Cd and impurity redistribution at the pn junction of CIGS based solar cells resolved by atom-probe tomography. *2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC)*, 1–6.
- Koprek, A., Cojocar-Mirédin, O., Wuerz, R., Freysoldt, C., Gault, B., & Raabe, D. (2016). Cd and impurity redistribution at the CdS/CIGS interface after annealing of CIGS-based solar cells resolved by atom probe tomography. *IEEE Journal of Photovoltaics*, *7*(1), 313–321. <https://doi.org/10.1109/JPHOTOV.2016.2629841>

- Körmann, F., Li, Z., Raabe, D., & Sluiter, M. H. F. (2021). Iron-rich High Entropy Alloys. In *High-Performance Ferrous Alloys* (pp. 389–421). Springer.
- Korte-Kerzel, S., Hickel, T., Huber, L., Raabe, D., Sandlöbes-Haut, S., Todorova, M., & Neugebauer, J. (2022). Defect phases—thermodynamics and impact on material properties. *International Materials Reviews*, *67*(1), 89–117. <https://doi.org/10.1080/09506608.2021.1930734>
- Kovács, A., Pradeep, K. G., Herzer, G., Raabe, D., & Dunin-Borkowski, R. E. (2016). Magnetic microstructure in a stress-annealed Fe₇₃. 5Si₁₅. 5B₇Nb₃Cu₁ soft magnetic alloy observed using off-axis electron holography and Lorentz microscopy. *Aip Advances*, *6*(5), 56501.
- Koyama, M., Akiyama, E., Lee, Y. K., Raabe, D., & Tsuzaki, K. (2017). Overview of hydrogen embrittlement in high-Mn steels. *International Journal of Hydrogen Energy*, *42*(17), 12706–12723. <https://doi.org/10.1016/j.ijhydene.2017.02.214>
- Koyama, M., Akiyama, E., Sawaguchi, T., Raabe, D., & Tsuzaki, K. (2012). Hydrogen-induced cracking at grain and twin boundaries in an Fe-Mn-C austenitic steel. *Scripta Materialia*, *66*(7), 459–462. <https://doi.org/10.1016/j.scriptamat.2011.12.015>
- Koyama, M., Akiyama, E., Tsuzaki, K., & Raabe, D. (2013). Hydrogen-assisted failure in a twinning-induced plasticity steel studied under in situ hydrogen charging by electron channeling contrast imaging. *Acta Materialia*, *61*(12), 4607–4618. <https://doi.org/10.1016/j.actamat.2013.04.030>
- Koyama, M., Bashir, A., Rohwerder, M., Merzlikin, S. V., Akiyama, E., Tsuzaki, K., & Raabe, D. (2015). Spatially and kinetically resolved mapping of hydrogen in a twinning-induced plasticity steel by use of Scanning Kelvin Probe Force Microscopy. *Journal of the Electrochemical Society*, *162*(12), C638–C647. <https://doi.org/10.1149/2.0131512jes>
- Koyama, M., Rohwerder, M., Tasan, C. C., Bashir, A., Akiyama, E., Takai, K., Raabe, D., & Tsuzaki, K. (2017). Recent progress in microstructural hydrogen mapping in steels: quantification, kinetic analysis, and multi-scale characterisation. *Materials Science and Technology (United Kingdom)*, *33*(13), 1481–1496. <https://doi.org/10.1080/02670836.2017.1299276>
- Koyama, M., Springer, H., Merzlikin, S. V., Tsuzaki, K., Akiyama, E., & Raabe, D. (2014). Hydrogen embrittlement associated with strain localization in a precipitation-hardened Fe-Mn-Al-C light weight austenitic steel. *International Journal of Hydrogen Energy*, *39*(9), 4634–4646. <https://doi.org/10.1016/j.ijhydene.2013.12.171>
- Koyama, M., Tasan, C. C., Akiyama, E., Tsuzaki, K., & Raabe, D. (2014). Hydrogen-assisted decohesion and localized plasticity in dual-phase steel. *Acta Materialia*, *70*, 174–187. <https://doi.org/10.1016/j.actamat.2014.01.048>
- Koyama, M., Tasan, C. C., Nagashima, T., Akiyama, E., Raabe, D., & Tsuzaki, K. (2016). Hydrogen-assisted damage in austenite/martensite dual-phase steel. *Philosophical Magazine Letters*, *96*(1), 9–18. <https://doi.org/10.1080/09500839.2015.1130275>
- Koyama, M., Zhang, Z., Wang, M., Ponge, D., Raabe, D., Tsuzaki, K., Noguchi, H., & Tasan, C. C. (2017). Bone-like crack resistance in hierarchical metastable nanolaminate steels. *Science*, *355*(6329), 1055–1057. <https://doi.org/10.1126/science.aal2766>

- Kraska, M., Doig, M., Tikhomirov, D., Raabe, D., & Roters, F. (2009). Virtual material testing for stamping simulations based on polycrystal plasticity. *Computational Materials Science*, *46*(2), 383–392. <https://doi.org/10.1016/j.commatsci.2009.03.025>
- Krause, F. F., Ahl, J.-P. P., Tytko, D., Choi, P.-P. P., Egoavil, R., Schowalter, M., Mehrtens, T., Müller-Caspary, K., Verbeeck, J., Raabe, D., Hertkorn, J., Engl, K., & Rosenauer, A. (2015). Homogeneity and composition of AlInGaN: A multiprobe nanostructure study. *Ultramicroscopy*, *156*(2015), 29–36. <https://doi.org/10.1016/j.ultramic.2015.04.012>
- Kresse, T., Li, Y. J., Boll, T., Borchers, C., Choi, P., Al-Kassab, T., Raabe, D., & Kirchheim, R. (2013). Influence of supersaturated carbon on the diffusion of Ni in ferrite determined by atom probe tomography. *Scripta Materialia*, *69*(5), 424–427. <https://doi.org/10.1016/j.scriptamat.2013.05.039>
- Krüger, T., Gross, M., Raabe, D., & Varnik, F. (2013). Crossover from tumbling to tank-treading-like motion in dense simulated suspensions of red blood cells. *Soft Matter*, *9*(37), 9008–9015.
- Krüger, T., Varnik, F., & Raabe, D. (2009). Shear stress in lattice Boltzmann simulations. *Physical Review E - Statistical, Nonlinear, and Soft Matter Physics*, *79*(4), 1–14. <https://doi.org/10.1103/PhysRevE.79.046704>
- Krüger, T., Varnik, F., & Raabe, D. (2010). Second-order convergence of the deviatoric stress tensor in the standard Bhatnagar-Gross-Krook lattice Boltzmann method. *Physical Review E*, *82*(2), 25701. <https://doi.org/10.1103/PhysRevE.82.025701>
- Krüger, T., Varnik, F., & Raabe, D. (2011). Efficient and accurate simulations of deformable particles immersed in a fluid using a combined immersed boundary lattice Boltzmann finite element method. *Computers and Mathematics with Applications*, *61*(12), 3485–3505. <https://doi.org/10.1016/j.camwa.2010.03.057>
- Krüger, T., Varnik, F., & Raabe, D. (2011). Particle stress in suspensions of soft objects. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, *369*(1945), 2414–2421. <https://doi.org/10.1098/rsta.2011.0090>
- Krywka, C., Sternemann, C., Paulus, M., Javid, N., Winter, R., Al-Sawalmih, A., Yi, S., Raabe, D., & Tolan, M. (2007). The small-angle and wide-angle X-ray scattering set-up at beamline BL9 of DELTA. *Journal of Synchrotron Radiation*, *14*(3), 244–251. <https://doi.org/10.1107/S0909049507009727>
- Kumar, D., Bieler, T. R., Eisenlohr, P., Mason, D. E., Crimp, M. A., Roters, F., & Raabe, D. (2008). On predicting nucleation of microcracks due to slip-twin interactions at grain boundaries in duplex Near gamma-TiAl. *Journal Of Engineering Materials And Technology-Transactions Of The Asme*, *130*(2), 0210121–02101212. <https://doi.org/10.1115/1.2841620>
- Kundin, J., Raabe, D., & Emmerich, H. (2011). A phase-field model for incoherent martensitic transformations including plastic accommodation processes in the austenite. *Journal of the Mechanics and Physics of Solids*, *59*(10), 2082–2102. <https://doi.org/10.1016/j.jmps.2011.07.001>
- Kuo, J.-C. C., Zaefferer, S., Zhao, Z., Winning, M., & Raabe, D. (2003). Deformation behavior of aluminum bicrystals. *Advanced Engineering Materials*, *5*(8), 563–566. <https://doi.org/10.1002/adem.200300372>

- Kürnsteiner, P., Bajaj, P., Gupta, A., Wilms, M. B., Weisheit, A., Li, X., Leinenbach, C., Gault, B., Jäggle, E. A., & Raabe, D. (2020). Control of thermally stable core-shell nano-precipitates in additively manufactured Al-Sc-Zr alloys. *Additive Manufacturing*, *32*.
<https://doi.org/10.1016/j.addma.2019.100910>
- Kürnsteiner, P., Hariharan, A., Jung, H. Y., Peter, N., Wilms, M. B., Weisheit, A., Barriobero-Vila, P., Gault, B., Raabe, D., & Jäggle, E. A. (2019). Application of Atom Probe Tomography to Complex Microstructures of Laser Additively Manufactured Samples. *Microscopy and Microanalysis*, *25*(S2), 2514–2515. <https://doi.org/10.1017/s1431927619013308>
- Kürnsteiner, P., Wilms, M. B., Weisheit, A., Barriobero-Vila, P., Jäggle, E. A., & Raabe, D. (2017). Massive nanoprecipitation in an Fe-19Ni-xAl maraging steel triggered by the intrinsic heat treatment during laser metal deposition. *Acta Materialia*, *129*, 52–60.
<https://doi.org/10.1016/j.actamat.2017.02.069>
- Kürnsteiner, P., Wilms, M. B., Weisheit, A., Barriobero-Vila, P., Gault, B., Jäggle, E. A., & Raabe, D. (2017). In-process Precipitation During Laser Additive Manufacturing Investigated by Atom Probe Tomography. *Microscopy and Microanalysis*, *23*(S1), 694–695.
<https://doi.org/10.1017/s1431927617004135>
- Kürnsteiner, P., Wilms, M. B., Weisheit, A., Gault, B., Jäggle, E. A., & Raabe, D. (2020). High-strength Damascus steel by additive manufacturing. *Nature*, *582*(7813), 515–519.
<https://doi.org/10.1038/s41586-020-2409-3>
- Kuzmina, M., Herbig, M., Ponge, D., Sandlöbes, S., & Raabe, D. (2015). Linear complexions: Confined chemical and structural states at dislocations. *Science*, *349*(6252), 1080–1083.
<https://doi.org/10.1126/science.aab2633>
- Kuzmina, M., Ponge, D., & Raabe, D. (2015). Grain boundary segregation engineering and austenite reversion turn embrittlement into toughness: Example of a 9 wt.% medium Mn steel. *Acta Materialia*, *86*, 182–192. <https://doi.org/10.1016/j.actamat.2014.12.021>
- Kwiatkowski da Silva, A., Inden, G., Kumar, A., Ponge, D., Gault, B., & Raabe, D. (2018). Competition between formation of carbides and reversed austenite during tempering of a medium-manganese steel studied by thermodynamic-kinetic simulations and atom probe tomography. *Acta Materialia*, *147*, 165–175. <https://doi.org/10.1016/j.actamat.2018.01.022>
- Kwiatkowski da Silva, A., Kamachali, R. D., Ponge, D., Gault, B., Neugebauer, J., & Raabe, D. (2019). Thermodynamics of grain boundary segregation, interfacial spinodal and their relevance for nucleation during solid-solid phase transitions. *Acta Materialia*, *168*, 109–120.
<https://doi.org/10.1016/j.actamat.2019.02.005>
- Kwiatkowski da Silva, A., Leyson, G., Kuzmina, M., Ponge, D., Herbig, M., Sandlöbes, S., Gault, B., Neugebauer, J., & Raabe, D. (2017). Confined chemical and structural states at dislocations in Fe-9wt%Mn steels: A correlative TEM-atom probe study combined with multiscale modelling. *Acta Materialia*, *124*, 305–315. <https://doi.org/10.1016/j.actamat.2016.11.013>
- Kwiatkowski Da Silva, A., Ponge, D., Peng, Z., Inden, G., Lu, Y., Breen, A., Gault, B., & Raabe, D. (2018). Phase nucleation through confined spinodal fluctuations at crystal defects evidenced in Fe-Mn alloys. *Nature Communications*, *9*(1), 1–11. <https://doi.org/10.1038/s41467-018-03591-4>

- Kwiatkowski da Silva, A., Souza Filho, I. R., Lu, W., Zilnyk, K. D., Hupaló, M. F., Alves, L. M., Ponge, D., Gault, B., & Raabe, D. (2022). A sustainable ultra-high strength Fe₁₈Mn₃Ti maraging steel through controlled solute segregation and α -Mn nanoprecipitation. *Nature Communications*, *13*(1), 1–8. <https://doi.org/10.1038/s41467-022-30019-x>
- Lai, M. J., Li, T., & Raabe, D. (2018). ω phase acts as a switch between dislocation channeling and joint twinning-and transformation-induced plasticity in a metastable β titanium alloy. *Acta Materialia*, *151*, 67–77. <https://doi.org/10.1016/j.actamat.2018.03.053>
- Lai, M. J., Li, Y. J., Lillpopf, L., Ponge, D., Will, S., & Raabe, D. (2018). On the origin of the improvement of shape memory effect by precipitating VC in Fe–Mn–Si-based shape memory alloys. *Acta Materialia*, *155*, 222–235. <https://doi.org/10.1016/j.actamat.2018.06.008>
- Lai, M. J., Tasan, C. C., & Raabe, D. (2015). Deformation mechanism of ω -enriched Ti-Nb-based gum metal: Dislocation channeling and deformation induced ω - β transformation. *Acta Materialia*, *100*, 290–300. <https://doi.org/10.1016/j.actamat.2015.08.047>
- Lai, M. J., Tasan, C. C., & Raabe, D. (2016). On the mechanism of {332} twinning in metastable β titanium alloys. *Acta Materialia*, *111*, 173–186. <https://doi.org/10.1016/j.actamat.2016.03.040>
- Lai, M. J., Tasan, C. C., Zhang, J., Grabowski, B., Huang, L. F., & Raabe, D. (2015). Origin of shear induced β to ω transition in Ti-Nb-based alloys. *Acta Materialia*, *92*, 55–63. <https://doi.org/10.1016/j.actamat.2015.03.040>
- Lapauw, T., Tytko, D., Vanmeensel, K., Huang, S., Choi, P.-P., Raabe, D., Caspi, E. N., Ozeri, O., To Baben, M., & Schneider, J. M. (2016). (Nb_x, Zr_{1-x})₄AlC₃ MAX Phase Solid Solutions: Processing, Mechanical Properties, and Density Functional Theory Calculations. *Inorganic Chemistry*, *55*(11), 5445–5452.
- Laplanche, G., Kostka, A., Horst, O. M., Eggeler, G., & George, E. P. (2016). Microstructure evolution and critical stress for twinning in the CrMnFeCoNi high-entropy alloy. *Acta Materialia*, *118*, 152–163. <https://doi.org/10.1016/j.actamat.2016.07.038>
- Lee, D.-H., Sun, B., Lee, S., Ponge, D., Jäggle, E. A., & Raabe, D. (2021). Comparative study of hydrogen embrittlement resistance between additively and conventionally manufactured 304L austenitic stainless steels. *Materials Science and Engineering: A*, *803*, 140499.
- Lei, Z., Liu, X., Wu, Y. Y., Wang, H. H., Jiang, S., Wang, S., Hui, X., Wu, Y. Y., Gault, B., Kontis, P., Raabe, D., Gu, L., Zhang, Q., Chen, H., Wang, H. H., Liu, J., An, K., Zeng, Q., Nieh, T. G., ... Z. Lei Y. Wu, H. Wang, S. Jiang, S. Wang, X. Hui, Y. Wu, B. Gault, P. Kontis, D. Raabe, L. Gu, Q. Zhang, H. Chen, H. Wang, J. Liu, K. An, Q. Zeng, T. Nieh, Z. Lu, X. L. (2018). Enhanced strength and ductility in a high-entropy alloy via ordered oxygen complexes. *Nature*, *563*(7732), 546–550. <https://doi.org/10.1038/s41586-018-0685-y>
- Lei, Z., Wu, Y., He, J., Liu, X., Wang, H., Jiang, S., Gu, L., Zhang, Q., Gault, B., Raabe, D., & Lu, Z. (2020). Snoek-type damping performance in strong and ductile high-entropy alloys. *Science Advances*, *6*(25), eaba7802. <https://doi.org/10.1126/sciadv.aba7802>
- Lemmens, B., Springer, H., De Graeve, I., De Strycker, J., Raabe, D., & Verbeken, K. (2017). Effect of silicon on the microstructure and growth kinetics of intermetallic phases formed during hot-dip

- aluminizing of ferritic steel. *Surface and Coatings Technology*, 319, 104–109. <https://doi.org/10.1016/j.surfcoat.2017.03.040>
- Lemmens, B., Springer, H., De Graeve, I., De Strycker, J., Raabe, D., & Verbeken, K. (2017). Phases formed during hot-dip aluminizing of ferritic steel. *Surface & Coatings Technology*, 319, 104–109.
- Lemmens, B., Springer, H., Duarte, M. J., De Graeve, I., De Strycker, J., Raabe, D., & Verbeken, K. (2016). Atom probe tomography of intermetallic phases and interfaces formed in dissimilar joining between Al alloys and steel. *Materials Characterization*, 120, 268–272. <https://doi.org/10.1016/j.matchar.2016.09.008>
- Lemmens, B., Springer, H., Peeters, M., De Graeve, I., De Strycker, J., Raabe, D., & Verbeken, K. (2018). Deformation induced degradation of hot-dip aluminized steel. *Materials Science and Engineering: A*, 710(July 2017), 385–391. <https://doi.org/10.1016/j.msea.2017.10.094>
- Li, F., Barani, A. A., Ponge, D., & Raabe, D. (2006). Austenite Grain Coarsening Behaviour in a Medium Carbon Si-Cr Spring Steel with and without Vanadium. *Steel Research International*, 77(8), 590–594. <https://doi.org/10.1002/srin.200606434>
- Li, J., Lu, W., Gibson, J., Zhang, S., Chen, T., Korte-Kerzel, S., & Raabe, D. (2018). Eliminating deformation incompatibility in composites by gradient nanolayer architectures. *Scientific Reports*, 8(1), 1–9. <https://doi.org/10.1038/s41598-018-34369-9>
- Li, J., Lu, W., Gibson, J., Zhang, S., Korte-Kerzel, S., & Raabe, D. (2020). Compatible deformation and extra strengthening by heterogeneous nanolayer composites. *Scripta Materialia*, 179, 30–35.
- Li, J., Lu, W., Zhang, S., & Raabe, D. (2017). Large strain synergetic material deformation enabled by hybrid nanolayer architectures. *Scientific Reports*, 7(1), 1–10. <https://doi.org/10.1038/s41598-017-11001-w>
- Li, L., Li, Z., Kwiatkowski da Silva, A., Peng, Z., Zhao, H., Gault, B., & Raabe, D. (2019). Segregation-driven grain boundary spinodal decomposition as a pathway for phase nucleation in a high-entropy alloy. *Acta Materialia*, 178, 1–9. <https://doi.org/10.1016/j.actamat.2019.07.052>
- Li, Q., Yan, F. K., Tao, N. R., Ponge, D., Raabe, D., & Lu, K. (2019). Deformation compatibility between nanotwinned and recrystallized grains enhances resistance to interface cracking in cyclic loaded stainless steel. *Acta Materialia*, 165, 87–98. <https://doi.org/10.1016/j.actamat.2018.11.033>
- Li, T., Kasian, O., Cherevko, S., Zhang, S., Geiger, S., Scheu, C., Felfer, P., Raabe, D., Gault, B., & Mayrhofer, K. J. J. J. (2018). Atomic-scale insights into surface species of electrocatalysts in three dimensions. *Nature Catalysis*, 1(4), 300–305. <https://doi.org/10.1038/s41929-018-0043-3>
- Li, Y. J. J., Kostka, A., Choi, P., Goto, S., Ponge, D., Kirchheim, R., & Raabe, D. (2015). Mechanisms of subgrain coarsening and its effect on the mechanical properties of carbon-supersaturated nanocrystalline hypereutectoid steel. *Acta Materialia*, 84, 110–123. <https://doi.org/10.1016/j.actamat.2014.10.027>
- Li, Y. J., Choi, P., Borchers, C., Westerkamp, S., Goto, S., Raabe, D., & Kirchheim, R. (2011). Atomic-scale mechanisms of deformation-induced cementite decomposition in pearlite. *Acta Materialia*, 59(10), 3965–3977. <https://doi.org/10.1016/j.actamat.2011.03.022>

- Li, Y. J., Choi, P., Goto, S., Borchers, C., Raabe, D., & Kirchheim, R. (2013). Atomic scale investigation of redistribution of alloying elements in pearlitic steel wires upon cold-drawing and annealing. *Ultramicroscopy*, *132*, 233–238. <https://doi.org/10.1016/j.ultramic.2012.10.010>
- Li, Y. J., Choi, P., Goto, S., Borchers, C., Raabe, D., & Kirchheim, R. (2012). Evolution of strength and microstructure during annealing of heavily cold-drawn 6.3 GPa hypereutectoid pearlitic steel wire. *Acta Materialia*, *60*(9), 4005–4016. <https://doi.org/10.1016/j.actamat.2012.03.006>
- Li, Y. J., Herbig, M., Goto, S., & Raabe, D. (2016). Formation of nanosized grain structure in martensitic 100Cr6 bearing steels upon rolling contact loading studied by atom probe tomography. *Materials Science and Technology*, *32*(11), 1100–1105. <https://doi.org/10.1080/02670836.2015.1120458>
- Li, Y. J., Herbig, M., Goto, S., & Raabe, D. (2017). Atomic scale characterization of white etching area and its adjacent matrix in a martensitic 100Cr6 bearing steel. *Materials Characterization*, *123*, 349–353. <https://doi.org/10.1016/j.matchar.2016.12.002>
- Li, Y. J., Ponge, D., Choi, P., & Raabe, D. (2015). Segregation of boron at prior austenite grain boundaries in a quenched martensitic steel studied by atom probe tomography. *Scripta Materialia*, *96*(C), 13–16. <https://doi.org/10.1016/j.scriptamat.2014.09.031>
- Li, Y., Raabe, D., Herbig, M., Choi, P.-P. P., Goto, S., Kostka, A., Yarita, H., Borchers, C., & Kirchheim, R. (2014). Segregation stabilizes nanocrystalline bulk steel with near theoretical strength. *Physical Review Letters*, *113*(10), 106104. <https://doi.org/10.1103/PhysRevLett.113.106104>
- Li, Y., Yuan, G., Li, L., Kang, J., Yan, F., Du, P., Raabe, D., & Wang, G. (2023). Ductile 2-GPa steels with hierarchical substructure. *Science (New York, N.Y.)*, *379*(6628), 168–173. <https://doi.org/10.1126/science.add7857>
- Li, Z., & Raabe, D. (2017). Designing novel high-entropy alloys towards superior properties. *Frontiers in Materials Processing Applications, Research and Technology (FIMPART'2017)*.
- Li, Z., & Raabe, D. (2017). Strong and Ductile Non-equiatomic High-Entropy Alloys: Design, Processing, Microstructure, and Mechanical Properties. *JOM*, *69*(11), 2099–2106. <https://doi.org/10.1007/s11837-017-2540-2>
- Li, Z., Körmann, F., Grabowski, B., Neugebauer, J., & Raabe, D. (2017). Ab initio assisted design of quinary dual-phase high-entropy alloys with transformation-induced plasticity. *Acta Materialia*, *136*, 262–270. <https://doi.org/10.1016/j.actamat.2017.07.023>
- Li, Z., Ludwig, A., Savan, A., Springer, H., & Raabe, D. (2018). Combinatorial metallurgical synthesis and processing of high-entropy alloys. *Journal of Materials Research*, *33*(19), 3156–3169. <https://doi.org/10.1557/jmr.2018.214>
- Li, Z., Pradeep, K. G., Deng, Y., Raabe, D., & Tasan, C. C. (2016). Metastable high-entropy dual-phase alloys overcome the strength-ductility trade-off. *Nature*, *534*(7606), 227–230. <https://doi.org/10.1038/nature17981>
- Li, Z., Tasan, C. C., Pradeep, K. G., & Raabe, D. (2017). A TRIP-assisted dual-phase high-entropy alloy: Grain size and phase fraction effects on deformation behavior. *Acta Materialia*, *131*, 323–335. <https://doi.org/10.1016/j.actamat.2017.03.069>

- Li, Z., Tasan, C. C., Springer, H., Gault, B., & Raabe, D. (2017). Interstitial atoms enable joint twinning and transformation induced plasticity in strong and ductile high-entropy alloys. *Scientific Reports*, 7(January), 1–7. <https://doi.org/10.1038/srep40704>
- Lia, Y. J., Choi, P., Borchers, C., Chen, Y. Z., Goto, S., Raabe, D., Kirchheim, R., Li, Y. J., Choi, P., Borchers, C., Chen, Y. Z., Goto, S., Raabe, D., & Kirchheim, R. (2011). Atom probe tomography characterization of heavily cold drawn pearlitic steel wire. *Ultramicroscopy*, 111(6), 628–632. <https://doi.org/10.1016/j.ultramic.2010.11.010>
- Liebscher, C. H., Stoffers, A., Alam, M., Lymperakis, L., Cojocaru-Mirédin, O., Gault, B., Neugebauer, J., Dehm, G., Scheu, C., & Raabe, D. (2018). Strain-induced asymmetric line segregation at faceted Si grain boundaries. *Physical Review Letters*, 121(1), 15702. <https://doi.org/10.1103/PhysRevLett.121.015702>
- Liebscher, C. H., Stoffers, A., Cojocaru-Mirédin, O., Gault, B., Scheu, C., Dehm, G., & Raabe, D. (2016). Topological Impurity Segregation at Faceted Silicon Grain Boundaries Studied by Correlative Atomic-Resolution STEM and APT. *Microscopy and Microanalysis*, 22(S5), 46–47.
- Liebscher, C. H., Yao, M., Dey, P., Lipińska-Chwalek, M., Berkels, B., Gault, B., Hickel, T., Herbig, M., Mayer, J., Neugebauer, J., Raabe, D., Dehm, G., & Scheu, C. (2018). Tetragonal fcc-Fe induced by κ -carbide precipitates: Atomic scale insights from correlative electron microscopy, atom probe tomography, and density functional theory. *Physical Review Materials*, 2(2), 23804. <https://doi.org/10.1103/PhysRevMaterials.2.023804>
- Lim, J., Ghoncheh Kasiri, D., Sahu, R., Schweinar, K., Hengge, K., Raabe, D., La Mantia, F., & Scheu, C. (2020). Irreversible Structural Changes of Copper Hexacyanoferrate Used as a Cathode in Zn-Ion Batteries. *Chemistry (Weinheim an Der Bergstrasse, Germany)*, 26(22), 4917.
- Lima, E. B. F., Pyzalla, A. R., Reimers, W., Kuo, J.-C., & Raabe, D. (2003). Mosaic Size Distributions in an Aluminum Bi-crystal Deformed by Channel Die Plane Strain Compression. *Journal of Neutron Research*, 11(4), 209–214.
- Lins, J. F. C. C., Sandim, H. R. Z. Z., Kestenbach, H.-J. J., Raabe, D., & Vecchio, K. S. (2007). A microstructural investigation of adiabatic shear bands in an interstitial free steel. *Materials Science and Engineering: A*, 457(1–2), 205–218. <https://doi.org/10.1016/j.msea.2006.12.019>
- Liu, B., Eisenlohr, P., Roters, F., & Raabe, D. (2012). Simulation of dislocation penetration through a general low-angle grain boundary. *Acta Materialia*, 60(13–14), 5380–5390. <https://doi.org/10.1016/j.actamat.2012.05.002>
- Liu, B., Raabe, D., Eisenlohr, P., Roters, F., Arsenlis, A., & Hommes, G. (2011). Dislocation interactions and low-angle grain boundary strengthening. *Acta Materialia*, 59(19), 7125–7134. <https://doi.org/10.1016/j.actamat.2011.07.067>
- Liu, B., Raabe, D., Roters, F., & Arsenlis, A. (2014). Interfacial dislocation motion and interactions in single-crystal superalloys. *Acta Materialia*, 79, 216–233. <https://doi.org/10.1016/j.actamat.2014.06.048>
- Liu, B., Raabe, D., Roters, F., Eisenlohr, P., & Lebensohn, R. A. (2010). Comparison of finite element and fast Fourier transform crystal plasticity solvers for texture prediction. *Modelling and*

Simulation in Materials Science and Engineering, 18(8). <https://doi.org/10.1088/0965-0393/18/8/085005>

- Liu, C., Garner, A., Zhao, H., Prangnell, P. B., Gault, B., Raabe, D., & Shanthraj, P. (2021). CALPHAD-informed phase-field modeling of grain boundary microchemistry and precipitation in Al-Zn-Mg-Cu alloys. *Acta Materialia*, 214, 116966. <https://doi.org/10.1016/j.actamat.2021.116966>
- Liu, C., Lu, W., Xia, W., Du, C., Rao, Z., Best, J. P., Brinckmann, S., Lu, J., Gault, B., Dehm, G., Wu, G., Li, Z., & Raabe, D. (2022). Massive interstitial solid solution alloys achieve near-theoretical strength. *Nature Communications*, 13(1). <https://doi.org/10.1038/s41467-022-28706-w>
- Liu, C., Shanthraj, P., Diehl, M., Roters, F., Dong, S., Dong, J., Ding, W., & Raabe, D. (2018). An integrated crystal plasticity-phase field model for spatially resolved twin nucleation, propagation, and growth in hexagonal materials. *International Journal of Plasticity*, 106(March), 203–227. <https://doi.org/10.1016/j.ijplas.2018.03.009>
- Liu, C., Shanthraj, P., Robson, J. D. J. D., Diehl, M., Dong, S., Dong, J., Ding, W., & Raabe, D. (2019). On the interaction of precipitates and tensile twins in magnesium alloys. *Acta Materialia*, 178(August), 146–162. <https://doi.org/10.1016/j.actamat.2019.07.046>
- Liu, J., Chen, C., Feng, Q., Fang, X., Wang, H., Liu, F., Lu, J., & Raabe, D. (2017). Dislocation activities at the martensite phase transformation interface in metastable austenitic stainless steel: An in-situ TEM study. *Materials Science and Engineering: A*, 703(July), 236–243. <https://doi.org/10.1016/j.msea.2017.06.107>
- Liu, T., Pinto, H., Brito, P., Sales, L. A., & Raabe, D. (2009). Residual stress analysis in chemical-vapor-deposition diamond films. *Applied Physics Letters*, 94(20), 201902. <https://doi.org/10.1063/1.3139083>
- Liu, T., Raabe, D., & Zaefferer, S. (2008). A 3D tomographic EBSD analysis of a CVD diamond thin film. *Science and Technology of Advanced Materials*, 9(3). <https://doi.org/10.1088/1468-6996/9/3/035013>
- Liu, T., Raabe, D., Mao, W., & Zaefferer, S. (2009). Microtexture and grain boundaries in freestanding CVD diamond films: Growth and twinning mechanisms. *Advanced Functional Materials*, 19(24), 3880–3891. <https://doi.org/10.1002/adfm.200901231>
- Liu, W. C., Li, Z., Man, C. S., Raabe, D., & Morris, J. G. (2006). Effect of precipitation on rolling texture evolution in continuous cast AA 3105 aluminum alloy. *Materials Science and Engineering A*, 434(1–2), 105–113. <https://doi.org/10.1016/j.msea.2006.06.102>
- Liu, W. C., Man, C. S., & Raabe, D. (2010). Effect of strain hardening on texture development in cold rolled Al-Mg alloy. *Materials Science and Engineering A*, 527(4–5), 1249–1254. <https://doi.org/10.1016/j.msea.2009.09.059>
- Liu, W. C., Man, C. S., Raabe, D., & Morris, J. G. (2005). Effect of hot and cold deformation on the recrystallization texture of continuous cast AA 5052 aluminum alloy. *Scripta Materialia*, 53(11), 1273–1277. <https://doi.org/10.1016/j.scriptamat.2005.07.040>

- Lomuscio, A., Rödel, T., Schwarz, T., Gault, B., Melchiorre, M., Raabe, D., & Siebentritt, S. (2019). Quasi-Fermi-Level Splitting of Cu-Poor and Cu-Rich Cu In S₂ Absorber Layers. *Physical Review Applied*, *11*(5), 54052.
- Lu, W., Guo, W., Wang, Z., Li, J., An, F., Dehm, G., Raabe, D., Liebscher, C. H., & Li, Z. (2023). Advancing strength and counteracting embrittlement by displacive transformation in heterogeneous high-entropy alloys containing sigma phase. *Acta Materialia*, *246*, 118717. <https://doi.org/10.1016/j.ACTAMAT.2023.118717>
- Lu, W., Herbig, M., Liebscher, C. H., Morsdorf, L., Marceau, R. K. W., Dehm, G., & Raabe, D. (2018). Formation of eta carbide in ferrous martensite by room temperature aging. *Acta Materialia*, *158*, 297–312. <https://doi.org/10.1016/j.actamat.2018.07.071>
- Lu, W., Liebscher, C. H., Dehm, G., Raabe, D., & Li, Z. (2018). Bidirectional transformation enables hierarchical nanolaminate dual-phase high-entropy alloys. *Advanced Materials*, *30*(44), 1804727.
- Lu, W., Liebscher, C. H., Dehm, G., Raabe, D., & Li, Z. (2018). Bidirectional Transformation Enables Hierarchical Nanolaminate Dual-Phase High-Entropy Alloys. *Advanced Materials*, *30*(44), 1–10. <https://doi.org/10.1002/adma.201804727>
- Lu, W., Liebscher, C. H., Yan, F., Fang, X., Li, L., Li, J., Guo, W., Dehm, G., Raabe, D., & Li, Z. (2019). Interfacial nanophases stabilize nanotwins in high-entropy alloys. *Acta Materialia*, *185*, 218–232. <https://doi.org/10.1016/j.actamat.2019.12.010>
- Lu, W., Liebscher, C. H., Yan, F., Fang, X., Li, L., Li, J., Guo, W., Dehm, G., Raabe, D., & Li, Z. (2020). Interfacial nanophases stabilize nanotwins in high-entropy alloys. *Acta Materialia*, *185*, 218–232. <https://doi.org/10.1016/j.actamat.2019.12.010>
- Lu, X., Zhang, X., Shi, M., Roters, F., Kang, G., & Raabe, D. (2019). Dislocation mechanism based size-dependent crystal plasticity modeling and simulation of gradient nano-grained copper. *International Journal of Plasticity*, *113*(September), 52–73. <https://doi.org/10.1016/j.ijplas.2018.09.007>
- Lübke, A., Enax, J., Loza, K., Prymak, O., Gaengler, P., Fabritius, H.-O. O., Raabe, D., & Epple, M. (2015). Dental lessons from past to present: ultrastructure and composition of teeth from plesiosaurs, dinosaurs, extinct and recent sharks. *RSC Advances*, *5*(76), 61612–61622. <https://doi.org/10.1039/c5ra11560d>
- Lübke, A., Enax, J., Wey, K., Fabritius, H.-O. O., Raabe, D., & Epple, M. (2016). Composites of fluoroapatite and methylmethacrylate-based polymers (PMMA) for biomimetic tooth replacement. *Bioinspiration & Biomimetics*, *11*(3), 35001. <https://doi.org/10.1088/1748-3190/11/3/035001>
- Lücke, R. K., Raabe, D., & Lücke, K. (1992). Texture and microstructure of hot rolled steel. *Scripta Metallurgica et Materialia*, *26*(8), 1221–1226. [https://doi.org/10.1016/0956-716X\(92\)90567-X](https://doi.org/10.1016/0956-716X(92)90567-X)
- Luebke, A., Loza, K., Patnaik, R., Enax, J., Raabe, D., Prymak, O., Fabritius, H. O., Gaengler, P., & Epple, M. (2017). Reply to the “Comments on ‘dental lessons from past to present: Ultrastructure and composition of teeth from plesiosaurs, dinosaurs, extinct and recent sharks’” by H. Botella: Et

- al., RSC Adv., 2016, 6, 74384-74388. *RSC Advances*, 7(11), 6215–6222.
<https://doi.org/10.1039/c6ra27121a>
- Luo, H., Li, Z., & Raabe, D. (2017). Hydrogen enhances strength and ductility of an equiatomic high-entropy alloy. *Scientific Reports*, 7(1), 1–7. <https://doi.org/10.1038/s41598-017-10774-4>
- Luo, H., Li, Z., Chen, Y. H., Ponge, D., Rohwerder, M., & Raabe, D. (2017). Hydrogen effects on microstructural evolution and passive film characteristics of a duplex stainless steel. *Electrochemistry Communications*, 79, 28–32. <https://doi.org/10.1016/j.elecom.2017.04.013>
- Luo, H., Li, Z., Lu, W., Ponge, D., & Raabe, D. (2018). Hydrogen embrittlement of an interstitial equimolar high-entropy alloy. *Corrosion Science*, 136(September 2017), 403–408.
<https://doi.org/10.1016/j.corsci.2018.03.040>
- Luo, H., Li, Z., Mingers, A. M., & Raabe, D. (2018). Corrosion behavior of an equiatomic CoCrFeMnNi high-entropy alloy compared with 304 stainless steel in sulfuric acid solution. *Corrosion Science*, 134(February), 131–139. <https://doi.org/10.1016/j.corsci.2018.02.031>
- Luo, H., Lu, W., Fang, X., Ponge, D., Li, Z., & Raabe, D. (2018). Beating hydrogen with its own weapon: Nano-twin gradients enhance embrittlement resistance of a high-entropy alloy. *Materials Today*, 21(10), 1003–1009. <https://doi.org/10.1016/j.mattod.2018.07.015>
- Luo, H., Sohn, S. S., Lu, W., Li, L., Li, X., Soundararajan, C. K., Krieger, W., Li, Z., & Raabe, D. (2020). A strong and ductile medium-entropy alloy resists hydrogen embrittlement and corrosion. *Nature Communications*, 11(1), 1–8. <https://doi.org/10.1038/s41467-020-16791-8>
- M.J. Lai, C.C. Tasan, J. Zhang, B. Grabowski, L.F. Huang, & D. Raabe. (2015). Origin of shear induced b to x transition in Ti–Nb-based alloys. *Acta Materialia*, 92, 55–63. https://ac.els-cdn.com/S1359645415002165/1-s2.0-S1359645415002165-main.pdf?_tid=4539944a-ddb3-11e7-a6ce-00000aab0f02&acdnat=1512914957_e79dc047cd90722ff740afce0b6594df
- Ma, A., Roters, F., & Raabe, D. (2004). Numerical study of textures and Lankford values for FCC polycrystals by use of a modified Taylor model. *Computational Materials Science*, 29(3), 353–361. <https://doi.org/10.1016/j.commatsci.2003.10.011>
- Ma, A., Roters, F., & Raabe, D. (2006). A dislocation density based constitutive model for crystal plasticity FEM including geometrically necessary dislocations. *Acta Materialia*, 54(8), 2169–2179. <https://doi.org/10.1016/j.actamat.2006.01.005>
- Ma, A., Roters, F., & Raabe, D. (2006). On the consideration of interactions between dislocations and grain boundaries in crystal plasticity finite element modeling - Theory, experiments, and simulations. *Acta Materialia*, 54(8), 2181–2194. <https://doi.org/10.1016/j.actamat.2006.01.004>
- Ma, A., Roters, F., & Raabe, D. (2006). Studying the effect of grain boundaries in dislocation density based crystal-plasticity finite element simulations. *International Journal of Solids and Structures*, 43(24), 7287–7303. <https://doi.org/10.1016/j.ijsolstr.2006.07.006>
- Ma, A., Roters, F., & Raabe, D. (2007). A dislocation density based constitutive law for BCC materials in crystal plasticity FEM. *Computational Materials Science*, 39(1 SPEC. ISS.), 91–95. <https://doi.org/10.1016/j.commatsci.2006.04.014>

- Ma, D., Eisenlohr, P., Epler, E., Volkert, C. A., Shanthraj, P., Diehl, M., Roters, F., & Raabe, D. (2016). Crystal plasticity study of monocrystalline stochastic honeycombs under in-plane compression. *Acta Materialia*, *103*, 796–808. <https://doi.org/10.1016/j.actamat.2015.11.016>
- Ma, D., Eisenlohr, P., Shanthraj, P., Diehl, M., Roters, F., & Raabe, D. (2015). Analytical bounds of in-plane Young's modulus and full-field simulations of two-dimensional monocrystalline stochastic honeycomb structures. *Computational Materials Science*, *109*, 323–329. <https://doi.org/10.1016/j.commatsci.2015.07.041>
- Ma, D., Friák, M., Neugebauer, J., Raabe, D., & Roters, F. (2008). Multiscale simulation of polycrystal mechanics of textured β -Ti alloys using ab initio and crystal-based finite element methods. *Physica Status Solidi (B) Basic Research*, *245*(12), 2642–2648. <https://doi.org/10.1002/pssb.200844227>
- Ma, D., Friák, M., von Pezold, J., Neugebauer, J., & Raabe, D. (2015). Ab initio study of compositional trends in solid solution strengthening in metals with low Peierls stresses. *Acta Materialia*, *98*, 367–376. <https://doi.org/10.1016/j.actamat.2015.07.054>
- Ma, D., Friák, M., Von Pezold, J., Raabe, D., & Neugebauer, J. (2015). Computationally efficient and quantitatively accurate multiscale simulation of solid-solution strengthening by ab initio calculation. *Acta Materialia*, *85*, 53–66. <https://doi.org/10.1016/j.actamat.2014.10.044>
- Ma, D., Friák, M., von Pezold, J., Raabe, D., Neugebauer, J., Pezold, J. Von, Raabe, D., & Neugebauer, J. (2013). Ab initio identified design principles of solid-solution strengthening in Al. *Science and Technology of Advanced Materials*, *14*(2), 25001. <https://doi.org/10.1088/1468-6996/14/2/025001>
- Ma, D., Grabowski, B., Körmann, F., Neugebauer, J., & Raabe, D. (2015). Ab initio thermodynamics of the CoCrFeMnNi high entropy alloy: Importance of entropy contributions beyond the configurational one. *Acta Materialia*, *100*, 90–97. <https://doi.org/10.1016/j.actamat.2015.08.050>
- Ma, D., Yao, M., Pradeep, K. G., Tasan, C. C., Springer, H., & Raabe, D. (2015). Phase stability of non-equiatomic CoCrFeMnNi high entropy alloys. *Acta Materialia*, *98*, 288–296. <https://doi.org/10.1016/j.actamat.2015.07.030>
- Ma, Y., Souza Filho, I. R., Bai, Y., Schenk, J., Patisson, F., Beck, A., van Bokhoven, J. A., Willinger, M. G., Li, K., Xie, D., Ponge, D., Zaefferer, S., Gault, B., Mianroodi, J. R., & Raabe, D. (2022). Hierarchical nature of hydrogen-based direct reduction of iron oxides. *Scripta Materialia*, 114571. <https://doi.org/10.1016/j.scriptamat.2022.114571>
- Ma, Y., Souza Filho, I. R., Zhang, X., Nandy, S., Barriobero-Vila, P., Requena, G., Vogel, D., Rohwerder, M., Ponge, D., Springer, H., & Raabe, D. (2022). Hydrogen-based direct reduction of iron oxide at 700°C: Heterogeneity at pellet and microstructure scales. *International Journal of Minerals, Metallurgy and Materials*, *29*(10), 1901–1907. <https://doi.org/10.1007/s12613-022-2440-5>
- Ma, Y., Sun, B., Schökel, A., Song, W., Ponge, D., Raabe, D., & Bleck, W. (2020). Phase boundary segregation-induced strengthening and discontinuous yielding in ultrafine-grained duplex medium-Mn steels. *Acta Materialia*, *200*, 389–403.

- Maaß, R., Van Petegem, S., Ma, D., Zimmermann, J., Grolimund, D., Roters, F., Van Swygenhoven, H., & Raabe, D. (2009). Smaller is stronger: The effect of strain hardening. *Acta Materialia*, *57*(20), 5996–6005. <https://doi.org/10.1016/j.actamat.2009.08.024>
- MacDonald, B. E., Fu, Z., Wang, X., Li, Z., Chen, W., Zhou, Y., Raabe, D., Schoenung, J., Hahn, H., & Lavernia, E. J. (2019). Influence of phase decomposition on mechanical behavior of an equiatomic CoCuFeMnNi high entropy alloy. *Acta Materialia*, *181*, 25–35. <https://doi.org/10.1016/j.actamat.2019.09.030>
- Makineni, S. K., Kini, A. R., Jäggle, E. A., Springer, H., Raabe, D., & Gault, B. (2018). Synthesis and stabilization of a new phase regime in a Mo-Si-B based alloy by laser-based additive manufacturing. *Acta Materialia*, *151*, 31–40. <https://doi.org/10.1016/j.actamat.2018.03.037>
- Makineni, S. K., Kumar, A., Lenz, M., Kontis, P., Meiners, T., Zenk, C., Zaefferer, S., Eggeler, G., Neumeier, S., Spiecker, E., Raabe, D., & Gault, B. (2018). On the diffusive phase transformation mechanism assisted by extended dislocations during creep of a single crystal CoNi-based superalloy. *Acta Materialia*, *155*, 362–371. <https://doi.org/10.1016/j.actamat.2018.05.074>
- Makineni, S. K., Lenz, M., Kontis, P., Li, Z., Kumar, A., Felfer, P. J., Neumeier, S., Herbig, M., Spiecker, E., Raabe, D., & Gault, B. (2018). Correlative Microscopy—Novel Methods and Their Applications to Explore 3D Chemistry and Structure of Nanoscale Lattice Defects: A Case Study in Superalloys. *JOM*, *70*(9), 1736–1743. <https://doi.org/10.1007/s11837-018-2802-7>
- Makineni, S. K., Lenz, M., Neumeier, S., Spiecker, E., Raabe, D., & Gault, B. (2018). Elemental segregation to antiphase boundaries in a crept CoNi-based single crystal superalloy. *Scripta Materialia*, *157*, 62–66. <https://doi.org/10.1016/j.scriptamat.2018.07.042>
- Mandal, S., Chikkadi, V., Nienhuis, B., Raabe, D., Schall, P., & Varnik, F. (2013). Single-particle fluctuations and directional correlations in driven hard-sphere glasses. *Physical Review E*, *88*(2), 22129. <https://doi.org/10.1103/PhysRevE.88.022129>
- Mandal, S., Gross, M., Raabe, D., & Varnik, F. (2012). Heterogeneous shear in hard sphere glasses. *Physical Review Letters*, *108*(9), 98301. <https://doi.org/10.1103/PhysRevLett.108.098301>
- Mandal, S., Lang, S., Gross, M., Oettel, M., Raabe, D., Franosch, T., & Varnik, F. (2014). Multiple reentrant glass transitions in confined hard-sphere glasses. *Nature Communications*, *5*(1), 1–8. <https://doi.org/10.1038/ncomms5435>
- Mandal, S., Pradeep, K. G., Zaefferer, S., & Raabe, D. (2014). A novel approach to measure grain boundary segregation in bulk polycrystalline materials in dependence of the boundaries' five rotational degrees of freedom. *Scripta Materialia*, *81*, 16–19. <https://doi.org/10.1016/j.scriptamat.2014.02.016>
- Maniruzzaman, M., Rahman, M. A., Gafur, M. A., Fabritius, H., & Raabe, D. (2012). Modification of pineapple leaf fibers and graft copolymerization of acrylonitrile onto modified fibers. *Journal of Composite Materials*, *46*(1), 79–90. <https://doi.org/10.1177/0021998311410486>
- Marceau, R. K. W. W., Ceguerra, A. V., Breen, A. J., Raabe, D., & Ringer, S. P. (2015). Quantitative chemical-structure evaluation using atom probe tomography: Short-range order analysis of Fe–Al. *Ultramicroscopy*, *157*, 12–20. <https://doi.org/10.1016/j.ultramic.2015.05.001>

- Marceau, R. K. W., Ceguerra, A. V., Breen, A. J., Palm, M., Stein, F., Ringer, S. P., & Raabe, D. (2015). Atom probe tomography investigation of heterogeneous short-range ordering in the 'komplex' phase state (K-state) of Fe-18Al (at.%). *Intermetallics*, *64*, 23–31.
- Marceau, R. K. W., Ceguerra, A. V., Breen, A. J., Palm, M., Stein, F., Ringer, S. P., & Raabe, D. (2015). Atom probe tomography investigation of heterogeneous short-range ordering in the "komplex" phase state (K-state) of Fe-18Al (at.%). *Intermetallics*, *64*, 23–31. <https://doi.org/10.1016/j.intermet.2015.04.005>
- Marceau, R. K. W., Choi, P., & Raabe, D. (2013). Understanding the detection of carbon in austenitic high-Mn steel using atom probe tomography. *Ultramicroscopy*, *132*, 239–247. <https://doi.org/10.1016/j.ultramic.2013.01.010>
- Marceau, R. K. W., Gutierrez-Urrutia, I., Herbig, M., Moore, K. L., Lozano-Perez, S., & Raabe, D. (2013). Multi-scale correlative microscopy investigation of both structure and chemistry of deformation twin bundles in Fe-Mn-C steel. *Microscopy and Microanalysis*, *19*(6), 1581–1585. <https://doi.org/10.1017/S1431927613013494>
- Marquis, E. A., Choi, P.-P., Danoix, F., Kruska, K., Lozano-Perez, S., Ponge, D., Raabe, D., & Williams, C. A. (2012). New Insights into the Atomic-Scale Structures and Behavior of Steels. *Microscopy Today*, *20*(4), 44–48. <https://doi.org/10.1017/s1551929512000387>
- Marx, V., Raabe, D., Engler, O., & Gottstein, G. (1997). Simulation of the Texture Evolution During Annealing of Cold Rolled Bcc and Fcc Metals Using a Cellular Automation Approach. *Textures and Microstructures*, *28*(3–4), 211–218.
- Mattern, N., Han, J. H., Pradeep, K. G., Kim, K. C., Park, E. M., Kim, D. H., Yokoyama, Y., Raabe, D., & Eckert, J. (2014). *J Alloys and Compounds 2014 APT metallic glass Mattern Pradeep Raabe Eckert*. *607*, 285–290.
- Mattern, N., Han, J. H., Pradeep, K. G., Kim, K. C., Park, E. M., Kim, D. H., Yokoyama, Y., Raabe, D., & Eckert, J. (2014). Structure of rapidly quenched (Cu_{0.5}Zr_{0.5})_{100-x}Ag_x alloys (x= 0–40 at.%). *Journal of Alloys and Compounds*, *607*, 285–290.
- Mattern, N., Han, J. H., Pradeep, K. G., Kim, K. C., Park, E. M., Kim, D. H., Yokoyama, Y., Raabe, D., & Eckert, J. (2014). Structure of rapidly quenched (Cu_{0.5}Zr_{0.5})_{100-x}Ag_x alloys (x = 0–40 at.%). *Journal of Alloys and Compounds*, *607*, 285–290. <https://doi.org/10.1016/j.jallcom.2014.04.047>
- Mattissen, D., Raabe, D., & Heringhaus, F. (1999). Experimental investigation and modeling of the influence of microstructure on the resistive conductivity of a Cu–Ag–Nb in situ composite. *Acta Materialia*, *47*(5), 1627–1634. [https://doi.org/10.1016/S1359-6454\(99\)00026-9](https://doi.org/10.1016/S1359-6454(99)00026-9)
- Matuszewski, K., Rettig, R., Matysiak, H., Peng, Z., Povstugar, I., Choi, P., Müller, J., Raabe, D., Spiecker, E., Kurzydłowski, K. J., & Singer, R. F. (2015). Effect of ruthenium on the precipitation of topologically close packed phases in Ni-based superalloys of 3rd and 4th generation. *Acta Materialia*, *95*, 274–283. <https://doi.org/10.1016/j.actamat.2015.05.033>
- Medrano, S., Zhao, H., De Geuser, F., Gault, B., Stephenson, L. T., Deschamps, A., Ponge, D., Raabe, D., & Sinclair, C. W. (2018). Cluster hardening in Al-3Mg triggered by small Cu additions. *Acta Materialia*, *161*, 12–20. <https://doi.org/10.1016/j.actamat.2018.08.050>

- Mehrtens, T., Bley, S., Schowalter, M., Sebald, K., Seyfried, M., Gutowski, J., Gerstl, S. S. A., Choi, P. P., Raabe, D., & Rosenauer, A. (2011). A (S)TEM and atom probe tomography study of InGaN. *Journal of Physics: Conference Series*, *326*(1), 1–5. <https://doi.org/10.1088/1742-6596/326/1/012029>
- Mehrtens, T., Bley, S., Schowalter, M., Sebald, K., Seyfried, M., Gutowski, J., Gerstl, S. S. A., Choi, P.-P., Raabe, D., & Rosenauer, A. (2011). A (S) TEM and atom probe tomography study of InGaN. *Journal of Physics: Conference Series*, *326*(1), 12029.
- Mehrtens, T., Schowalter, M., Tytko, D., Choi, P., Raabe, D., Hoffmann, L., Jönen, H., Rossow, U., Hangleiter, A., & Rosenauer, A. (2013). Measurement of the indium concentration in high indium content InGaN layers by scanning transmission electron microscopy and atom probe tomography. *Applied Physics Letters*, *102*(13), 100–103. <https://doi.org/10.1063/1.4799382>
- Mianroodi, J. R., H. Siboni, N., & Raabe, D. (2021). Teaching solid mechanics to artificial intelligence—a fast solver for heterogeneous materials. *Npj Computational Materials*, *7*(1), 1–10. <https://doi.org/10.1038/s41524-021-00571-z>
- Mianroodi, J. R., Rezaei, S., Siboni, N. H., Xu, B.-X., & Raabe, D. (2021). Lossless Multi-Scale Constitutive Elastic Relations with Artificial Intelligence. *Npj Computational Materials*, *8*(67), 1–12. <https://doi.org/10.1038/s41524-022-00753-3>
- Mianroodi, J. R., Shanthraj, P., Kontis, P., Cormier, J., Gault, B., Svendsen, B., & Raabe, D. (2019). Atomistic phase field chemomechanical modeling of dislocation-solute-precipitate interaction in Ni–Al–Co. *Acta Materialia*, *175*(2018), 250–261. <https://doi.org/10.1016/j.actamat.2019.06.008>
- Mianroodi, J. R., Shanthraj, P., Svendsen, B., & Raabe, D. (2021). Phase-Field Modeling of Chemoelastic Binodal/Spinodal Relations and Solute Segregation to Defects in Binary Alloys. *Materials*, *14*(7), 1787.
- Mianroodi, J. R., Siboni, N. H., & Raabe, D. (2022). Computational Discovery of Energy-Efficient Heat Treatment for Microstructure Design using Deep Reinforcement Learning. *ArXiv E-Prints*. <https://doi.org/10.48550/arxiv.2209.11259>
- Millan, J., Ponge, D., Raabe, D., Choi, P., & Dmitrieva, O. (2011). Characterization of Nano-Sized Precipitates in a Mn-Based Lean Maraging Steel by Atom Probe Tomography. *Steel Research International*, *82*(2), 137–145.
- Millán, J., Ponge, D., Raabe, D., Choi, P., & Dmitrieva, O. (2011). Characterization of nano-sized precipitates in a Mn-based lean maraging steel by atom probe tomography. *Steel Research International*, *82*(2), 137–145. <https://doi.org/10.1002/srin.201000274>
- Millán, J., Sandlöbes, S., Al-Zubi, A., Hickel, T., Choi, P., Neugebauer, J., Ponge, D., & Raabe, D. (2014). Designing Heusler nanoprecipitates by elastic misfit stabilization in Fe-Mn maraging steels. *Acta Materialia*, *76*, 94–105. <https://doi.org/10.1016/j.actamat.2014.05.016>
- Moon, J., Ha, H.-Y., Kim, K.-W., Park, S.-J., Lee, T.-H., Kim, S.-D., Jang, J. H., Jo, H.-H., Hong, H.-U., & Lee, B. H. (2020). A new class of lightweight, stainless steels with ultra-high strength and large ductility. *Scientific Reports*, *10*(1), 1–10.

- Morales-Rivas, L., Archie, F., Zaefferer, S., Benito-Alfonso, M., Tsai, S.-P. P., Yang, J.-R. R., Raabe, D., Garcia-Mateo, C., & Caballero, F. G. (2018). Crystallographic examination of the interaction between texture evolution, mechanically induced martensitic transformation and twinning in nanostructured bainite. *Journal of Alloys and Compounds*, *752*, 505–519. <https://doi.org/10.1016/j.jallcom.2018.04.189>
- Moravcik, I., Hadraba, H., Li, L., Dlouhy, I., Raabe, D., & Li, Z. (2020). Yield strength increase of a CoCrNi medium entropy alloy by interstitial nitrogen doping at maintained ductility. *Scripta Materialia*, *178*, 391–397. <https://doi.org/10.1016/j.scriptamat.2019.12.007>
- Moravcik, I., Hornik, V., Minárik, P., Li, L., Dlouhy, I., Janovska, M., Raabe, D., Li, Z., Moravcik, I., Hornik, V., Min, P., Minárik, P., Li, L., Dlouhy, I., Janovska, M., Raabe, D., & Li, Z. (2020). Interstitial doping enhances the strength-ductility synergy in a CoCrNi medium entropy alloy. *Materials Science and Engineering: A*, *781*(October 2019), 1–14. <https://doi.org/10.1016/j.msea.2020.139242>
- Morgado, F. F., Katnagallu, S., Freysoldt, C., Klaes, B., Vurpillot, F., Neugebauer, J., Raabe, D., Neumeier, S., Gault, B., & Stephenson, L. T. (2021). Revealing atomic-scale vacancy-solute interaction in nickel. *Scripta Materialia*, *203*, 114036.
- Morsdorf, L., Jeannin, O., Barbier, D., Mitsuhara, M., Raabe, D., & Tasan, C. C. (2016). Multiple mechanisms of lath martensite plasticity. *Acta Materialia*, *121*, 202–214. <https://doi.org/10.1016/j.actamat.2016.09.006>
- Morsdorf, L., Mayweg, D., Li, Y., Diederichs, A., Raabe, D., & Herbig, M. (2020). Moving cracks form white etching areas during rolling contact fatigue in bearings. *Materials Science and Engineering: A*, *771*, 138659.
- Morsdorf, L., Pradeep, K. G., Herzer, G., Kovács, A., Dunin-Borkowski, R. E., Povstugar, I., Konygin, G., Choi, P., & Raabe, D. (2016). Phase selection and nanocrystallization in Cu-free soft magnetic FeSiNbB amorphous alloy upon rapid annealing. *Journal of Applied Physics*, *119*(12), 124903. <https://doi.org/10.1063/1.4944595>
- Morsdorf, L., Tasan, C. C., Ponge, D., & Raabe, D. (2015). 3D structural and atomic-scale analysis of lath martensite: Effect of the transformation sequence. *Acta Materialia*, *95*, 366–377. <https://doi.org/10.1016/j.actamat.2015.05.023>
- Mouton, I., Breen, A. J., Wang, S., Chang, Y., Szczepaniak, A., Kontis, P., Stephenson, L. T., Raabe, D., Herbig, M., Britton, T. Ben, & Gault, B. (2019). Quantification Challenges for Atom Probe Tomography of Hydrogen and Deuterium in Zircaloy-4. *Microscopy and Microanalysis*, *25*(2), 481–488. <https://doi.org/10.1017/S143192761801615X>
- Nagashima, T., Koyama, M., Bashir, A., Rohwerder, M., Tasan, C. C., Akiyama, E., Raabe, D., & Tsuzaki, K. (2017). Interfacial hydrogen localization in austenite/martensite dual-phase steel visualized through optimized silver decoration and scanning Kelvin probe force microscopy. *Materials and Corrosion*, *68*(3), 306–310. <https://doi.org/10.1002/maco.201609104>
- Nakada, N., Fukagawa, R., Tsuchiyama, T., Takaki, S., Ponge, D., & Raabe, D. (2013). Inheritance of dislocations and crystallographic texture during martensitic reversion into austenite. *ISIJ International*, *53*(7), 1286–1288. <https://doi.org/10.2355/isijinternational.53.1286>

- Nakada, N., Tsuchiyama, T., Takaki, S., Ponge, D., & Raabe, D. (2013). Transition from diffusive to displacive austenite reversion in low-alloy steel. *ISIJ International*, *53*(12), 2275–2277. <https://doi.org/10.2355/isijinternational.53.2275>
- Nellessen, J., Sandlöbes, S., & Raabe, D. (2015). Effects of strain amplitude, cycle number and orientation on low cycle fatigue microstructures in austenitic stainless steel studied by electron channelling contrast imaging. *Acta Materialia*, *87*, 86–99. <https://doi.org/10.1016/j.actamat.2014.12.024>
- Nellessen, J., Sandlöbes, S., & Raabe, D. (2016). Low cycle fatigue in aluminum single and bi-crystals: On the influence of crystal orientation. *Materials Science and Engineering: A*, *668*, 166–179. <https://doi.org/10.1016/j.msea.2016.05.054>
- Nematollahi, G. A., Grabowski, B., Raabe, D., & Neugebauer, J. (2016). Multiscale description of carbon-supersaturated ferrite in severely drawn pearlitic wires. *Acta Materialia*, *111*, 321–334. <https://doi.org/10.1016/j.actamat.2016.03.052>
- Nematollahi, G. A., Von Pezold, J., Neugebauer, J., & Raabe, D. (2013). Thermodynamics of carbon solubility in ferrite and vacancy formation in cementite in strained pearlite. *Acta Materialia*, *61*(5), 1773–1784. <https://doi.org/10.1016/j.actamat.2012.12.001>
- Nene, S. S., Liu, K., Frank, M., Mishra, R. S., Brennan, R. E., Cho, K. C., Li, Z., & Raabe, D. (2017). Enhanced strength and ductility in a friction stir processing engineered dual phase high entropy alloy. *Scientific Reports*, *7*(1), 1–7. <https://doi.org/10.1038/s41598-017-16509-9>
- Niendorf, T., Wegener, T., Li, Z., & Raabe, D. (2018). Unexpected cyclic stress-strain response of dual-phase high-entropy alloys induced by partial reversibility of deformation. *Scripta Materialia*, *143*, 63–67. <https://doi.org/10.1016/j.scriptamat.2017.09.013>
- Nikolov, S., & Raabe, D. (2006). Yielding of polyethylene through propagation of chain twist defects: Temperature, stem length and strain-rate dependence. *Polymer*, *47*(5), 1696–1703.
- Nikolov, S., & Raabe, D. (2008). Hierarchical modeling of the elastic properties of bone at submicron scales: The role of extrafibrillar mineralization. *Biophysical Journal*, *94*(11), 4220–4232. <https://doi.org/10.1529/biophysj.107.125567>
- Nikolov, S., Fabritius, H. O., Friák, M., Raabe, D., & Neugebauer, J. (2012). Hierarchical modeling of biological nanocomposites. *Mechanics of Nanomaterials and Nanotechnology (Series in Applied Mathematics and Mechanics)*, 199–224.
- Nikolov, S., Fabritius, H., Petrov, M., Friák, M., Lymperakis, L., Sachs, C., Raabe, D., & Neugebauer, J. (2011). Robustness and optimal use of design principles of arthropod exoskeletons studied by ab initio-based multiscale simulations. *Journal of the Mechanical Behavior of Biomedical Materials*, *4*(2), 129–145. <https://doi.org/10.1016/j.jmbbm.2010.09.015>
- Nikolov, S., Han, C.-S., & Raabe, D. (2007). On the origin of size effects in small-strain elasticity of solid polymers. *International Journal of Solids and Structures*, *44*(5), 1582–1592.
- Nikolov, S., Lebensohn, R. A., & Raabe, D. (2006). Self-consistent modeling of large plastic deformation, texture and morphology evolution in semi-crystalline polymers. *Journal of the Mechanics and Physics of Solids*, *54*(7), 1350–1375. <https://doi.org/10.1016/j.jmps.2006.01.008>

- Nikolov, S., Petrov, M., Lymperakis, L., Friák, M., Sachs, C., Fabritius, H. O., Raabe, D., & Neugebauer, J. (2010). Revealing the design principles of high-performance biological composites using Ab initio and multiscale simulations: The example of lobster cuticle. *Advanced Materials*, *22*(4), 519–526. <https://doi.org/10.1002/adma.200902019>
- Oh, H. S., Kim, S. J., Odbadrakh, K., Ryu, W. H., Yoon, K. N., Mu, S., Körmann, F., Ikeda, Y., Tasan, C. C., Raabe, D., Egami, T., & Park, E. S. (2019). Engineering atomic-level complexity in high-entropy and complex concentrated alloys. *Nature Communications*, *10*(1). <https://doi.org/10.1038/s41467-019-10012-7>
- Oh, H. S., Ma, D., Leyson, G. P., Grabowski, B., Park, E. S., Körmann, F., & Raabe, D. (2016). Lattice distortions in the FeCoNiCrMn high entropy alloy studied by theory and experiment. *Entropy*, *18*(9), 1–9. <https://doi.org/10.3390/e18090321>
- Oliveira, V. B., Sandim, H. R. Z., & Raabe, D. (2017). Abnormal grain growth in Eurofer-97 steel in the ferrite phase field. *Journal of Nuclear Materials*, *485*, 23–38.
- Orava, J., Balachandran, S., Han, X., Shuleshova, O., Nurouzi, E., Soldatov, I., Oswald, S., Gutowski, O., Ivashko, O., Dippel, A.-C., Zimmermann, M. v., Ivanov, Y. P., Greer, A. L., Raabe, D., Herbig, M., & Kaban, I. (2021). In situ correlation between metastable phase-transformation mechanism and kinetics in a metallic glass. *Nature Communications*, *12*(1), 1–13. <https://doi.org/10.1038/s41467-021-23028-9>
- Otto, F., Dlouhý, A., Pradeep, K. G. G., Kuběnová, M., Raabe, D., Eggeler, G., & George, E. P. P. (2016). Decomposition of the single-phase high-entropy alloy CrMnFeCoNi after prolonged anneals at intermediate temperatures. *Acta Materialia*, *112*, 40–52. <https://doi.org/10.1016/j.actamat.2016.04.005>
- Palanisamy, D., Ener, S., Maccari, F., Schäfer, L., Skokov, K. P., Gutfleisch, O., Raabe, D., & Gault, B. (2020). Grain boundary segregation, phase formation, and their influence on the coercivity of rapidly solidified SmFe₁₁Ti hard magnetic alloys. *Physical Review Materials*, *4*(5), 54404. <https://doi.org/10.1103/physrevmaterials.4.054404>
- Palanisamy, D., Kovács, A., Hegde, O., Dunin-Borkowski, R. E., Raabe, D., Hickel, T., & Gault, B. (2021). Influence of crystalline defects on magnetic nanodomains in a rare-earth-free magnetocrystalline anisotropic alloy. *Physical Review Materials*, *5*(6), 64403.
- Palanisamy, D., Raabe, D., & Gault, B. (2018). Elemental segregation to twin boundaries in a MnAl ferromagnetic Heusler alloy. *Scripta Materialia*, *155*, 144–148. <https://doi.org/10.1016/j.scriptamat.2018.06.037>
- Palanisamy, D., Raabe, D., & Gault, B. (2019). On the compositional partitioning during phase transformation in a binary ferromagnetic MnAl alloy. *Acta Materialia*, *174*, 227–236. <https://doi.org/10.1016/j.actamat.2019.05.037>
- Pandey, P., Makineni, S. K., Samanta, A., Sharma, A., Das, S. M., Nithin, B., Srivastava, C., Singh, A. K., Raabe, D., Gault, B., & Chattopadhyay, K. (2019). Elemental site occupancy in the L1₂ A3B ordered intermetallic phase in Co-based superalloys and its influence on the microstructure. *Acta Materialia*, *163*, 140–153. <https://doi.org/10.1016/j.actamat.2018.09.049>

- Park, Y. B., Raabe, D., & Yim, T. H. (1996). Cold rolling textures of Fe-Ni soft magnetic alloys. *Scripta Materialia*, 35(11), 1277–1284. [https://doi.org/10.1016/1359-6462\(96\)00308-9](https://doi.org/10.1016/1359-6462(96)00308-9)
- Park, Y. B., Raabe, D., & Yim, T. H. (1996). Rolling and recrystallization textures in Fe-Ni alloys. *Metals and Materials*, 2(3), 151–157.
- Parsa, A. B., Wollgramm, P., Buck, H., Somsen, C., Kostka, A., Povstugar, I., Choi, P. P., Raabe, D., Dlouhy, A., Müller, J., Spiecker, E., Demtroder, K., Schreuer, J., Neuking, K., & Eggeler, G. (2015). Advanced scale bridging microstructure analysis of single crystal Ni-base superalloys. *Advanced Engineering Materials*, 17(2), 216–230. <https://doi.org/10.1002/adem.201400136>
- Pavlic, O., Ibarra-Hernandez, W., Valencia-Jaime, I., Singh, S., Avendano-Franco, G., Raabe, D., Romero, A. H., Avendaño-Franco, G., Raabe, D., & Romero, A. H. (2017). Design of Mg alloys: The effects of Li concentration on the structure and elastic properties in the Mg-Li binary system by first principles calculations. *Journal of Alloys and Compounds*, 691, 15–25. <https://doi.org/10.1016/j.jallcom.2016.08.217>
- Pei, Z., Friák, M., Sandlöbes, S., Nazarov, R., Svendsen, B., Raabe, D., & Neugebauer, J. (2015). Rapid theory-guided prototyping of ductile Mg alloys: from binary to multi-component materials. *New Journal of Physics*, 17(9), 93009. <https://doi.org/10.1088/1367-2630/17/9/093009>
- Pei, Z., Ma, D., Friák, M., Svendsen, B., Raabe, D., & Neugebauer, J. (2015). From generalized stacking fault energies to dislocation properties: Five-energy-point approach and solid solution effects in magnesium. *Physical Review B*, 92(6), 64107.
- Pei, Z., Yin, J., Liaw, P. K., & Raabe, D. (2023). Toward the design of ultrahigh-entropy alloys via mining six million texts. *Nature Communications*, 14, 54. <https://doi.org/10.1038/s41467-022-35766-5>
- Pei, Z., Zhu, L.-F. F., Friák, M., Sandlöbes, S., von Pezold, J., Sheng, H. W., Race, C. P., Zaefferer, S., Svendsen, B., Raabe, D., & Neugebauer, J. (2013). Ab initio and atomistic study of generalized stacking fault energies in Mg and Mg–Y alloys. *New Journal of Physics*, 15(4), 43020. <https://doi.org/10.1088/1367-2630/15/4/043020>
- Peivaste, I., Siboni, N. H., Alahyarizadeh, G., Ghaderi, R., Svendsen, B., Raabe, D., & Mianroodi, J. R. (2022). Machine-learning-based surrogate modeling of microstructure evolution using phase-field. *Computational Materials Science*, 214, 111750. <https://doi.org/10.1016/j.commatsci.2022.111750>
- Peng, Z., Choi, P. P., Gault, B., & Raabe, D. (2017). Evaluation of Analysis Conditions for Laser-Pulsed Atom Probe Tomography: Example of Cemented Tungsten Carbide. *Microscopy and Microanalysis*, 23(2), 431–442. <https://doi.org/10.1017/S1431927616012654>
- Peng, Z., Gault, B., Raabe, D., Ashton, M. W., Sinnott, S. B., Choi, P.-P., & Li, Y. (2017). On the Multiple Event Detection in Atom Probe Tomography. *Microscopy and Microanalysis*, 23(S1), 618–619. <https://doi.org/10.1017/s1431927617003762>
- Peng, Z., Lu, Y., Hatzoglou, C., Kwiatkowski Da Silva, A., Vurpillot, F., Ponge, D., Raabe, D., & Gault, B. (2019). An Automated Computational Approach for Complete In-Plane Compositional Interface Analysis by Atom Probe Tomography. *Microscopy and Microanalysis*, 25(2), 389–400. <https://doi.org/10.1017/S1431927618016112>

- Peng, Z., Povstugar, I., Matuszewski, K., Rettig, R., Singer, R., Kostka, A., Choi, P. P., & Raabe, D. (2015). Effects of Ru on elemental partitioning and precipitation of topologically close-packed phases in Ni-based superalloys. *Scripta Materialia*, *101*, 44–47. <https://doi.org/10.1016/j.scriptamat.2015.01.014>
- Peng, Z., Rohwerder, M., Choi, P. P., Gault, B., Meiners, T., Friedrichs, M., Kreilkamp, H., Klocke, F., & Raabe, D. (2017). Atomic diffusion induced degradation in bimetallic layer coated cemented tungsten carbide. *Corrosion Science*, *120*, 1–13. <https://doi.org/10.1016/j.corsci.2017.01.007>
- Peng, Z., Vurpillot, F., Choi, P. P., Li, Y., Raabe, D., & Gault, B. (2018). On the detection of multiple events in atom probe tomography. *Ultramicroscopy*, *189*, 54–60. <https://doi.org/10.1016/j.ultramic.2018.03.018>
- Peng, Z., Zanuttini, D., Gervais, B., Jacquet, E., Blum, I., Choi, P. P., Raabe, D., Vurpillot, F., & Gault, B. (2019). Unraveling the Metastability of Cn^{2+} ($n = 2-4$) Clusters. *Journal of Physical Chemistry Letters*, *10*(3), 581–588. <https://doi.org/10.1021/acs.jpcclett.8b03449>
- Peranio, N., Li, Y. J., Roters, F., & Raabe, D. (2010). Microstructure and texture evolution in dual-phase steels: Competition between recovery, recrystallization, and phase transformation. *Materials Science and Engineering A*, *527*(16–17), 4161–4168. <https://doi.org/10.1016/j.msea.2010.03.028>
- Pierce, D. T., Jiménez, J. A., Bentley, J., Raabe, D., & Wittig, J. E. (2015). The influence of stacking fault energy on the microstructural and strain-hardening evolution of Fe–Mn–Al–Si steels during tensile deformation. *Acta Materialia*, *100*, 178–190. <https://doi.org/10.1016/j.actamat.2015.08.030>
- Pierce, D. T., Jiménez, J. A., Bentley, J., Raabe, D., Oskay, C., & Wittig, J. E. (2014). The influence of manganese content on the stacking fault and austenite/ ϵ -martensite interfacial energies in Fe–Mn–(Al–Si) steels investigated by experiment and theory. *Acta Materialia*, *68*, 238–253. <https://doi.org/10.1016/j.actamat.2014.01.001>
- Plancher, E., Tasan, C. C., Sandloebes, S., & Raabe, D. (2013). On dislocation involvement in Ti – Nb gum metal plasticity Author ' s personal copy. *Scripta Materialia*, *68*, 805–808.
- Plancher, E., Tasan, C. C., Sandloebes, S., & Raabe, D. (2013). On dislocation involvement in Ti-Nb gum metal plasticity. *Scripta Materialia*, *68*(10), 805–808. <https://doi.org/10.1016/j.scriptamat.2013.01.034>
- Povstugar, I., Choi, P. P., Neumeier, S., Bauer, A., Zenk, C. H., Göken, M., & Raabe, D. (2014). Elemental partitioning and mechanical properties of Ti- and Ta-containing Co-Al-W-base superalloys studied by atom probe tomography and nanoindentation. *Acta Materialia*, *78*, 78–85. <https://doi.org/10.1016/j.actamat.2014.06.020>
- Povstugar, I., Choi, P.-P. P., Tytko, D., Ahn, J.-P. P., & Raabe, D. (2013). Interface-directed spinodal decomposition in TiAlN/CrN multilayer hard coatings studied by atom probe tomography. *Acta Materialia*, *61*(20), 7534–7542. <https://doi.org/10.1016/j.actamat.2013.08.028>
- Povstugar, I., Zenk, C. H., Li, R., Choi, P.-P. P., Neumeier, S., Dolotko, O., Hoelzel, M., Göken, M., & Raabe, D. (2016). Elemental partitioning, lattice misfit and creep behaviour of Cr containing

- gamma prime strengthened Co base superalloys. *Materials Science and Technology (United Kingdom)*, 32(3), 220–225. <https://doi.org/10.1179/1743284715Y.0000000112>
- Pradeep, K. G., Herzer, G., & Raabe, D. (2015). Atomic scale study of CU clustering and pseudo-homogeneous Fe-Si nanocrystallization in soft magnetic FeSiNbB(CU) alloys. *Ultramicroscopy*, 159, 285–291. <https://doi.org/10.1016/j.ultramic.2015.04.006>
- Pradeep, K. G., Herzer, G., Choi, P., & Raabe, D. (2014). Atom probe tomography study of ultrahigh nanocrystallization rates in FeSiNbBCu soft magnetic amorphous alloys on rapid annealing. *Acta Materialia*, 68, 295–309. <https://doi.org/10.1016/j.actamat.2014.01.031>
- Pradeep, K. G., Tasan, C. C., Yao, M. J., Deng, Y., Springer, H., & Raabe, D. (2015). Non-equiatom high entropy alloys: Approach towards rapid alloy screening and property-oriented design. *Materials Science and Engineering A*, 648, 183–192. <https://doi.org/10.1016/j.msea.2015.09.010>
- Pradeep, K. G., Wanderka, N., Choi, P., Banhart, J., Murty, B. S., & Raabe, D. (2013). Atomic-scale compositional characterization of a nanocrystalline AlCrCuFeNiZn high-entropy alloy using atom probe tomography. *Acta Materialia*, 61(12), 4696–4706. <https://doi.org/10.1016/j.actamat.2013.04.059>
- Prakash, A., Guérolé, J., Wang, J., Müller, J., Spiecker, E., Mills, M. J., Povstugar, I., Choi, P., Raabe, D., & Bitzek, E. (2015). Atom probe informed simulations of dislocation-precipitate interactions reveal the importance of local interface curvature. *Acta Materialia*, 92, 33–45. <https://doi.org/10.1016/j.actamat.2015.03.050>
- Pristovsek, M., Han, Y., Zhu, T., Oehler, F., Tang, F., Oliver, R. A., Humphreys, C. J., Tytko, D., Choi, P., & Raabe, D. (2016). Structural and optical properties of (11 $\bar{2}$ 2) InGaN quantum wells compared to (0001) and (11 $\bar{2}$ 0). *Semiconductor Science and Technology*, 31(8), 85007.
- Pristovsek, M., Han, Y., Zhu, T., Oehler, F., Tang, F., Oliver, R. A., Humphreys, C. J., Tytko, D., Choi, P., Raabe, D., Brunner, F., & Weyers, M. (2016). Structural and optical properties of (1122) InGaN quantum wells compared to (0001) and (1120). *Semiconductor Science and Technology*, 31(8), 1–8. <https://doi.org/10.1088/0268-1242/31/8/085007>
- Prymak, O., Enax, J., Fabritius, H., Raabe, D., & Epple, M. (2013). Correlation of composition and structure of shark teeth. *Engineering of Biomaterials*, 16.
- Qian, X., Cao, Y., Zhang, J., Raabe, D., Yao, Z., & Fei, B. (2008). An inverse approach to determine the mechanical properties of elastoplastic materials using indentation tests. *Cmc-Computers Materials & Continua*, 7(1), 33–41.
- Raabe, D. (1994). Modelling of grain rotations during compression deformation of polycrystalline intermetallic L12 compounds. *Materials Science and Engineering: A*, 186(1–2), L1–L3.
- Raabe, D. (1994). Modelling of texture evolution during rolling and compression deformation of intermetallic Ni3Al and NiAl polycrystals. *Computational Materials Science*, 3(2), 231–240.
- Raabe, D. (1994). Simulation of texture evolution during rolling deformation of an intermetallic Fe-28Al-5Cr polycrystal. *Materials Letters*, 19(1–2), 75–78.

- Raabe, D. (1995). Contribution of $\{123\}$ $\langle 111 \rangle$ slip systems to deformation of b.c.c. metals. *Physica Status Solidi (A)*, 149(2), 575–581. <https://doi.org/10.1002/pssa.2211490208>
- Raabe, D. (1995). Experimental investigation and simulation of crystallographic rolling textures of Fe–11Cr steel. *Materials Science and Technology*, 11(10), 985–993.
- Raabe, D. (1995). Inhomogeneity of the crystallographic texture in a hot-rolled austenitic stainless steel. *Journal of Materials Science*, 30(1), 47–52. <https://doi.org/10.1007/BF00352130>
- Raabe, D. (1995). Investigation of contribution of $\{123\}$ slip planes to development of rolling textures in bcc metals by use of Taylor models. *Materials Science and Technology*, 11(5), 455–460. <https://doi.org/10.1179/mst.1995.11.5.455>
- Raabe, D. (1995). Investigation of the iterative series expansion method by means of standard functions. *Materials Letters*, 22(5–6), 313–318. [https://doi.org/10.1016/0167-577X\(94\)00252-5](https://doi.org/10.1016/0167-577X(94)00252-5)
- Raabe, D. (1995). Investigation of the orientation dependence of recovery in low-carbon steel by use of single orientation determination. *Steel Research*, 66(5), 222–229.
- Raabe, D. (1995). Microstructure and crystallographic texture of strip-cast and hot-rolled austenitic stainless steel. *Metallurgical and Materials Transactions A*, 26(4), 991–998. <https://doi.org/10.1007/BF02649096>
- Raabe, D. (1995). Modelling of active slip systems, Taylor factors and grain rotations during rolling and compression deformation of polycrystalline intermetallic L12 compounds. *Acta Metallurgica et Materialia*, 43(4), 1531–1540.
- Raabe, D. (1995). On the orientation dependence of static recovery in low-carbon steels. *Scripta Metallurgica et Materialia*, 33(5).
- Raabe, D. (1995). Simulation of rolling textures of b.c.c. metals considering grain interactions and crystallographic slip on $\{110\}$, $\{112\}$ and $\{123\}$ planes. *Materials Science and Engineering A*, 197(1), 31–37. [https://doi.org/10.1016/0921-5093\(94\)09770-4](https://doi.org/10.1016/0921-5093(94)09770-4)
- Raabe, D. (1995). Simulation of the resistivity of heavily cold worked Cu-20 wt.% Nb wires. *Computational Materials Science*, 3(3), 402–412. [https://doi.org/10.1016/0927-0256\(94\)00079-R](https://doi.org/10.1016/0927-0256(94)00079-R)
- Raabe, D. (1995). Texture simulation for hot rolling of aluminium by use of a Taylor model considering grain interactions. *Acta Metallurgica Et Materialia*, 43(3), 1023–1028. [https://doi.org/10.1016/0956-7151\(94\)00302-X](https://doi.org/10.1016/0956-7151(94)00302-X)
- Raabe, D. (1995). Textures of strip cast and hot rolled ferritic and austenitic stainless steel. *Materials Science and Technology (United Kingdom)*, 11(5), 461–468. <https://doi.org/10.1179/mst.1995.11.5.461>
- Raabe, D. (1996). On the contribution of screw dislocations to internal stress fields associated with dislocation cell structures. *Philosophical Magazine A*, 73(5), 1363–1383. <https://doi.org/10.1080/01418619608245139>

- Raabe, D. (1996). On the influence of the chromium content on the evolution of rolling textures in ferritic stainless steels. *Journal of Materials Science*, 31(14), 3839–3845. <https://doi.org/10.1007/BF00352800>
- Raabe, D. (1996). Simulation of Dislocation Statics by Using 3D Field Equations for Dislocation Segments in Anisotropic Media/Simulation der Versetzungsstatik mit dreidimensionalen Feldgleichungen für Versetzungssegmente in anisotropen Medien. *International Journal of Materials Research*, 87(6), 493–497.
- Raabe, D. (1996). Taylor simulation and experimental investigation of rolling textures of polycrystalline iron aluminides with special regard to slip on {112} planes. *Acta Materialia*, 44(3), 937–951. [https://doi.org/10.1016/1359-6454\(95\)00243-X](https://doi.org/10.1016/1359-6454(95)00243-X)
- Raabe, D. (1997). Texture and microstructure evolution during cold rolling of a strip cast and of a hot rolled austenitic stainless steel. *Acta Materialia*, 45(3), 1137–1151. [https://doi.org/10.1016/S1359-6454\(96\)00222-4](https://doi.org/10.1016/S1359-6454(96)00222-4)
- Raabe, D. (1998). Computational Materials Science. In *Computational Materials Science*. Wiley-VCH Verlag GmbH & Co. KGaA. <https://doi.org/10.1002/3527601945>
- Raabe, D. (1998). On the consideration of climb in discrete dislocation dynamics. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, 77(3), 751–759. <https://doi.org/10.1080/01418619808224081>
- Raabe, D. (1999). Introduction of a scalable three-dimensional cellular automaton with a probabilistic switching rule for the discrete mesoscale simulation of recrystallization phenomena. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, 79(10), 2339–2358. <https://doi.org/10.1080/01418619908214288>
- RAABE, D. (1999). Introduction of a scalable three-dimensional cellular automaton, with a probabilistic switching rule for the discrete mesoscale simulation of recrystallization phenomena. *Philosophical Magazine A*, 79(10), 2339–2358.
- Raabe, D. (2000). Scaling Monte Carlo kinetics of the Potts model using rate theory. *Acta Materialia*, 48(7), 1617–1628. [https://doi.org/10.1016/S1359-6454\(99\)00451-6](https://doi.org/10.1016/S1359-6454(99)00451-6)
- Raabe, D. (2000). Yield surface simulation for partially recrystallized aluminum polycrystals on the basis of spatially discrete data. *Computational Materials Science*, 19(1–4), 13–26. [https://doi.org/10.1016/S0927-0256\(00\)00135-X](https://doi.org/10.1016/S0927-0256(00)00135-X)
- Raabe, D. (2002). Cellular Automata in Materials Science with Particular Reference to Recrystallization Simulation. *Annual Review of Materials Science*, 32(1), 53–76. <https://doi.org/10.1146/annurev.matsci.32.090601.152855>
- Raabe, D. (2002). Challenges in computational materials science. *Advanced Materials*, 14(9), 639–650. [https://doi.org/10.1002/1521-4095\(20020503\)14:9<639::AID-ADMA639>3.0.CO;2-7](https://doi.org/10.1002/1521-4095(20020503)14:9<639::AID-ADMA639>3.0.CO;2-7)
- Raabe, D. (2002). Don't trust your simulation - Computational materials science on its way to maturity? *Advanced Engineering Materials*, 4(5), 255–267. [https://doi.org/10.1002/1527-2648\(20020503\)4:5<255::AID-ADEM255>3.0.CO;2-R](https://doi.org/10.1002/1527-2648(20020503)4:5<255::AID-ADEM255>3.0.CO;2-R)

- Raabe, D. (2004). Mesoscale simulation of spherulite growth during polymer crystallization by use of a cellular automaton. *Acta Materialia*, 52(9), 2653–2664. <https://doi.org/10.1016/j.actamat.2004.02.013>
- Raabe, D. (2004). Overview of the lattice Boltzmann method for nano- And microscale fluid dynamics in materials science and engineering. *Modelling and Simulation in Materials Science and Engineering*, 12(6), R13–R46. <https://doi.org/10.1088/0965-0393/12/6/R01>
- Raabe, D. (2005). Recrystallization Simulation by Use of Cellular Automata. In *Handbook of Materials Modeling* (pp. 2173–2203). https://doi.org/10.1007/978-1-4020-3286-8_113
- Raabe, D. (2006). A texture-component Avrami model for predicting recrystallization textures, kinetics and grain size. *Modelling and Simulation in Materials Science and Engineering*, 15(2), 39. <https://doi.org/10.1088/0965-0393/15/2/004>
- Raabe, D. (2023). The Materials Science behind Sustainable Metals and Alloys. *Chemical Reviews*, 123(5), 2436–2608. <https://doi.org/10.1021/acs.chemrev.2c00799>
- Raabe, D., & Becker, R. C. (2000). Coupling of a crystal plasticity finite-element model with a probabilistic cellular automaton for simulating primary static recrystallization in aluminium. *Modelling and Simulation in Materials Science and Engineering*, 8(4), 445. <https://doi.org/10.1088/0965-0393/8/4/304>
- Raabe, D., & Ge, J. (2004). Experimental study on the thermal stability of Cr filaments in a Cu-Cr-Ag in situ composite. *Scripta Materialia*, 51(9), 915–920. <https://doi.org/10.1016/j.scriptamat.2004.06.016>
- Raabe, D., & Ge, J. (2004). Experimental study on the thermal stability of Cr filaments in a Cu–Cr–Ag in situ composite. *Scripta Materialia*, 51(9), 915–920.
- Raabe, D., & Godara, A. (2005). Mesoscale simulation of the kinetics and topology of spherulite growth during crystallization of isotactic polypropylene (iPP) by using a cellular automaton. *Modelling and Simulation in Materials Science and Engineering*, 13(5), 733. <https://doi.org/10.1088/0965-0393/13/5/007>
- Raabe, D., & Hangen, U. (1995). Introduction of a modified linear rule of mixtures for the modelling of the yield strength of heavily wire drawn in situ composites. *Composites Science and Technology*, 55(1), 57–61. [https://doi.org/10.1016/0266-3538\(95\)00094-1](https://doi.org/10.1016/0266-3538(95)00094-1)
- Raabe, D., & Hangen, U. (1995). Investigation of structurally less-ordered areas in the Nb filaments of a heavily cold-rolled Cu-20 wt. % Nb in situ composite. *Journal of Materials Research*, 10(12), 3050–3061. <https://doi.org/10.1557/JMR.1995.3050>
- Raabe, D., & Hangen, U. (1995). Observation of amorphous areas in a heavily cold rolled Cu-20 wt% Nb composite. *Materials Letters*, 22(3–4), 155–161. [https://doi.org/10.1016/0167-577X\(94\)00248-7](https://doi.org/10.1016/0167-577X(94)00248-7)
- Raabe, D., & Hangen, U. (1996). Correlation of microstructure and type II superconductivity of a heavily cold rolled Cu-20mass% Nb in situ composite. *Acta Materialia*, 44(3), 953–961. [https://doi.org/10.1016/1359-6454\(95\)00239-1](https://doi.org/10.1016/1359-6454(95)00239-1)

- Raabe, D., & Hangen, U. (1996). On the anisotropy of the superconducting properties of a heavily cold rolled Cu-20 mass% Nb in situ composite. *Physica Status Solidi (A) Applied Research*, 154(2), 715–726. <https://doi.org/10.1002/pssa.2211540224>
- Raabe, D., & Hangen, U. (1996). Simulation of the yield strength of wire drawn Cu-based in-situ composites. *Computational Materials Science*, 5(1–3), 195–202. [https://doi.org/10.1016/0927-0256\(95\)00072-0](https://doi.org/10.1016/0927-0256(95)00072-0)
- Raabe, D., & Hantcherli, L. (2005). 2D cellular automaton simulation of the recrystallization texture of an if sheet steel under consideration of Zener pinning. *Computational Materials Science*, 34(4), 299–313. <https://doi.org/10.1016/j.commatsci.2004.12.067>
- Raabe, D., & Heringhaus, F. (1994). Correlation of superconductivity and microstructure in an in-situ formed Cu–20%Nb composite. *Physica Status Solidi (A)*, 142(2), 473–481. <https://doi.org/10.1002/pssa.2211420221>
- Raabe, D., & Hessling, D. (2010). Synthesis of hollow metallic particles via ultrasonic treatment of a metal emulsion. *Scripta Materialia*, 62(9), 690–692. <https://doi.org/10.1016/j.scriptamat.2010.01.028>
- Raabe, D., & Keichel, J. (1995). Development of the microstructure and crystallographic texture during annealing of a rolled polycrystalline Fe₃Al alloy. *Materials Science and Engineering A*, 203(1–2), 208–216. [https://doi.org/10.1016/0921-5093\(95\)09872-0](https://doi.org/10.1016/0921-5093(95)09872-0)
- Raabe, D., & Keichel, J. (1996). On the inhomogeneity of the crystallographic rolling texture of polycrystalline Fe₃Al. *Journal of Materials Research*, 11(7), 1694–1701.
- Raabe, D., & Lucke, K. (1992). INFLUENCE OF PARTICLES ON RECRYSTALLIZATION TEXTURES OF FERRITIC STAINLESS-STEELS. *Steel Research-Dusseldorf*, 63(10), 457–464.
- Raabe, D., & Lücke, K. (1992). Rolling and annealing textures of bcc metals. *Scripta Metallurgica et Materiala*, 27(pt 1), 597–610. <https://doi.org/10.4028/www.scientific.net/msf.157-162.597>
- Raabe, D., & Lücke, K. (1992). Selective particle drag during primary recrystallization of Fe-Cr alloys. *Scripta Metallurgica et Materiala*, 26(1), 19–24. [https://doi.org/10.1016/0956-716X\(92\)90361-H](https://doi.org/10.1016/0956-716X(92)90361-H)
- Raabe, D., & Lücke, K. (1993). Investigation of the ADC Method for Direct ODF Approximation by Means of Standard Functions. *Physica Status Solidi (B)*, 180(1), 59–65. <https://doi.org/10.1002/pssb.2221800103>
- Raabe, D., & Lücke, K. (1993). Textures of ferritic stainless steels. *Materials Science and Technology (United Kingdom)*, 9(4), 302–312. <https://doi.org/10.1179/mst.1993.9.4.302>
- Raabe, D., & Mao, W. (1995). Experimental investigation and simulation of the texture evolution during rolling deformation of an intermetallic Fe-28 at.% Al–2 at.% Cr polycrystal at elevated temperatures. *Philosophical Magazine A*, 71(4), 805–813. <https://doi.org/10.1080/01418619508236221>
- Raabe, D., & Mattissen, D. (1998). Microstructure and mechanical properties of a cast and wire-drawn ternary Cu-Ag-Nb in situ composite. *Acta Materialia*, 46(16), 5973–5984. [https://doi.org/10.1016/S1359-6454\(98\)00218-3](https://doi.org/10.1016/S1359-6454(98)00218-3)

- Raabe, D., & Mattissen, D. (1999). Experimental investigation and ginzburg-landau modeling of the microstructure dependence of superconductivity in Cu-Ag-Nb wires. *Acta Materialia*, 47(3), 769–777. [https://doi.org/10.1016/S1359-6454\(98\)00406-6](https://doi.org/10.1016/S1359-6454(98)00406-6)
- Raabe, D., & Mattissen, D. (1999). Experimental investigation and Ginzburg–Landau modeling of the microstructure dependence of superconductivity in Cu–Ag–Nb wires. *Acta Materialia*, 47(3), 769–777.
- Raabe, D., & Roters, F. (2004). Using texture components in crystal plasticity finite element simulations. *International Journal of Plasticity*, 20(3), 339–361. [https://doi.org/10.1016/S0749-6419\(03\)00092-5](https://doi.org/10.1016/S0749-6419(03)00092-5)
- Raabe, D., & Ylitalo, M. (1996). Experimental investigation of the transformation texture in hotrolled ferritic stainless steel using single orientation determination. *Metallurgical and Materials Transactions A*, 27(1), 49–57. <https://doi.org/10.1007/BF02647746>
- Raabe, D., Al-Sawalmih, A., Yi, S. B., & Fabritius, H. (2007). Preferred crystallographic texture of α -chitin as a microscopic and macroscopic design principle of the exoskeleton of the lobster *Homarus americanus*. *Acta Biomaterialia*, 3(6), 882–895. <https://doi.org/10.1016/j.actbio.2007.04.006>
- Raabe, D., Ball, J., & Gottstein, G. (1992). Rolling Textures of a Cu–20 Nb Composite. *Scripta Metallurgica et Materialia(USA)*, 27(2), 211–216.
- Raabe, D., Chen, N., & Chen, L. (2004). Crystallographic texture, amorphization, and recrystallization in rolled and heat treated polyethylene terephthalate (PET). *Polymer*, 45(24), 8265–8277. <https://doi.org/10.1016/j.polymer.2004.09.045>
- Raabe, D., Choi, P. P., Li, Y., Kostka, A., Sauvage, X., Lecouturier, F., Hono, K., Kirchheim, R., Pippan, R., & Embury, D. (2010). Metallic composites processed via extreme deformation: Toward the limits of strength in bulk materials. *MRS Bulletin*, 35(12), 982–991. <https://doi.org/10.1557/mrs2010.703>
- Raabe, D., Choi, P., Li, Y., Kostka, A., Sauvage, X., Lecouturier, F., Hono, K., Kirchheim, R., Pippan, R., & Embury, D. (2010). *MRS_Bulletin-2010 Raabe Metals at extremes mechanical alloying*. 35(December), 982–991.
- Raabe, D., Degenhardt, R., Seliger, R., Klos, W., Sachtleber, M., & Ernenputsch, L. (2008). Advances in the Optimization of Thin Strip Cast Austenitic 304 Stainless Steel. *Steel Research International*, 79(6), 440–444. <https://doi.org/10.1002/srin.200806150>
- Raabe, D., Helming, K., Roters, F., Zhao, Z., & Hirsch, J. (2002). A texture component crystal plasticity finite element method for scalable large strain anisotropy simulations. *Materials Science Forum*, 408–412(I), 257–262. <https://doi.org/10.4028/www.scientific.net/msf.396-402.31>
- Raabe, D., Herbig, M., Sandlöbes, S., Li, Y., Tytko, D., Kuzmina, M., Ponge, D., & Choi, P. P. (2014). Grain boundary segregation engineering in metallic alloys: A pathway to the design of interfaces. *Current Opinion in Solid State and Materials Science*, 18(4), 253–261. <https://doi.org/10.1016/j.cossms.2014.06.002>

- Raabe, D., Heringhaus, F., Hangen, U., & Gottstein, G. (1995). Investigation of a Cu-20 mass% Nb in situ Composite, Part II: Electromagnetic Properties and Application. *Zeitschrift Fuer Metallkunde/Materials Research and Advanced Techniques Für Metallkunde*, 86, 416.
- Raabe, D., Heringhaus, F., Hangen, U., & Gottstein, G. (1995). Investigation of a Cu-20 mass% Nb in situ composite, part I: fabrication, microstructure and mechanical properties. *Zeitschrift Für Metallkunde*, 86(6), 405–415.
- Raabe, D., Keichel, J., & Gottstein, G. (1997). Investigation of crystallographic slip in polycrystalline Fe3Al using slip trace measurement and microtexture determination. *Acta Materialia*, 45(7), 2839–2849. [https://doi.org/10.1016/S1359-6454\(96\)00373-4](https://doi.org/10.1016/S1359-6454(96)00373-4)
- Raabe, D., Keichel, J., & Sun, Z. (1996). Microstructure and crystallographic texture of rolled polycrystalline Fe3Al. *Journal of Materials Science*, 31(2), 339–344. <https://doi.org/10.1007/BF01139149>
- Raabe, D., Klose, P., Engl, B., Imlau, K. P., Friedel, F., & Roters, F. (2002). Concepts for integrating plastic anisotropy into metal forming simulations. *Advanced Engineering Materials*, 4(4), 169–180. [https://doi.org/10.1002/1527-2648\(200204\)4:4<169::AID-ADEM169>3.0.CO;2-G](https://doi.org/10.1002/1527-2648(200204)4:4<169::AID-ADEM169>3.0.CO;2-G)
- Raabe, D., Li, Z., & Ponge, D. (2019). Metastability alloy design. *MRS Bulletin*, 44(4), 266–272. <https://doi.org/10.1557/mrs.2019.72>
- Raabe, D., Lücke, K., Raahe, D., Licke, K., Raabe, D., & Lucke, K. (1994). Rolling textures of niobium and molybdenum. *Zeitschrift Für Metallkunde/Materials Research and Advanced Techniques. Metallkd*, 85(5), 302–307. <http://cat.inist.fr/?aModele=afficheN&cpsidt=4188559>
- Raabe, D., Ma, D., & Roters, F. (2007). Effects of initial orientation, sample geometry and friction on anisotropy and crystallographic orientation changes in single crystal microcompression deformation: A crystal plasticity finite element study. *Acta Materialia*, 55(13), 4567–4583. <https://doi.org/10.1016/j.actamat.2007.04.023>
- Raabe, D., Mianroodi, J. R., & Neugebauer, J. (2023). Accelerating the design of compositionally complex materials via physics-informed artificial intelligence. *Nature Computational Science*, 3(March), 198–209. <https://doi.org/10.1038/s43588-023-00412-7>
- Raabe, D., Miyake, K., & Takahara, H. (2000). Processing, microstructure, and properties of ternary high-strength Cu-Cr-Ag in situ composites. *Materials Science and Engineering A*, 291(1), 186–197. [https://doi.org/10.1016/S0921-5093\(00\)00981-3](https://doi.org/10.1016/S0921-5093(00)00981-3)
- Raabe, D., Ohsaki, S., & Hono, K. (2009). Mechanical alloying and amorphization in Cu-Nb-Ag in situ composite wires studied by transmission electron microscopy and atom probe tomography. *Acta Materialia*, 57(17), 5254–5263. <https://doi.org/10.1016/j.actamat.2009.07.028>
- Raabe, D., Ponge, D., Dmitrieva, O., & Sander, B. (2009). Designing ultrahigh strength steels with good ductility by combining transformation induced plasticity and martensite aging. *Advanced Engineering Materials*, 11(7), 547–555. <https://doi.org/10.1002/adem.200900061>
- Raabe, D., Ponge, D., Dmitrieva, O., & Sander, B. (2009). Nanoprecipitate-hardened 1.5 GPa steels with unexpected high ductility. *Scripta Materialia*, 60(12), 1141–1144. <https://doi.org/10.1016/j.scriptamat.2009.02.062>

- Raabe, D., Ponge, D., Kirchheim, R., Assadi, H., Li, Y., Goto, S., Kostka, A., Herbig, M., Sandl, S., Kuzmina, M., Millán, J., Yuan, L., Choi, P. P., Sandlöbes, S., & Kuzmina, M. (2013). Interface segregation in advanced steels studied at the atomic scale. *Microstructural Design of Advanced Engineering Materials*, 267–298. <https://doi.org/10.1002/9783527652815.ch11>
- Raabe, D., Ponge, D., Uggowitzer, P. J., Roscher, M., Paolantonio, M., Liu, C., Antrekowitsch, H., Kozeschnik, E., Seidmann, D., Gault, B., De Geuser, F., Deschamps, A., Hutchinson, C., Liu, C., Li, Z., Prangnell, P., Robson, J., Shanthraj, P., Vakili, S., ... Pogatscher, S. (2022). Making sustainable aluminum by recycling scrap: The science of “dirty” alloys. *Progress in Materials Science*, 128, 100947. <https://doi.org/10.1016/j.pmatsci.2022.100947>
- Raabe, D., Ponge, D., Wang, M. M., Herbig, M., Belde, M., & Springer, H. (2017). 1 billion tons of nanostructure - Segregation engineering enables confined transformation effects at lattice defects in steels. *IOP Conference Series: Materials Science and Engineering*, 219(1). <https://doi.org/10.1088/1757-899X/219/1/012006>
- Raabe, D., Reher, F., Hölscher, M., & Lücke, K. (1993). Textures of strip cast Fe16%Cr. *Scripta Metallurgica et Materiala*, 29(1), 113–116. [https://doi.org/10.1016/0956-716X\(93\)90264-S](https://doi.org/10.1016/0956-716X(93)90264-S)
- Raabe, D., Rezaei Mianroodi, J., & Neugebauer, J. (2023). Computational design of compositionally complex materials. *Nature Computational Science*, 3, 198–209. <https://www.nature.com/articles/s43588-023-00412-7>
- Raabe, D., Romano, P., Sachs, C., Al-Sawalmih, A., Brokmeier, H. G., Yi, S. B., Servos, G., & Hartwig, H. G. (2005). Discovery of a honeycomb structure in the twisted plywood patterns of fibrous biological nanocomposite tissue. *Journal of Crystal Growth*, 283(1–2), 1–7. <https://doi.org/10.1016/j.jcrysgro.2005.05.077>
- Raabe, D., Romano, P., Sachs, C., Fabritius, H., Al-Sawalmih, A., Yi, S. B., Servos, G., & Hartwig, H. G. (2006). Microstructure and crystallographic texture of the chitin-protein network in the biological composite material of the exoskeleton of the lobster *Homarus americanus*. *Materials Science and Engineering A*, 421(1–2), 143–153. <https://doi.org/10.1016/j.msea.2005.09.115>
- Raabe, D., Roters, F., & Gottstein, G. (1996). Simulation of the statics of 2D and 3D dislocation networks. *Computational Materials Science*, 5(1–3), 203–209.
- Raabe, D., Roters, F., Barlat, F., & Chen, L.-Q. (2004). Continuum Scale Simulation of Engineering Materials. In *Continuum Scale Simulation of Engineering Materials*. John Wiley & Sons. <https://doi.org/10.1002/3527603786>
- Raabe, D., Roters, F., Neugebauer, J., Gutierrez-Urrutia, I., Hickel, T., Bleck, W., Schneider, J. M., Wittig, J. E., & Mayer, J. (2016). Ab initio-guided design of twinning-induced plasticity steels. *MRS Bulletin*, 41(4), 320–325. <https://doi.org/10.1557/mrs.2016.63>
- Raabe, D., Sachs, C., & Romano, P. (2005). The crustacean exoskeleton as an example of a structurally and mechanically graded biological nanocomposite material. *Acta Materialia*, 53(15), 4281–4292. <https://doi.org/10.1016/j.actamat.2005.05.027>
- Raabe, D., Sachtleber, M., Vega, L. F., & Weiland, H. (2002). Surface micromechanics of polymer coated aluminium sheets during plastic deformation. *Advanced Engineering Materials*, 4(11), 859–864. <https://doi.org/10.1002/1527-2648>

- Raabe, D., Sachtleber, M., Weiland, H., Scheele, G., & Zhao, Z. (2003). Grain-scale micromechanics of polycrystal surfaces during plastic straining. *Acta Materialia*, *51*(6), 1539–1560. [https://doi.org/10.1016/S1359-6454\(02\)00557-8](https://doi.org/10.1016/S1359-6454(02)00557-8)
- Raabe, D., Sachtleber, M., Zhao, Z., Roters, F., & Zaeferrer, S. (2001). Micromechanical and macromechanical effects in grain scale polycrystal plasticity experimentation and simulation. *Acta Materialia*, *49*(17), 3433–3441. [https://doi.org/10.1016/S1359-6454\(01\)00242-7](https://doi.org/10.1016/S1359-6454(01)00242-7)
- Raabe, D., Sander, B., Friák, M., Ma, D., & Neugebauer, J. (2007). Theory-guided bottom-up design of β -titanium alloys as biomaterials based on first principles calculations: Theory and experiments. *Acta Materialia*, *55*(13), 4475–4487. <https://doi.org/10.1016/j.actamat.2007.04.024>
- Raabe, D., Sandlöbes, S., Millán, J., Ponge, D., Assadi, H., Herbig, M., & Choi, P. P. (2013). Segregation engineering enables nanoscale martensite to austenite phase transformation at grain boundaries: A pathway to ductile martensite. *Acta Materialia*, *61*(16), 6132–6152. <https://doi.org/10.1016/j.actamat.2013.06.055>
- Raabe, D., Schlenkert, G., Weisshaupt, H., & Lücke, K. (1994). Texture and microstructure of rolled and annealed tantalum. *Materials Science and Technology (United Kingdom)*, *10*(4), 299–305. <https://doi.org/10.1179/mst.1994.10.4.299>
- Raabe, D., Springer, H., Gutierrez-Urrutia, I., Roters, F., Bausch, M., Seol, J. B., Koyama, M., Choi, P. P., & Tsuzaki, K. (2014). Alloy Design, Combinatorial Synthesis, and Microstructure–Property Relations for Low-Density Fe-Mn-Al-C Austenitic Steels. *JOM*, *66*(9), 1845–1856. <https://doi.org/10.1007/s11837-014-1032-x>
- Raabe, D., Sun, B., Kwiatkowski Da Silva, A., Gault, B., Yen, H. W., Sedighiani, K., Thoudden Sukumar, P., Souza Filho, I. R., Katnagallu, S., Jägle, E., Kürsteiner, P., Kusampudi, N., Stephenson, L., Herbig, M., Liebscher, C. H., Springer, H., Zaeferrer, S., Shah, V., Wong, S. L., ... Ponge, D. (2020). Current Challenges and Opportunities in Microstructure-Related Properties of Advanced High-Strength Steels. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, *51*(11), 5517–5586. <https://doi.org/10.1007/s11661-020-05947-2>
- Raabe, D., Tasan, C. C., & Olivetti, E. A. (2019). Strategies for improving the sustainability of structural metals. *Nature*, *575*(7781), 64–74. <https://doi.org/10.1038/s41586-019-1702-5>
- Raabe, D., Tasan, C. C., Springer, H., & Bausch, M. (2015). From high-entropy alloys to high-entropy steels. *Steel Research International*, *86*(10), 1127–1138. <https://doi.org/10.1002/srin.201500133>
- Raabe, D., Wang, Y., & Roters, F. (2005). Crystal plasticity simulation study on the influence of texture on earing in steel. *Computational Materials Science*, *34*(3), 221–234. <https://doi.org/10.1016/j.commatsci.2004.12.072>
- Raabe, D., Zhao, Z., & Mao, W. (2002). On the dependence of in-grain subdivision and deformation texture of aluminum on grain interaction. *Acta Materialia*, *50*(17), 4379–4394. [https://doi.org/10.1016/S1359-6454\(02\)00276-8](https://doi.org/10.1016/S1359-6454(02)00276-8)
- Raabe, D., Zhao, Z., & Roters, F. (2004). Study on the orientational stability of cube-oriented FCC crystals under plane strain by use of a texture component crystal plasticity finite element method. *Scripta Materialia*, *50*(7), 1085–1090. <https://doi.org/10.1016/j.scriptamat.2003.11.061>

- Raabe, D., Zhao, Z., Park, S. J., & Roters, F. (2002). Theory of orientation gradients in plastically strained crystals. *Acta Materialia*, *50*(2), 421–440. [https://doi.org/10.1016/S1359-6454\(01\)00323-8](https://doi.org/10.1016/S1359-6454(01)00323-8)
- Ram, F., Li, Z., Zaefferer, S., Hafez Haghighat, S. M., Zhu, Z., Raabe, D., Reed, R. C., Haghighat, S. M. H., Zhu, Z., Raabe, D., & Reed, R. C. (2016). On the origin of creep dislocations in a Ni-base, single-crystal superalloy: an ECCI, EBSD, and dislocation dynamics-based study. *Acta Materialia*, *109*, 151–161. <https://doi.org/10.1016/j.actamat.2016.02.038>
- Ram, F., Zaefferer, S., & Raabe, D. (2014). Kikuchi bandlet method for the accurate deconvolution and localization of Kikuchi bands in Kikuchi diffraction patterns. *Journal of Applied Crystallography*, *47*(1), 264–275.
- Ram, F., Zaefferer, S., Jäpel, T., & Raabe, D. (2015). Error analysis of the crystal orientations and disorientations obtained by the classical electron backscatter diffraction technique. *Journal of Applied Crystallography*, *48*(3), 797–813.
- Rao, Z., Çakır, A., Özgün, Ö., Ponge, D., Raabe, D., Li, Z., & Acet, M. (2021). 3 d transition-metal high-entropy Invar alloy developed by adjusting the valence-electron concentration. *Physical Review Materials*, *5*(4), 44406.
- Rao, Z., Dutta, B., Körmann, F., Lu, W., Zhou, X., Liu, C., da Silva, A. K., Wiedwald, U., Spasova, M., & Farle, M. (2021). Beyond Solid Solution High-Entropy Alloys: Tailoring Magnetic Properties via Spinodal Decomposition. *Advanced Functional Materials*, *31*(7), 2007668.
- Rao, Z., Dutta, B., Körmann, F., Ponge, D., Li, L., He, J., Stephenson, L., Schäfer, L., Skokov, K., & Gutfleisch, O. (2020). Unveiling the mechanism of abnormal magnetic behavior of FeNiCoMnCu high-entropy alloys through a joint experimental-theoretical study. *Physical Review Materials*, *4*(1), 14402.
- Rao, Z., Ponge, D., Körmann, F., Ikeda, Y., Schneeweiss, O., Friák, M., Neugebauer, J., Raabe, D., & Li, Z. (2019). Invar effects in FeNiCo medium entropy alloys: From an Invar treasure map to alloy design. *Intermetallics*, *111*(May), 106520. <https://doi.org/10.1016/j.intermet.2019.106520>
- Rao, Z., Tung, P., Xie, R., Wei, Y., Zhang, H., Ferrari, A., Klaver, T. P. C., Körmann, F., Sukumar, P. T., da Silva, A. K., Chen, Y., Li, Z., Ponge, D., Neugebauer, J., Gutfleisch, O., Bauer, S., & Raabe, D. (2022). Machine learning-enabled high-entropy alloy discovery. *Science*, *85*(October), 78–85. <https://doi.org/10.1126/science.abo4940>
- Rapp, B. (2006). Materials for extreme environments. Defense, aviation, and space agencies are beginning to look at the advanced composite materials necessary for hypersonic speeds. In *Materials Today* (Vol. 9, Issue 5, p. 6). [https://doi.org/10.1016/S1369-7021\(06\)71471-7](https://doi.org/10.1016/S1369-7021(06)71471-7)
- Ratanaphan, S., Raabe, D., Sarochawikasit, R., Olmsted, D. L., Rohrer, G. S., & Tu, K.-N. (2017). Grain boundary character distribution in electroplated nanotwinned copper. *Journal of Materials Science*, *52*(7), 4070–4085.
- Raters, F., & Raabe, D. (1996). Numerical simulation of stress fields of dislocation networks with special regard to interface dislocations. *Materials Science and Technology*, *12*(4), 281–289.

- Raue, L., Klein, H., & Raabe, D. (2010). The exoskeleton of the American lobster- From texture to anisotropic properties. *Solid State Phenomena*, *160*(5), 287–294. <https://doi.org/10.4028/www.scientific.net/SSP.160.287>
- Ravi Kumar, B., Raabe, D., Kumar, B. R., & Raabe, D. (2012). Tensile deformation characteristics of bulk ultrafine-grained austenitic stainless steel produced by thermal cycling. *Scripta Materialia*, *66*(9), 634–637. <https://doi.org/10.1016/j.scriptamat.2012.01.052>
- Reeh, S., Music, D., Gebhardt, T., Kasprzak, M., Jäpel, T., Zaefferer, S., Raabe, D., Richter, S., Schwedt, A., Mayer, J., Wietbrock, B., Hirt, G., & Schneider, J. M. (2012). Elastic properties of face-centred cubic Fe–Mn–C studied by nanoindentation and ab initio calculations. *Acta Materialia*, *60*(17), 6025–6032. <https://doi.org/10.1016/j.actamat.2012.07.038>
- Renner, F. U., Ankah, G. N., Bashir, A., Ma, D., Biedermann, P. U., Shrestha, B. R., Nellesen, M., Khorashadizadeh, A., Losada-Pérez, P., Duarte, M. J., Losada-Pérez, P., Duarte, M. J., Raabe, D., & Valtiner, M. (2015). Star-Shaped Crystallographic Cracking of Localized Nanoporous Defects. *Advanced Materials*, *27*(33), 4877–4882. <https://doi.org/10.1002/adma.201405565>
- Renzetti, R. A., Sandim, H. R. Z., Padilha, A. F., Raabe, D., Lindau, R., & Möslang, A. (2011). Annealing Effects on the Microstructure of Ferritic-Martensitic ODS-Eurofer Steel. *Fusion Science and Technology*, *60*(1T), 22–26.
- Renzetti, R. A., Sandim, H. R. Z., Sandim, M. J. R., Santos, A. D., Möslang, A., & Raabe, D. (2011). Annealing effects on microstructure and coercive field of ferritic-martensitic ODS Eurofer steel. *Materials Science and Engineering A*, *528*(3), 1442–1447. <https://doi.org/10.1016/j.msea.2010.10.051>
- Reuber, C., Eisenlohr, P., Roters, F., & Raabe, D. (2014). Dislocation density distribution around an indent in single-crystalline nickel: Comparing nonlocal crystal plasticity finite-element predictions with experiments. *Acta Materialia*, *71*, 333–348. <https://doi.org/10.1016/j.actamat.2014.03.012>
- Ristig, S., Prymak, O., Loza, K., Gocyla, M., Meyer-Zaika, W., Heggen, M., Raabe, D., & Epple, M. (2015). Nanostructure of wet-chemically prepared, polymer-stabilized silver–gold nanoalloys (6 nm) over the entire composition range. *Journal of Materials Chemistry B*, *3*(23), 4654–4662.
- Rollett, A. D., & Raabe, D. (2001). A hybrid model for mesoscopic simulation of recrystallization. *Computational Materials Science*, *21*(1), 69–78. [https://doi.org/10.1016/S0927-0256\(00\)00216-0](https://doi.org/10.1016/S0927-0256(00)00216-0)
- Romano, P., Fabritius, H., & Raabe, D. (2007). The exoskeleton of the lobster *Homarus americanus* as an example of a smart anisotropic biological material. *Acta Biomaterialia*, *3*(3 SPEC. ISS.), 301–309. <https://doi.org/10.1016/j.actbio.2006.10.003>
- Roters, F., Diehl, M., Shanthraj, P., Eisenlohr, P., Reuber, C., Wong, S. L., Maiti, T., Ebrahimi, A., Hochrainer, T., Fabritius, H. O., Nikolov, S., Friák, M., Fujita, N., Grilli, N., Janssens, K. G. F., Jia, N., Kok, P. J. J., Ma, D., Meier, F., ... Raabe, D. (2019). DAMASK – The Düsseldorf Advanced Material Simulation Kit for modeling multi-physics crystal plasticity, thermal, and damage phenomena from the single crystal up to the component scale. *Computational Materials Science*, *158*(January), 420–478. <https://doi.org/10.1016/j.commatsci.2018.04.030>

- Roters, F., Eisenlohr, P., Bieler, T. R., & Raabe, D. (2011). Crystal plasticity finite element methods: in materials science and engineering. In *Crystal Plasticity Finite Element Methods: In Materials Science and Engineering*. John Wiley & Sons. <https://doi.org/10.1002/9783527631483>
- Roters, F., Eisenlohr, P., Hantcherli, L., Tjahjanto, D. D., Bieler, T. R., & Raabe, D. (2010). Overview of constitutive laws, kinematics, homogenization and multiscale methods in crystal plasticity finite-element modeling: Theory, experiments, applications. *Acta Materialia*, *58*(4), 1152–1211. <https://doi.org/10.1016/j.actamat.2009.10.058>
- Roters, F., Eisenlohr, P., Kords, C., Tjahjanto, D. D., Diehl, M., & Raabe, D. (2012). DAMASK: The Düsseldorf advanced material simulation kit for studying crystal plasticity using an fe based or a spectral numerical solver. *Procedia IUTAM*, *3*, 3–10. <https://doi.org/10.1016/j.piutam.2012.03.001>
- Roters, F., Raabe, D., & Gottstein, G. (1996). Calculation of stress—strain curves by using 2 dimensional dislocation dynamics. *Computational Materials Science*, *7*(1–2), 56–62.
- Roters, F., Raabe, D., & Gottstein, G. (2000). Work hardening in heterogeneous alloys - a microstructural approach based on three internal state variables. *Acta Materialia*, *48*(17), 4181–4189. [https://doi.org/10.1016/S1359-6454\(00\)00289-5](https://doi.org/10.1016/S1359-6454(00)00289-5)
- Roters, F., Wang, Y., Kuo, J. J. C., & Raabe, D. (2004). Comparison of single crystal simple shear deformation experiments with crystal plasticity finite element simulations. *Advanced Engineering Materials*, *6*(8), 653–656. <https://doi.org/10.1002/adem.200400079>
- Rusitzka, K. A. K., Stephenson, L. T., Szczepaniak, A., Gremer, L., Raabe, D., Willbold, D., & Gault, B. (2018). A near atomic-scale view at the composition of amyloid-beta fibrils by atom probe tomography. *Scientific Reports*, *8*(1). <https://doi.org/10.1038/s41598-018-36110-y>
- Sachs, C., Fabritius, H., & Raabe, D. (2006). Experimental investigation of the elastic-plastic deformation of mineralized lobster cuticle by digital image correlation. *Journal of Structural Biology*, *155*(3), 409–425. <https://doi.org/10.1016/j.jsb.2006.06.004>
- Sachs, C., Fabritius, H., & Raabe, D. (2006). Hardness and elastic properties of dehydrated cuticle from the lobster *Homarus americanus* obtained by nanoindentation. *Journal of Materials Research*, *21*(8), 1987–1995. <https://doi.org/10.1557/jmr.2006.0241>
- Sachs, C., Fabritius, H., & Raabe, D. (2008). Influence of microstructure on deformation anisotropy of mineralized cuticle from the lobster *Homarus americanus*. *Journal of Structural Biology*, *161*(2), 120–132. <https://doi.org/10.1016/j.jsb.2007.09.022>
- Sachtleber, M., Raabe, D., & Weiland, H. (2004). Surface roughening and color changes of coated aluminum sheets during plastic straining. *Journal of Materials Processing Technology*, *148*(1), 68–76. <https://doi.org/10.1016/j.jmatprotec.2004.01.041>
- Sachtleber, M., Zhao, Z., & Raabe, D. (2002). Experimental investigation of plastic grain interaction. *Materials Science and Engineering A*, *336*(1–2), 81–87. [https://doi.org/10.1016/S0921-5093\(01\)01974-8](https://doi.org/10.1016/S0921-5093(01)01974-8)

- Sander, B., & Raabe, D. (2008). Texture inhomogeneity in a Ti-Nb-based β -titanium alloy after warm rolling and recrystallization. *Materials Science and Engineering A*, 479(1–2), 236–247. <https://doi.org/10.1016/j.msea.2007.06.077>
- Sandim, H. R. Z. R. Z., Bolmaro, R. E., Renzetti, R. A., Sandim, M. J. R. J. R., Hartwig, K. T., Vogel, S. C., & Raabe, D. (2014). Texture Evolution as Determined by In situ Neutron Diffraction During Annealing of Iron Deformed by Equal Channel Angular Pressing. *Metallurgical and Materials Transactions A*, 45(10), 4235–4246. <https://doi.org/10.1007/s11661-014-2401-3>
- Sandim, H. R. Z. Z., & Raabe, D. (2005). EBSD study of grain subdivision of a Goss grain in coarse-grained cold-rolled niobium. *Scripta Materialia*, 53(2), 207–212. <https://doi.org/10.1016/j.scriptamat.2005.03.045>
- Sandim, H. R. Z. Z., Hayama, A. O. F. F., & Raabe, D. (2006). Recrystallization of the ODS superalloy PM-1000. *Materials Science and Engineering: A*, 430(1–2), 172–178. <https://doi.org/10.1016/j.msea.2006.05.110>
- Sandim, H. R. Z. Z., Renzetti, R. A., Padilha, A. F., Möslang, A., Lindau, R., & Raabe, D. (2012). Annealing behavior of RAFM ODS-Eurofer steel. *Fusion Science and Technology*, 61(2), 136–140. <https://doi.org/10.13182/FST12-A13379>
- Sandim, H. R. Z., Bernardi, H. H., Verlinden, B., & Raabe, D. (2007). Equal channel angular extrusion of niobium single crystals. *Materials Science and Engineering: A*, 467(1–2), 44–52.
- Sandim, H. R. Z., Renzetti, R. A., Padilha, A. F., Raabe, D., Klimenkov, M., Lindau, R., & Möslang, A. (2010). Annealing behavior of ferritic-martensitic 9%Cr-ODS-Eurofer steel. *Materials Science and Engineering A*, 527(15), 3602–3608. <https://doi.org/10.1016/j.msea.2010.02.051>
- Sandim, H. R. Z., Renzetti, R. A., Padilha, A. F., Raabe, D., Klimenkov, M., Lindau, R., & Möslang, A. (2010). Annealing behavior of ferritic–martensitic 9% Cr–ODS–Eurofer steel. *Materials Science and Engineering: A*, 527(15), 3602–3608.
- Sandim, H. R. Z., Sandim, M. J. R., Bernardi, H. H., Lins, J. F. C., & Raabe, D. (2004). Annealing effects on the microstructure and texture of a multifilamentary Cu-Nb composite wire. *Scripta Materialia*, 51(11), 1099–1104. <https://doi.org/10.1016/j.scriptamat.2004.07.026>
- Sandim, H. R. Z., Sandim, M. J. R., Bernardi, H. H., Lins, J. F. C., & Raabe, D. (2004). Annealing effects on the microstructure and texture of a multifilamentary Cu–Nb composite wire. *Scripta Materialia*, 51(11), 1099–1104.
- Sandim, M. J. R. R., Stamopoulos, D., Aristomenopoulou, E., Zaefferer, S., Raabe, D., Awaji, S., & Watanabe, K. (2012). Grain structure and irreversibility line of a bronze route CuNb reinforced Nb3Sn multifilamentary wire. *Physics Procedia*, 36, 1504–1509. <https://doi.org/10.1016/j.phpro.2012.06.122>
- Sandim, M. J. R. R., Stamopoulos, D., Sandim, H. R. Z. Z., Ghivelder, L., Thilly, L., Vidal, V., Lecouturier, F., & Raabe, D. (2006). Size effects on the magnetic properties of Cu–Nb nanofilamentary wires processed by severe plastic deformation. *Superconductor Science and Technology*, 19(12), 1233. <https://doi.org/10.1088/0953-2048/19/12/002>

- Sandim, M. J. R., Sandim, H. R. Z., Zaefferer, S., Raabe, D., Awaji, S., & Watanabe, K. (2010). Electron backscatter diffraction study of Nb₃Sn superconducting multifilamentary wire. *Scripta Materialia*, *62*(2), 59–62.
- Sandim, M. J. R., Souza Filho, I. R., Bredda, E. H., Kostka, A., Raabe, D., & Sandim, H. R. Z. (2017). Coarsening of Y-rich oxide particles in 9% Cr-ODS Eurofer steel annealed at 1350 C. *J. Nucl. Mater.*, *484*, 283–287.
- Sandim, M. J. R., Tytko, D., Kostka, A., Choi, P., Awaji, S., Watanabe, K., & Raabe, D. (2013). Grain boundary segregation in a bronze-route Nb₃Sn superconducting wire studied by atom probe tomography. *Superconductor Science and Technology*, *26*(5), 2–8. <https://doi.org/10.1088/0953-2048/26/5/055008>
- Sandlöbes, S., Friák, M., Korte-Kerzel, S., Pei, Z., Neugebauer, J., & Raabe, D. (2017). A rare-earth free magnesium alloy with improved intrinsic ductility. *Scientific Reports*, *7*(1), 1–8. <https://doi.org/10.1038/s41598-017-10384-0>
- Sandlöbes, S., Friák, M., Neugebauer, J., & Raabe, D. (2013). Basal and non-basal dislocation slip in Mg–Y. *Materials Science and Engineering: A*, *576*, 61–68. <https://doi.org/10.1016/j.msea.2013.03.006>
- Sandlöbes, S., Friák, M., Zaefferer, S., Dick, A., Yi, S., Letzig, D., Pei, Z., Zhu, L. F., Neugebauer, J., & Raabe, D. (2012). The relation between ductility and stacking fault energies in Mg and Mg–Y alloys. *Acta Materialia*, *60*(6–7), 3011–3021. <https://doi.org/10.1016/j.actamat.2012.02.006>
- Sandlöbes, S., Korte-Kerzel, S., & Raabe, D. (2019). On the influence of the heat treatment on microstructure formation and mechanical properties of near- α Ti–Fe alloys. *Materials Science and Engineering A*, *748*(September 2018), 301–312. <https://doi.org/10.1016/j.msea.2018.12.071>
- Sasidhar, K. N., Siboni, N. H., Mianroodi, J. R., Rohwerder, M., Neugebauer, J., & Raabe, D. (2023). Enhancing corrosion-resistant alloy design through natural language processing and deep learning. *Science Advances*, *9*, 7992. <https://doi.org/10.1126/sciadv.adg7992>
- Sasidhar, K. N., Siboni, N. H., Mianroodi, J. R., Rohwerder, M., Neugebauer, J., & Raabe, D. (2022). Deep learning framework for uncovering compositional and environmental contributions to pitting resistance in passivating alloys. *Npj Materials Degradation*, *6*(1). <https://doi.org/10.1038/s41529-022-00281-x>
- Scharifi, E., Tasan, C. C., Hoefnagels, J. P. M., & Raabe, D. (2012). Microstructural analysis of strain rate sensitivity of dual-phase steel. *Materials Science Engineering (MSE) 2012*.
- Schemmann, L., Zaefferer, S., Raabe, D., Friedel, F., & Mattissen, D. (2015). Alloying effects on microstructure formation of dual phase steels. *Acta Materialia*, *95*, 386–398. <https://doi.org/10.1016/j.actamat.2015.05.005>
- Scherrer, B., Li, T., Tsyganok, A., Döbeli, M., Gupta, B., Malviya, K. D., Kasian, O., Maman, N., Gault, B., Grave, D. A., Mehlman, A., Visoly-Fisher, I., Raabe, D., Rothschild, A., Döbeli, M., Gupta, B., Malviya, K. D., Kasian, O., Maman, N., ... Grave, D. A. (2019). Defect segregation and its effect on the photoelectrochemical properties of Ti-doped hematite photoanodes for solar water

- splitting. *Chemistry of Materials*, 32(3), 1031–1040.
<https://doi.org/10.1021/acs.chemmater.9b03704>
- Schnabel, V., Jaya, B. N., Köhler, M., Music, D., Kirchlechner, C., Dehm, G., Raabe, D., & Schneider, J. M. (2016). Electronic hybridisation implications for the damage-tolerance of thin film metallic glasses. *Scientific Reports*, 6(1), 1–12. <https://doi.org/10.1038/srep36556>
- Schnabel, V., Köhler, M., Evertz, S., Gamcova, J., Bednarcik, J., Music, D., Raabe, D., & Schneider, J. M. (2016). Revealing the relationships between chemistry, topology and stiffness of ultrastrong Co-based metallic glass thin films: A combinatorial approach. *Acta Materialia*, 107, 213–219. <https://doi.org/10.1016/j.actamat.2016.01.060>
- Schnabel, V., Köhler, M., Music, D., Bednarcik, J., Clegg, W. J., Raabe, D., & Schneider, J. M. (2017). Ultra-stiff metallic glasses through bond energy density design. *Journal of Physics: Condensed Matter*, 29(26), 265502. <https://doi.org/10.1088/1361-648X/aa72cb>
- Schönhöbel, A. M., Madugundo, R., Barandiarán, J. M., Hadjipanayis, G. C., Palanisamy, D., Schwarz, T., Gault, B., Raabe, D., Skokov, K., Gutfleisch, O., Fischbacher, J., & Schrefl, T. (2020). Nanocrystalline Sm-based 1: 12 magnets. *Acta Materialia*, 200, 652–658. <https://doi.org/10.1016/j.actamat.2020.08.075>
- Schwan, M., Naikade, M., Raabe, D., & Ratke, L. (2015). From hard to rubber-like: mechanical properties of resorcinol–formaldehyde aerogels. *Journal of Materials Science*, 50(16), 5482–5493. <https://doi.org/10.1007/s10853-015-9094-x>
- Schwarz, T., Cojocar-Mirédin, O., Choi, P., Mousel, M., Redinger, A., Siebentritt, S., & Raabe, D. (2013). Atom probe study of Cu₂ZnSnSe₄ thin-films prepared by co-evaporation and post-deposition annealing. *Applied Physics Letters*, 102(4). <https://doi.org/10.1063/1.4788815>
- Schwarz, T., Cojocar-Mirédin, O., Choi, P., Mousel, M., Redinger, A., Siebentritt, S., & Raabe, D. (2015). Atom probe tomography study of internal interfaces in Cu₂ZnSnSe₄ thin-films. *Journal of Applied Physics*, 118(9), 95302.
- Schwarz, T., Cojocar-Mirédin, O., Mousel, M., Redinger, A., Raabe, D., & Choi, P. P. (2017). Formation of nanometer-sized Cu-Sn-Se particles in Cu₂ZnSnSe₄ thin-films and their effect on solar cell efficiency. *Acta Materialia*, 132, 276–284. <https://doi.org/10.1016/j.actamat.2017.04.056>
- Schwarz, T., Cojocar-Mirédin, O., Raabe, D., Choi, P.-P., Marques, M. A. L., Botti, S., Mousel, M., Redinger, A., & Siebentritt, S. (2015). Detection of Cu₂Zn₅SnSe₈ and Cu₂Zn₆SnSe₉ phases in co-evaporated Cu₂ZnSnSe₄ thin-films. *Applied Physics Letters*, 107(17).
- Schwarz, T., Marques, M. A. L. L., Botti, S., Mousel, M., Redinger, A., Siebentritt, S., Cojocar-Mirédin, O., Raabe, D., & Choi, P.-P. P. (2015). Detection of Cu₂Zn₅SnSe₈ and Cu₂Zn₆SnSe₉ phases in co-evaporated Cu₂ZnSnSe₄ thin-films. *Applied Physics Letters*, 107(17), 172102. <https://doi.org/10.1063/1.4934847>
- Schwarz, T., Redinger, A., Siebentritt, S., Peng, Z., Gault, B., Raabe, D., & Choi, P.-P. (2019). Variable chemical decoration of extended defects in Cu-poor Cu₂ZnSnSe₄ thin films. *Physical Review Materials*, 3(3), 35402.

- Schwarz, T., Stechmann, G., Gault, B., Cojocar-Miréidin, O., Wuerz, R., & Raabe, D. (2018). Correlative transmission Kikuchi diffraction and atom probe tomography study of Cu(In,Ga)Se₂ grain boundaries. *Progress in Photovoltaics: Research and Applications*, 26(3), 196–204. <https://doi.org/10.1002/pip.2966>
- Schweinar, K., Beeg, S., Hartwig, C., Rajamathi, C. R., Kasian, O., Piccinin, S., Prieto, M. J., Tanase, L. C., Gottlob, D. M., Schmidt, T., Raabe, D., Schlögl, R., Gault, B., Jones, T. E., & Greiner, M. T. (2020). Formation of a 2D Meta-stable Oxide by Differential Oxidation of AgCu Alloys. *ACS Applied Materials & Interfaces*, 12(20), 23595–23605. <https://doi.org/10.1021/acsami.0c03963>
- Schweinar, K., Nicholls, R. L., Rajamathi, C. R., Zeller, P., Amati, M., Gregoratti, L., Raabe, D., Greiner, M., Gault, B., & Kasian, O. (2020). Probing catalytic surfaces by correlative scanning photoemission electron microscopy and atom probe tomography. *Journal of Materials Chemistry A*, 8(1), 388–400. <https://doi.org/10.1039/c9ta10818a>
- Sedighiani, K., Diehl, M., Traka, K., Roters, F., Sietsma, J., & Raabe, D. (2020). An efficient and robust approach to determine material parameters of crystal plasticity constitutive laws from macro-scale stress–strain curves. *International Journal of Plasticity*, 134(June), 102779. <https://doi.org/10.1016/j.ijplas.2020.102779>
- Sedighiani, K., Traka, K., Roters, F., Raabe, D., Sietsma, J., & Diehl, M. (2021). Determination and analysis of the constitutive parameters of temperature-dependent dislocation-density-based crystal plasticity models. *Mechanics of Materials*, 164, 104117. <https://doi.org/10.1016/j.mechmat.2021.104117>
- Sedighiani, K., Traka, K., Roters, F., Sietsma, J., Raabe, D., & Diehl, M. (2022). Crystal plasticity simulation of in-grain microstructural evolution during large deformation of IF-steel. *Acta Materialia*, 237, 118167. <https://doi.org/10.1016/j.actamat.2022.118167>
- Semiatin, S. L., Fagin, P. N., Glavicic, M. G., & Raabe, D. (2004). Deformation behavior of Waspaloy at hot-working temperatures. *Scripta Materialia*, 50(5), 625–629. <https://doi.org/10.1016/j.scriptamat.2003.11.030>
- Seok, M.-Y., Gopalan, H., Nandy, S., Zaefferer, S., Raabe, D., Kirchlechner, C., & Dehm, G. (2020). Microscale plastic anisotropy of basal and pyramidal I slip in pure magnesium tested in shear. *Materialia*, 14, 100932.
- Seol, J. B., Bae, J. W., Li, Z., Chan Han, J., Kim, J. G., Raabe, D., & Kim, H. S. (2018). Boron doped ultrastrong and ductile high-entropy alloys. *Acta Materialia*, 151, 366–376. <https://doi.org/10.1016/j.actamat.2018.04.004>
- Seol, J. B., Na, S. H., Gault, B., Kim, J. E., Han, J. C., Park, C. G., & Raabe, D. (2017). Core-shell nanoparticle arrays double the strength of steel. *Scientific Reports*, 7(January), 1–9. <https://doi.org/10.1038/srep42547>
- Seol, J. B., Raabe, D., Choi, P. P., Im, Y. R., & Park, C. G. (2012). Atomic scale effects of alloying, partitioning, solute drag and austempering on the mechanical properties of high-carbon bainitic-austenitic TRIP steels. *Acta Materialia*, 60(17), 6183–6199. <https://doi.org/10.1016/j.actamat.2012.07.064>

- Seol, J. B., Raabe, D., Choi, P., Park, H. S., Kwak, J. H., & Park, C. G. (2013). Direct evidence for the formation of ordered carbides in a ferrite-based low-density Fe-Mn-Al-C alloy studied by transmission electron microscopy and atom probe tomography. *Scripta Materialia*, *68*(6), 348–353. <https://doi.org/10.1016/j.scriptamat.2012.08.013>
- Shanthraj, P., Liu, C., Akbarian, A., Svendsen, B., & Raabe, D. (2020). Multi-component chemo-mechanics based on transport relations for the chemical potential. *Computer Methods in Applied Mechanics and Engineering*, *365*, 113029. <https://doi.org/10.1016/j.cma.2020.113029>
- Shanthraj, P., Sharma, L., Svendsen, B., Roters, F., & Raabe, D. (2016). A phase field model for damage in elasto-viscoplastic materials. *Computer Methods in Applied Mechanics and Engineering*, *312*, 167–185. <https://doi.org/10.1016/j.cma.2016.05.006>
- Shanthraj, P., Svendsen, B., Sharma, L., Roters, F., & Raabe, D. (2017). Elasto-viscoplastic phase field modelling of anisotropic cleavage fracture. *Journal of the Mechanics and Physics of Solids*, *99*(November), 19–34. <https://doi.org/10.1016/j.jmps.2016.10.012>
- Shen, Y. F., Jia, N., Wang, Y. D., Sun, X., Zuo, L., & Raabe, D. (2015). Suppression of twinning and phase transformation in an ultrafine grained 2 GPa strong metastable austenitic steel: Experiment and simulation. *Acta Materialia*, *97*, 305–315. <https://doi.org/10.1016/j.actamat.2015.06.053>
- Shen, Y. F., Qiu, L. N., Sun, X., Zuo, L., Liaw, P. K., & Raabe, D. (2015). Effects of retained austenite volume fraction, morphology, and carbon content on strength and ductility of nanostructured TRIP-assisted steels. *Materials Science and Engineering: A*, *636*, 551–564.
- Sheskin, A., Schwarz, T., Yu, Y., Zhang, S., Abdellaoui, L., Gault, B., Cojocar-Mirédin, O., Scheu, C., Raabe, D., Wuttig, M., & Amouyal, Y. (2018). Tailoring Thermoelectric Transport Properties of Ag-Alloyed PbTe: Effects of Microstructure Evolution. *ACS Applied Materials and Interfaces*, *10*(45), 38994–39001. <https://doi.org/10.1021/acsami.8b15204>
- Siboni, N. H., Raabe, D., & Varnik, F. (2013). Maintaining the equipartition theorem in small heterogeneous molecular dynamics ensembles. *Physical Review E*, *87*(3), 30101. <https://doi.org/10.1103/PhysRevE.87.030101>
- Siboni, N. H., Raabe, D., & Varnik, F. (2015). Aging in amorphous solids: A study of the first-passage time and persistence time distributions. *EPL (Europhysics Letters)*, *111*(4), 48004. <https://doi.org/10.1209/0295-5075/111/48004>
- Siqueira, R. P., Sandim, H. R. Z., Oliveira, T. R., & Raabe, D. (2011). Composition and orientation effects on the final recrystallization texture of coarse-grained Nb-containing AISI 430 ferritic stainless steels. *Materials Science and Engineering A*, *528*(9), 3513–3519. <https://doi.org/10.1016/j.msea.2011.01.007>
- Sohn, S. S., Kwiatkowski da Silva, A., Ikeda, Y., Körmann, F., Lu, W., Choi, W. S., Gault, B., Ponge, D., Neugebauer, J., & Raabe, D. (2019). Ultrastrong Medium-Entropy Single-Phase Alloys Designed via Severe Lattice Distortion. *Advanced Materials*, *31*(8), 1–8. <https://doi.org/10.1002/adma.201807142>
- Soler, R., Evirgen, A., Yao, M., Kirchlechner, C., Stein, F., Feuerbacher, M., Raabe, D., & Dehm, G. (2018). Microstructural and mechanical characterization of an equiatomic YGdTbDyHo high

- entropy alloy with hexagonal close-packed structure. *Acta Materialia*, 156, 86–96.
<https://doi.org/10.1016/j.actamat.2018.06.010>
- Song, J., Kostka, A., Veehmayer, M., & Raabe, D. (2011). Hierarchical microstructure of explosive joints: Example of titanium to steel cladding. *Materials Science and Engineering A*, 528(6), 2641–2647. <https://doi.org/10.1016/j.msea.2010.11.092>
- Song, R., Ponge, D., & Raabe, D. (2005). Improvement of the work hardening rate of ultrafine grained steels through second phase particles. *Scripta Materialia*, 52(11), 1075–1080.
<https://doi.org/10.1016/j.scriptamat.2005.02.016>
- Song, R., Ponge, D., & Raabe, D. (2005). Influence of Mn content on the microstructure and mechanical properties of ultrafine grained C-Mn steels. *ISIJ International*, 45(11), 1721–1726.
<https://doi.org/10.2355/isijinternational.45.1721>
- Song, R., Ponge, D., & Raabe, D. (2005). Mechanical properties of an ultrafine grained C-Mn steel processed by warm deformation and annealing. *Acta Materialia*, 53(18), 4881–4892.
<https://doi.org/10.1016/j.actamat.2005.07.009>
- Song, R., Ponge, D., Kaspar, R., & Raabe, D. (2004). Grain boundary characterization and grain size measurement in an ultrafine-grained steel. *Zeitschrift Fuer Metallkunde/Materials Research and Advanced Techniques*, 95(6), 513–517. <https://doi.org/10.3139/146.017983>
- Song, R., Ponge, D., Raabe, D., & Kaspar, R. (2005). Microstructure and crystallographic texture of an ultrafine grained C-Mn steel and their evolution during warm deformation and annealing. *Acta Materialia*, 53(3), 845–858. <https://doi.org/10.1016/j.actamat.2004.10.051>
- Song, R., Ponge, D., Raabe, D., Speer, J. G., & Matlock, D. K. (2006). Overview of processing, microstructure and mechanical properties of ultrafine grained bcc steels. *Materials Science and Engineering A*, 441(1–2), 1–17. <https://doi.org/10.1016/j.msea.2006.08.095>
- Song, W., Von Appen, J., Choi, P., Dronskowski, R., Raabe, D., & Bleck, W. (2013). Atomic-scale investigation of ϵ and θ precipitates in bainite in 100Cr6 bearing steel by atom probe tomography and ab initio calculations. *Acta Materialia*, 61(20), 7582–7590.
<https://doi.org/10.1016/j.actamat.2013.08.051>
- Soni, P., Cojocaru-Miredin, O., & Raabe, D. (2015). Interface engineering and nanoscale characterization of Zn(S,O) alternative buffer layer for CIGS thin film solar cells. *2015 IEEE 42nd Photovoltaic Specialist Conference, PVSC 2015*, 1–5.
<https://doi.org/10.1109/PVSC.2015.7355889>
- Soni, P., Raghuvanshi, M., Wuerz, R., Berghoff, B., Knoch, J., Raabe, D., & Cojocaru-Mirédin, O. (2019). Sputtering as a viable route for In₂S₃ buffer layer deposition in high efficiency Cu(In,Ga)Se₂ solar cells. *Energy Science and Engineering*, 7(2), 478–487. <https://doi.org/10.1002/ese3.295>
- Souza Filho, I. R. I. R., Dutta, A., Almeida Junior, D. R., Lu, W., Sandim, M. J. R. M. J. R., Ponge, D., Sandim, H. R. Z. H. R. Z., Raabe, D., Junior, D. R. A., Lu, W., Sandim, M. J. R. M. J. R., Ponge, D., Sandim, H. R. Z. H. R. Z., Raabe, D., Almeida Junior, D. R., Lu, W., Sandim, M. J. R. M. J. R., Ponge, D., Sandim, H. R. Z. H. R. Z., & Raabe, D. (2020). The impact of grain-scale strain localization on strain hardening of a high-Mn steel: Real-time tracking of the transition from the $\gamma \rightarrow \epsilon \rightarrow$

- α' transformation to twinning. *Acta Materialia*, 197, 123–136.
<https://doi.org/10.1016/j.actamat.2020.07.038>
- Souza Filho, I. R., Kwiatkowski da Silva, A., Sandim, M. J. R., Ponge, D., Gault, B., Sandim, H. R. Z., & Raabe, D. (2019). Martensite to austenite reversion in a high-Mn steel: Partitioning-dependent two-stage kinetics revealed by atom probe tomography, in-situ magnetic measurements and simulation. *Acta Materialia*, 166, 178–191. <https://doi.org/10.1016/j.actamat.2018.12.046>
- Souza Filho, I. R., Ma, Y., Kulse, M., Ponge, D., Gault, B., Springer, H., & Raabe, D. (2021). Sustainable steel through hydrogen plasma reduction of iron ore: Process, kinetics, microstructure, chemistry. *Acta Materialia*, 213, 116971. <https://doi.org/10.1016/j.actamat.2021.116971>
- Souza Filho, I. R., Sandim, M. J. R. J. R., Ponge, D., Sandim, H. R. Z. R. Z., & Raabe, D. (2019). Strain hardening mechanisms during cold rolling of a high-Mn steel: Interplay between submicron defects and microtexture. *Materials Science and Engineering: A*, 754(February), 636–649. <https://doi.org/10.1016/j.msea.2019.03.116>
- Souza Filho, I. R., Sandim, M. J. R., Cohen, R., Nagamine, L. C. C. M., Sandim, H. R. Z., & Raabe, D. (2019). Magnetic properties of a 17.6 Mn-TRIP steel: Study of strain-induced martensite formation, austenite reversion, and athermal α' -formation. *Journal of Magnetism and Magnetic Materials*, 473(June 2018), 109–118. <https://doi.org/10.1016/j.jmmm.2018.10.034>
- Souza Filho, I. R., Springer, H., Ma, Y., Mahajan, A., da Silva, C. C., Kulse, M., & Raabe, D. (2022). Green steel at its crossroads: Hybrid hydrogen-based reduction of iron ores. *Journal of Cleaner Production*, 340(January), 130805. <https://doi.org/10.1016/j.jclepro.2022.130805>
- Souza Filho, I.R., Ma, Y., Raabe, D., Springer, H. (2023). Fundamentals of green steel production: Role of pressure in hydrogen reduction of iron ores. *JOM: Journal of The Minerals, Metals & Materials Society*, May. <https://doi.org/10.1007/s11837-023-05829-z>
- Springer, H., & Raabe, D. (2012). Rapid alloy prototyping: Compositional and thermo-mechanical high throughput bulk combinatorial design of structural materials based on the example of 30Mn-1.2C-xAl triplex steels. *Acta Materialia*, 60(12), 4950–4959. <https://doi.org/10.1016/j.actamat.2012.05.017>
- Springer, H., Aparicio Fernandez, R., Duarte, M. J., Kostka, A., & Raabe, D. (2015). Microstructure refinement for high modulus in-situ metal matrix composite steels via controlled solidification of the system Fe-TiB₂. *Acta Materialia*, 96, 47–56. <https://doi.org/10.1016/j.actamat.2015.06.017>
- Springer, H., Baron, C., Szczepaniak, A., Jäggle, E. A., Wilms, M. B., Weisheit, A., & Raabe, D. (2016). Efficient additive manufacturing production of oxide- and nitride-dispersion-strengthened materials through atmospheric reactions in liquid metal deposition. *Materials and Design*, 111, 60–69. <https://doi.org/10.1016/j.matdes.2016.08.084>
- Springer, H., Baron, C., Szczepaniak, A., Uhlenwinkel, V., & Raabe, D. (2017). Stiff, light, strong and ductile: nano-structured High Modulus Steel. *Scientific Reports*, 7(1), 17–22. <https://doi.org/10.1038/s41598-017-02861-3>
- Springer, H., Belde, M., & Raabe, D. (2013). Bulk combinatorial design of ductile martensitic stainless steels through confined martensite-to-austenite reversion. *Materials Science and Engineering: A*, 582, 235–244. <https://doi.org/10.1016/j.msea.2013.06.036>

- Springer, H., Belde, M., & Raabe, D. (2016). Combinatorial design of transitory constitution steels: Coupling high strength with inherent formability and weldability through sequenced austenite stability. *Materials and Design*, *90*, 1100–1109. <https://doi.org/10.1016/j.matdes.2015.11.050>
- Springer, H., Kostka, A., dos Santos, J. F., & Raabe, D. (2011). Influence of intermetallic phases and Kirkendall-porosity on the mechanical properties of joints between steel and aluminium alloys. *Materials Science and Engineering A*, *528*(13–14), 4630–4642. <https://doi.org/10.1016/j.msea.2011.02.057>
- Springer, H., Kostka, A., Payton, E. J., Raabe, D., Kaysser-Pyzalla, A., & Eggeler, G. (2011). On the formation and growth of intermetallic phases during interdiffusion between low-carbon steel and aluminum alloys. *Acta Materialia*, *59*(4), 1586–1600. <https://doi.org/10.1016/j.actamat.2010.11.023>
- Springer, H., Szczepaniak, A., & Raabe, D. (2015). On the role of zinc on the formation and growth of intermetallic phases during interdiffusion between steel and aluminium alloys. *Acta Materialia*, *96*, 203–211. <https://doi.org/10.1016/j.actamat.2015.06.028>
- Springer, H., Tasan, C., & Raabe, D. (2015). A novel roll-bonding methodology for the cross-scale analysis of phase properties and interactions in multiphase structural materials. *International Journal of Materials Research*, *106*(1), 3–14. <https://doi.org/10.3139/146.111156>
- Springer, H., Zhang, J. L., Szczepaniak, A., Belde, M., Gault, B., & Raabe, D. (2019). Light, strong and cost effective: Martensitic steels based on the Fe – Al – C system. *Materials Science and Engineering A*, *762*(May), 138088. <https://doi.org/10.1016/j.msea.2019.138088>
- Stechmann, G., Zaeferrer, S., & Raabe, D. (2018). Molecular statics simulation of CdTe grain boundary structures and energetics using a bond-order potential. *Modelling and Simulation in Materials Science and Engineering*, *26*(4). <https://doi.org/10.1088/1361-651X/aaba87>
- Stechmann, G., Zaeferrer, S., Konijnenberg, P., Raabe, D., Gretener, C., Kranz, L., Perrenoud, J., Buecheler, S., & Tiwari, A. N. (2016). 3-Dimensional microstructural characterization of CdTe absorber layers from CdTe/CdS thin film solar cells. *Solar Energy Materials and Solar Cells*, *151*, 66–80. <https://doi.org/10.1016/j.solmat.2016.02.023>
- Stechmann, G., Zaeferrer, S., Schwarz, T., Konijnenberg, P., Raabe, D., Gretener, C., Kranz, L., Perrenoud, J., Buecheler, S., Nath Tiwari, A., & Tiwari, A. N. (2017). A correlative investigation of grain boundary crystallography and electronic properties in CdTe thin film solar cells. *Solar Energy Materials and Solar Cells*, *166*(January), 108–120. <https://doi.org/10.1016/j.solmat.2017.03.022>
- Steinmetz, D. R., Ja, T., Wietbrock, B., Eisenlohr, P., Jäpel, T., Wietbrock, B., Eisenlohr, P., Gutierrez-Urrutia, I., Saeed-Akbari, A., Hickel, T., Roters, F., & Raabe, D. (2013). Author ' s personal copy Revealing the strain-hardening behavior of twinning-induced plasticity steels : Theory , simulations , experiments. *Acta Materialia*, *61*(2), 494–510. <https://doi.org/10.1016/j.actamat.2012.09.064>
- Stephenson, L. T., Szczepaniak, A., Mouton, I., Rusitzka, K. A. K. K., Breen, A. J., Tezins, U., Sturm, A., Vogel, D., Chang, Y., Kontis, P., Rosenthal, A., Shepard, J. D., Maier, U., Kelly, T. F., Raabe, D., & Gault, B. (2018). The Laplace Project: An integrated suite for preparing and transferring atom

- probe samples under cryogenic and UHV conditions. *Plos One*, *13*(12), e0209211. <https://doi.org/10.1371/journal.pone.0209211>
- Stoffers, A., Barthel, J., Liebscher, C. H., Gault, B., Cojocaru-Miréidin, O., Scheu, C., & Raabe, D. (2017). Correlating atom probe tomography with atomic-resolved scanning transmission electron microscopy: Example of segregation at silicon grain boundaries. *Microscopy and Microanalysis*, *23*(2), 291–299. <https://doi.org/10.1017/S1431927617000034>
- Stoffers, A., Cojocaru-Miréidin, O., Seifert, W., Zaefferer, S., Riepe, S., & Raabe, D. (2015). Grain boundary segregation in multicrystalline silicon: correlative characterization by EBSD, EBIC, and atom probe tomography. *Progress in Photovoltaics: Research and Applications*, *23*(12), 1742–1753.
- Stoffers, A., Ziebarth, B., Barthel, J., Cojocaru-Miréidin, O., Elsässer, C., & Raabe, D. (2015). Complex nanotwin substructure of an asymmetric Σ 9 tilt grain boundary in a silicon polycrystal. *Physical Review Letters*, *115*(23), 235502. <https://doi.org/10.1103/PhysRevLett.115.235502>
- Storojeva, L., Ponge, D., Kaspar, R., & Raabe, D. (2004). Development of microstructure and texture of medium carbon steel during heavy warm deformation. *Acta Materialia*, *52*(8), 2209–2220. <https://doi.org/10.1016/j.actamat.2004.01.024>
- Storojeva, L., Ponge, D., Raabe, D., & Kaspar, R. (2004). On the influence of heavy warm reduction on the microstructure and mechanical properties of a medium-carbon ferritic-pearlitic steel. *Zeitschrift Fuer Metallkunde/Materials Research and Advanced Techniques*, *95*(12), 1108–1114. <https://doi.org/10.3139/146.018060>
- Su, J., Raabe, D., & Li, Z. (2019). Hierarchical microstructure design to tune the mechanical behavior of an interstitial TRIP-TWIP high-entropy alloy. *Acta Materialia*, *163*, 40–54. <https://doi.org/10.1016/j.actamat.2018.10.017>
- Su, J., Wu, X., Raabe, D., & Li, Z. (2019). Deformation-driven bidirectional transformation promotes bulk nanostructure formation in a metastable interstitial high entropy alloy. *Acta Materialia*, *167*, 23–39. <https://doi.org/10.1016/j.actamat.2019.01.030>
- Sulzer, S., Li, Z., Zaefferer, S., Hafez Haghghat, S. M., Wilkinson, A., Raabe, D., & Reed, R. (2020). On the assessment of creep damage evolution in nickel-based superalloys through correlative HR-EBSD and cECCI studies. *Acta Materialia*, *185*, 13–27. <https://doi.org/10.1016/j.actamat.2019.07.018>
- Sun, B., Krieger, W., Rohwerder, M., Ponge, D., & Raabe, D. (2020). Dependence of hydrogen embrittlement mechanisms on microstructure-driven hydrogen distribution in medium Mn steels. *Acta Materialia*, *183*, 313–328. <https://doi.org/10.1016/j.actamat.2019.11.029>
- Sun, B., Kwiatkowski, A., Wu, Y., Ma, Y., Chen, H., Scott, C., & Ponge, D. (2022). Physical metallurgy of medium-Mn advanced high-strength steels. *International Materials Reviews*, *0*(0), 1–39. <https://doi.org/10.1080/09506608.2022.2153220>
- Sun, B., Lu, W., Gault, B., Ding, R., Makineni, S. K., Wan, D., Wu, C.-H. H., Chen, H., Ponge, D., & Raabe, D. (2021). Chemical heterogeneity enhances hydrogen resistance in high-strength steels. *Nature Materials*, *20*, 1629–1634. <https://doi.org/10.1038/s41563-021-01050-y>

- Sun, B., Ma, Y., Vanderesse, N., Varanasi, R. S., Song, W., Bocher, P., Ponge, D., & Raabe, D. (2019). Macroscopic to nanoscopic in situ investigation on yielding mechanisms in ultrafine grained medium Mn steels: Role of the austenite-ferrite interface. *Acta Materialia*, *178*, 10–25. <https://doi.org/10.1016/j.actamat.2019.07.043>
- Sun, B., Palanisamy, D., Ponge, D., Gault, B., Fazeli, F., Scott, C., Yue, S., & Raabe, D. (2019). Revealing fracture mechanisms of medium manganese steels with and without delta-ferrite. *Acta Materialia*, *164*, 683–696. <https://doi.org/10.1016/j.actamat.2018.11.029>
- Sun, D. K., Zhu, M. F., Dai, T., Cao, W. S., Chen, S. L., Raabe, D., & Hong, C. P. (2011). Modelling of dendritic growth in ternary alloy solidification with melt convection. *International Journal of Cast Metals Research*, *24*(3–4), 177–183. <https://doi.org/10.1179/136404611X13001912813988>
- Sun, D. K., Zhu, M. F., Pan, S. Y., Yang, C. R., & Raabe, D. (2011). Lattice Boltzmann modeling of dendritic growth in forced and natural convection. *Computers & Mathematics with Applications*, *61*(12), 3585–3592. <https://doi.org/10.1016/j.camwa.2010.11.001>
- Sun, D., Zhu, M., Pan, S., & Raabe, D. (2009). Lattice Boltzmann modeling of dendritic growth in a forced melt convection. *Acta Materialia*, *57*(6), 1755–1767. <https://doi.org/10.1016/j.actamat.2008.12.019>
- Sun, D., Zhu, M., Pan, S., & Raabe, D. (2009). Numerical modeling of dendritic growth in alloy solidification with forced convection. *International Journal of Modern Physics B*, *23*(06n07), 1609–1614.
- Sun, Z., Ma, Y., Ponge, D., Zaefferer, S., Jäggle, E. A., Gault, B., Rollett, A. D., & Raabe, D. (2022). Thermodynamics-guided alloy and process design for additive manufacturing. *Nature Communications*, *13*(1). <https://doi.org/10.1038/s41467-022-31969-y>
- Svendsen, B., Shanthraj, P., & Raabe, D. (2018). Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids. *Journal of the Mechanics and Physics of Solids*, *112*, 619–636. <https://doi.org/10.1016/j.jmps.2017.10.005>
- Swadener, J. G., Bögershausen, H., Sander, B., & Raabe, D. (2010). Crystal orientation effects in scratch testing with a spherical indenter. *Journal of Materials Research*, *25*(5), 921–926. <https://doi.org/10.1557/jmr.2010.0108>
- Szczepaniak, A., Fan, J., Kostka, A., & Raabe, D. (2012). On the Correlation Between Thermal Cycle and Formation of Intermetallic Phases at the Interface of Laser-Welded Aluminum-Steel Overlap Joints. *Advanced Engineering Materials*, *14*(7), 464–472.
- Szczepaniak, A., Fan, J., Kostka, A., & Raabe, D. (2012). On the correlation between thermal cycle and formation of intermetallic phases at the interface of laser-welded aluminum-steel overlap joints. *Advanced Engineering Materials*, *14*(7), 464–472. <https://doi.org/10.1002/adem.201200075>
- Szczepaniak, A., Springer, H., Aparicio-Fernández, R., Baron, C., & Raabe, D. (2017). Strengthening Fe – TiB₂ based high modulus steels by precipitations. *Materials and Design*, *124*, 183–193. <https://doi.org/10.1016/j.matdes.2017.03.042>
- Szczepaniak, A., Springer, H., Aparicio-Fernández, R., Baron, C., & Raabe, D. (2017). Strengthening Fe–TiB₂ based high modulus steels by precipitations. *Materials & Design*, *124*, 183–193.

- Tan, X. D., Xu, Y. B., Ponge, D., Yang, X. L., Hu, Z. P., Peng, F., Ju, X. W., Wu, D., & Raabe, D. (2016). Effect of intercritical deformation on microstructure and mechanical properties of a low-silicon aluminum-added hot-rolled directly quenched and partitioned steel. *Materials Science and Engineering A*, *656*, 200–215. <https://doi.org/10.1016/j.msea.2016.01.040>
- Tan, X., Ponge, D., Lu, W., Xu, Y., He, H., Yan, J., Wu, D., & Raabe, D. (2020). Joint investigation of strain partitioning and chemical partitioning in ferrite-containing TRIP-assisted steels. *Acta Materialia*, *186*, 374–388. <https://doi.org/10.1016/j.actamat.2019.12.050>
- Tan, X., Ponge, D., Lu, W., Xu, Y., Yang, X., Rao, X., Wu, D., & Raabe, D. (2019). Carbon and strain partitioning in a quenched and partitioned steel containing ferrite. *Acta Materialia*, *165*, 561–576. <https://doi.org/10.1016/j.actamat.2018.12.019>
- Tang, S., Wang, J. C., Svendsen, B., & Raabe, D. (2017). Competitive bcc and fcc crystal nucleation from non-equilibrium liquids studied by phase-field crystal simulation. *Acta Materialia*, *139*, 196–204. <https://doi.org/10.1016/j.actamat.2017.08.015>
- Tarzimoghadam, Z., Ponge, D., Klöwer, J., & Raabe, D. (2017). Hydrogen-assisted failure in Ni-based superalloy 718 studied under in situ hydrogen charging: The role of localized deformation in crack propagation. *Acta Materialia*, *128*, 365–374. <https://doi.org/10.1016/j.actamat.2017.02.059>
- Tarzimoghadam, Z., Rohwerder, M., Merzlikin, S. V., Bashir, A., Yedra, L., Eswara, S., Ponge, D., & Raabe, D. (2016). Multi-scale and spatially resolved hydrogen mapping in a Ni-Nb model alloy reveals the role of the δ phase in hydrogen embrittlement of alloy 718. *Acta Materialia*, *109*, 69–81. <https://doi.org/10.1016/j.actamat.2016.02.053>
- Tarzimoghadam, Z., Sandlöbes, S., Pradeep, K. G., & Raabe, D. (2015). Microstructure design and mechanical properties in a near- α Ti-4Mo alloy. *Acta Materialia*, *97*, 291–304. <https://doi.org/10.1016/j.actamat.2015.06.043>
- Tasan, C. C. C., Hoefnagels, J. P. M. P. M., Diehl, M., Yan, D., Roters, F., & Raabe, D. (2014). Strain localization and damage in dual phase steels investigated by coupled in-situ deformation experiments and crystal plasticity simulations. *International Journal of Plasticity*, *63*, 198–210. <https://doi.org/10.1016/j.ijplas.2014.06.004>
- Tasan, C. C., Deng, Y., Pradeep, K. G., Yao, M. J., Springer, H., & Raabe, D. (2014). Composition Dependence of Phase Stability, Deformation Mechanisms, and Mechanical Properties of the CoCrFeMnNi High-Entropy Alloy System. *JOM*, *66*(10), 1993–2001. <https://doi.org/10.1007/s11837-014-1133-6>
- Tasan, C. C., Diehl, M., Yan, D., Bechtold, M., Roters, F., Schemmann, L., Zheng, C., Peranio, N., Ponge, D., Koyama, M., Tsuzaki, K., & Raabe, D. (2015). An Overview of Dual-Phase Steels: Advances in Microstructure-Oriented Processing and Micromechanically Guided Design. *Annual Review of Materials Research*, *45*(1), 391–431. <https://doi.org/10.1146/annurev-matsci-070214-021103>
- Tasan, C. C., Diehl, M., Yan, D., Zambaldi, C., Shanthraj, P., Roters, F., & Raabe, D. (2014). Integrated experimental-simulation analysis of stress and strain partitioning in multiphase alloys. *Acta Materialia*, *81*, 386–400. <https://doi.org/10.1016/j.actamat.2014.07.071>

- Thomas, I., Zaefferer, S., Friedel, F., & Raabe, D. (2003). High-Resolution EBSD Investigation of Deformed and Partially Recrystallized IF Steel. *Advanced Engineering Materials*, 5(8), 566–570. <https://doi.org/10.1002/adem.200300373>
- Tikhovskiy, I., Raabe, D., & Roters, F. (2006). Simulation of the deformation texture of a 17%Cr ferritic stainless steel using the texture component crystal plasticity finite element method considering texture gradients. *Scripta Materialia*, 54(8), 1537–1542. <https://doi.org/10.1016/j.scriptamat.2005.12.038>
- Tikhovskiy, I., Raabe, D., & Roters, F. (2007). Simulation of earing during deep drawing of an Al-3% Mg alloy (AA 5754) using a texture component crystal plasticity FEM. *Journal of Materials Processing Technology*, 183(2–3), 169–175. <https://doi.org/10.1016/j.jmatprotec.2006.10.006>
- Tikhovskiy, I., Raabe, D., & Roters, F. (2008). Simulation of earing of a 17% Cr stainless steel considering texture gradients. *Materials Science and Engineering A*, 488(1–2), 482–490. <https://doi.org/10.1016/j.msea.2007.11.063>
- Timokhina, I. B., Liss, K.-D. D., Raabe, D., Rakha, K., Beladi, H., Xiong, X. Y., & Hodgson, P. D. (2016). Growth of bainitic ferrite and carbon partitioning during the early stages of bainite transformation in a 2 mass% silicon steel studied by in situ neutron diffraction, TEM and APT. *Journal of Applied Crystallography*, 49(2), 399–414. <https://doi.org/10.1107/S1600576716000418>
- Toji, Y., Matsuda, H., & Raabe, D. (2016). Effect of Si on the acceleration of bainite transformation by pre-existing martensite. *Acta Materialia*, 116, 250–262. <https://doi.org/10.1016/j.actamat.2016.06.044>
- Toji, Y., Matsuda, H., Herbig, M., Choi, P. P., & Raabe, D. (2014). Atomic-scale analysis of carbon partitioning between martensite and austenite by atom probe tomography and correlative transmission electron microscopy. *Acta Materialia*, 65, 215–228. <https://doi.org/10.1016/j.actamat.2013.10.064>
- Toji, Y., Miyamoto, G., & Raabe, D. (2015). Carbon partitioning during quenching and partitioning heat treatment accompanied by carbide precipitation. *Acta Materialia*, 86, 137–147. <https://doi.org/10.1016/j.actamat.2014.11.049>
- Tóth, L. S., Molinari, A., & Raabe, D. (1997). Modeling of rolling texture development in a ferritic chromium steel. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 28(11), 2343–2351. <https://doi.org/10.1007/s11661-997-0191-6>
- Traka, K., Sedighiani, K., Bos, C., Lopez, J. G., Angenendt, K., Raabe, D., & Sietsma, J. (2021). Topological aspects responsible for recrystallization evolution in an IF-steel sheet—Investigation with cellular-automaton simulations. *Computational Materials Science*, 198, 110643.
- Tytko, D., Choi, P. P., & Raabe, D. (2015). Thermal dissolution mechanisms of AlN/CrN hard coating superlattices studied by atom probe tomography and transmission electron microscopy. *Acta Materialia*, 85, 32–41. <https://doi.org/10.1016/j.actamat.2014.11.004>
- Tytko, D., Choi, P. P., & Raabe, D. (2017). Oxidation behavior of ALN/CRN multilayered hard coatings. *Nano Convergence*, 4(1), 2–6. <https://doi.org/10.1186/s40580-017-0109-y>

- Tytko, D., Choi, P. P., Klöwer, J., Kostka, A., Inden, G., & Raabe, D. (2012). Microstructural evolution of a Ni-based superalloy (617B) at 700 °C studied by electron microscopy and atom probe tomography. *Acta Materialia*, *60*(4), 1731–1740. <https://doi.org/10.1016/j.actamat.2011.11.020>
- Varnik, F., & Raabe, D. (2006). Scaling effects in microscale fluid flows at rough solid surfaces. *Modelling and Simulation in Materials Science and Engineering*, *14*(5), 857. <https://doi.org/10.1088/0965-0393/14/5/004>
- Varnik, F., & Raabe, D. (2007). Chaotic flows in microchannels: A lattice Boltzmann study. *Molecular Simulation*, *33*(7), 583–587. <https://doi.org/10.1080/08927020601030456>
- Varnik, F., & Raabe, D. (2008). Profile blunting and flow blockage in a yield-stress fluid: A molecular dynamics study. *Physical Review E*, *77*(1), 11504. <https://doi.org/10.1103/PhysRevE.77.011504>
- Varnik, F., Dorner, D., & Raabe, D. (2007). Roughness-induced flow instability: a lattice Boltzmann study. *Journal of Fluid Mechanics*, *573*, 191–209.
- Varnik, F., Gross, M., Moradi, N., Zikos, G., Uhlmann, P., Müller-Buschbaum, P., Magerl, D., Raabe, D., Steinbach, I., & Stamm, M. (2011). Stability and dynamics of droplets on patterned substrates: insights from experiments and lattice Boltzmann simulations. *Journal of Physics: Condensed Matter*, *23*(18), 184112. <https://doi.org/10.1088/0953-8984/23/18/184112>
- Varnik, F., Mandal, S., Chikkadi, V., Denisov, D., Olsson, P., Vågberg, D., Raabe, D., & Schall, P. (2014). Correlations of plasticity in sheared glasses. *Physical Review E*, *89*(4), 40301. <https://doi.org/10.1103/PhysRevE.89.040301>
- Varnik, F., Truman, P., Wu, B., Uhlmann, P., Raabe, D., & Stamm, M. (2008). Wetting gradient induced separation of emulsions: a combined experimental and lattice Boltzmann computer simulation study. *Physics of Fluids*, *20*(7), 72104. <https://doi.org/10.1063/1.2963958>
- Verbeken, K., Barbé, L., & Raabe, D. (2009). Evaluation of the crystallographic orientation relationships between FCC and BCC phases in TRIP steels. *ISIJ International*, *49*(10), 1601–1609. <https://doi.org/10.2355/isijinternational.49.1601>
- Verbeken, K., Van Caenegem, N., & Raabe, D. (2009). Identification of ϵ martensite in a Fe-based shape memory alloy by means of EBSD. *Micron*, *40*(1), 151–156. <https://doi.org/10.1016/j.micron.2007.12.012>
- Volz, N., Zenk, C. H., Cherukuri, R., Kalfhaus, T., Weiser, M., Makineni, S. K., Betzing, C., Lenz, M., Gault, B., Fries, S. G., Schreuer, J., Vaßen, R., Virtanen, S., Raabe, D., Spiecker, E., Neumeier, S., & Göken, M. (2018). Thermophysical and Mechanical Properties of Advanced Single Crystalline Co-base Superalloys. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, *49*(9), 4099–4109. <https://doi.org/10.1007/s11661-018-4705-1>
- Voß, S., Palm, M., Stein, F., & Raabe, D. (2011). Phase equilibria in the Fe-Nb system. *Journal of Phase Equilibria and Diffusion*, *32*(2), 97–104.
- Wang, D., Diehl, M., Roters, F., & Raabe, D. (2018). On the role of the collinear dislocation interaction in deformation patterning and laminate formation in single crystal plasticity. *Mechanics of Materials*, *125*(July), 70–79. <https://doi.org/10.1016/j.mechmat.2018.06.007>

- Wang, D., Shanthraj, P., Springer, H., & Raabe, D. (2018). Particle-induced damage in Fe–TiB₂ high stiffness metal matrix composite steels. *Materials & Design*, *160*, 557–571. <https://doi.org/10.1016/j.matdes.2018.09.033>
- Wang, F., Sandlöbes, S., Diehl, M., Sharma, L., Roters, F., & Raabe, D. (2014). In situ observation of collective grain-scale mechanics in Mg and Mg-rare earth alloys. *Acta Materialia*, *80*, 77–93. <https://doi.org/10.1016/j.actamat.2014.07.048>
- Wang, M. M., Tasan, C. C., Ponge, D., & Raabe, D. (2016). Spectral TRIP enables ductile 1.1 GPa martensite. *Acta Materialia*, *111*, 262–272. <https://doi.org/10.1016/j.actamat.2016.03.070>
- Wang, M. M., Tasan, C. C., Ponge, D., Kostka, A., & Raabe, D. (2014). Smaller is less stable: Size effects on twinning vs. transformation of reverted austenite in TRIP-maraging steels. *Acta Materialia*, *79*, 268–281. <https://doi.org/10.1016/j.actamat.2014.07.020>
- Wang, M., Li, Z., & Raabe, D. (2018). In-situ SEM observation of phase transformation and twinning mechanisms in an interstitial high-entropy alloy. *Acta Materialia*, *147*, 236–246. <https://doi.org/10.1016/j.actamat.2018.01.036>
- Wang, M., Tasan, C. C., Koyama, M., Ponge, D., & Raabe, D. (2015). Enhancing Hydrogen Embrittlement Resistance of Lath Martensite by Introducing Nano-Films of Interlath Austenite. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, *46*(9), 3797–3802. <https://doi.org/10.1007/s11661-015-3009-y>
- Wang, M., Tasan, C. C., Ponge, D., Dippel, A. C., & Raabe, D. (2015). Nano-laminate TRIP-TWIP steel with dynamic strain partitioning and enhanced damage resistance. *Acta Materialia*, *85*, 216–228.
- Wang, M.-M. M., Tasan, C. C. C., Ponge, D., Dippel, A.-C. C., Raabe, D. D., Dippel, A.-C. C., Tasan, C. C. C., Ponge, D., & Wang, M.-M. M. (2015). Nanolaminate transformation-induced plasticity-twinning-induced plasticity steel with dynamic strain partitioning and enhanced damage resistance. *Acta Materialia*, *85*, 216–228. <https://doi.org/10.1016/j.actamat.2014.11.010>
- Wang, X., Liu, C., Sun, B., Ponge, D., Jiang, C., & Raabe, D. (2022). The dual role of martensitic transformation in fatigue crack growth. *Proceedings of the National Academy of Sciences of the United States of America*, *119*(9). <https://doi.org/10.1073/pnas.2110139119>
- Wang, Y., Raabe, D., Klüber, C., & Roters, F. (2004). Orientation dependence of nanoindentation pile-up patterns and of nanoindentation microtextures in copper single crystals. *Acta Materialia*, *52*(8), 2229–2238. <https://doi.org/10.1016/j.actamat.2004.01.016>
- Wang, Z., Lu, W., An, F., Song, M., Ponge, D., Raabe, D., & Li, Z. (2022). High stress twinning in a compositionally complex steel of very high stacking fault energy. *Nature Communications*, *13*(1), 3598. <https://doi.org/10.1038/S41467-022-31315-2>
- Wang, Z., Lu, W., Raabe, D., & Li, Z. (2019). On the mechanism of extraordinary strain hardening in an interstitial high-entropy alloy under cryogenic conditions. *Journal of Alloys and Compounds*, *781*, 734–743. <https://doi.org/10.1016/j.jallcom.2018.12.061>

- Wang, Z., Lu, W., Zhao, H., He, J., Wang, K., Zhou, B., Ponge, D., Raabe, D., & Li, Z. (2020). Formation mechanism of κ -carbides and deformation behavior in Si-alloyed FeMnAlC lightweight steels. *Acta Materialia*, *198*, 258–270.
- Wang, Z., Lu, W., Zhao, H., Liebscher, C. H., He, J., Ponge, D., Raabe, D., & Li, Z. (2020). Ultrastrong lightweight compositionally complex steels via dual-nanoprecipitation. *Science Advances*, *6*(46), eaba9543.
- Weber, F., Schestakow, I., Roters, F., & Raabe, D. (2008). Texture evolution during bending of a single crystal copper nanowire studied by EBSD and crystal plasticity finite element simulations. *Advanced Engineering Materials*, *10*(8), 737–741. <https://doi.org/10.1002/adem.200800102>
- Wei, Y., Gault, B., Varanasi, R. S., Raabe, D., Herbig, M., & Breen, A. J. (2018). Machine-learning-based atom probe crystallographic analysis. *Ultramicroscopy*, *194*(July), 15–24. <https://doi.org/10.1016/j.ultramic.2018.06.017>
- Wei, Y., Varanasi, R. S., Schwarz, T., Gomell, L., Zhao, H., Larson, D. J., Sun, B., Liu, G., Chen, H., & Raabe, D. (2021). Machine-learning-enhanced time-of-flight mass spectrometry analysis. *Patterns*, *2*(2), 100192.
- Welsch, E., Ponge, D., Hafez Haghghat, S. M., Sandlöbes, S., Choi, P., Herbig, M., Zaefferer, S., & Raabe, D. (2016). Strain hardening by dynamic slip band refinement in a high-Mn lightweight steel. *Acta Materialia*, *116*, 188–199. <https://doi.org/10.1016/j.actamat.2016.06.037>
- Wen, Y. H. H., Peng, H. B., Si, H. T., Xiong, R. L., & Raabe, D. (2014). A novel high manganese austenitic steel with higher work hardening capacity and much lower impact deformation than Hadfield manganese steel. *Materials & Design*, *55*, 798–804. <https://doi.org/10.1016/j.matdes.2013.09.057>
- Wen, Y. H., Peng, H. B., Raabe, D., Gutierrez-Urrutia, I., Chen, J., & Du, Y. Y. (2014). Large recovery strain in Fe-Mn-Si-based shape memory steels obtained by engineering annealing twin boundaries. *Nature Communications*, *5*, 1–2. <https://doi.org/10.1038/ncomms5964>
- Wen, Y., Xiao, H., Peng, H., Li, N., & Raabe, D. (2015). Relationship between damping capacity and variations of vacancies concentration and segregation of carbon atom in an Fe-Mn alloy. *Metallurgical and Materials Transactions A*, *46*(11), 4828–4833.
- Woldemedhin, M. T., Raabe, D., & Hassel, A. W. (2010). Anodic oxides on a beta type Nb–Ti alloy and their characterization by electrochemical impedance spectroscopy. *Physica Status Solidi (A)*, *207*(4), 812–816. <https://doi.org/10.1002/pssa.200983324>
- Woldemedhin, M. T., Raabe, D., & Hassel, A. W. (2011). Grain boundary electrochemistry of β -type Nb–Ti alloy using a scanning droplet cell. *Physica Status Solidi (A)*, *208*(6), 1246–1251.
- Woldemedhin, M. T., Raabe, D., & Hassel, A. W. (2012). Characterization of thin anodic oxides of Ti–Nb alloys by electrochemical impedance spectroscopy. *Electrochimica Acta*, *82*, 324–332. <https://doi.org/10.1016/j.electacta.2012.06.029>
- Wong, S. L., Lapyteva, G., Brüggemann, T., Engler, O., Roters, F., Raabe, D., & Karhausen, K.-F. F. (2020). Microchemistry-dependent simulation of yield stress and flow stress in non-heat

- treatable Al sheet alloys. *Modelling and Simulation in Materials Science and Engineering*, 28(3), 35010. <https://doi.org/10.1088/1361-651X/ab71c0>
- Wong, S. L., Madivala, M., Prahl, U., Roters, F., & Raabe, D. (2016). A crystal plasticity model for twinning- and transformation-induced plasticity. *Acta Materialia*, 118, 140–151. <https://doi.org/10.1016/j.actamat.2016.07.032>
- Wu, G., Balachandran, S., Gault, B., Xia, W., Liu, C., Rao, Z., Wei, Y., Liu, S., Lu, J., & Herbig, M. (2020). Crystal–Glass High-Entropy Nanocomposites with Near Theoretical Compressive Strength and Large Deformability. *Advanced Materials*, 32(34), 2002619.
- Wu, X., Erbe, A., Raabe, D., & Fabritius, H. O. (2013). Extreme optical properties tuned through phase substitution in a structurally optimized biological photonic polycrystal. *Advanced Functional Materials*, 23(29), 3615–3620. <https://doi.org/10.1002/adfm.201203597>
- Wu, X., Li, Z., Rao, Z., Ikeda, Y., Dutta, B., Körmann, F., Neugebauer, J., & Raabe, D. (2020). Role of magnetic ordering for the design of quinary TWIP-TRIP high entropy alloys. *Physical Review Materials*, 4(3), 33601. <https://doi.org/10.1103/PhysRevMaterials.4.033601>
- Wu, X., Ma, D., Eisenlohr, P., Raabe, D., & Fabritius, H. O. (2016). From insect scales to sensor design: Modelling the mechanochromic properties of bicontinuous cubic structures. *Bioinspiration and Biomimetics*, 11(4). <https://doi.org/10.1088/1748-3190/11/4/045001>
- Wu, X., Makineni, S. K., Liebscher, C. H., Dehm, G., Rezaei Mianroodi, J., Shanthraj, P., Svendsen, B., Bürger, D., Eggeler, G., Raabe, D., & Gault, B. (2020). Unveiling the Re effect in Ni-based single crystal superalloys. *Nature Communications*, 11(1), 1–13. <https://doi.org/10.1038/s41467-019-14062-9>
- Yan, D., Tasan, C. C., & Raabe, D. (2015). High resolution in situ mapping of microstrain and microstructure evolution reveals damage resistance criteria in dual phase steels. *Acta Materialia*, 96, 399–409. <https://doi.org/10.1016/j.actamat.2015.05.038>
- Yan, F. K., Tao, N. R., Archie, F., Gutiérrez-Urrutia, I., Raabe, D., Lu, K. K., Gutierrez-Urrutia, I., Raabe, D., & Lu, K. K. (2014). Deformation mechanisms in an austenitic single-phase duplex microstructured steel with nanotwinned grains. *Acta Materialia*, 81, 487–500. <https://doi.org/10.1016/j.actamat.2014.08.054>
- Yan, F., Mouton, I., Stephenson, L. T., Breen, A. J., Chang, Y., Ponge, D., Raabe, D., & Gault, B. (2019). Atomic-scale investigation of hydrogen distribution in a Ti–Mo alloy. *Scripta Materialia*, 162, 321–325. <https://doi.org/10.1016/j.scriptamat.2018.11.040>
- Yan, F., Mouton, I., Stephenson, L. T., Breen, A. J., Chang, Y., Ponge, D., Raabe, D., & Gault, B. (2019). Atomic-scale investigation of hydrogen distribution in a TiMo alloy. *Scripta Materialia*, 162, 321–325.
- Yao, M. J., Dey, P., Seol, J. B., Choi, P., Herbig, M., Marceau, R. K. W., Hickel, T., Neugebauer, J., & Raabe, D. (2016). Combined atom probe tomography and density functional theory investigation of the Al off-stoichiometry of κ -carbides in an austenitic Fe–Mn–Al–C low density steel. *Acta Materialia*, 106, 229–238. <https://doi.org/10.1016/j.actamat.2016.01.007>

- Yao, M. J., Pradeep, K. G., Tasan, C. C., & Raabe, D. (2014). A novel, single phase, non-equiatomic FeMnNiCoCr high-entropy alloy with exceptional phase stability and tensile ductility. *Scripta Materialia*, 72–73, 5–8. <https://doi.org/10.1016/j.scriptamat.2013.09.030>
- Yao, M. J., Welsch, E., Ponge, D., Haghighat, S. M. H., Sandlöbes, S., Choi, P., Herbig, M., Bleskov, I., Hickel, T., Lipinska-Chwalek, M., Shanthraj, P., Scheu, C., Zaefferer, S., Gault, B., & Raabe, D. (2017). Strengthening and strain hardening mechanisms in a precipitation-hardened high-Mn lightweight steel. *Acta Materialia*, 140, 258–273. <https://doi.org/10.1016/j.actamat.2017.08.049>
- Yardley, V., Povstugar, I., Choi, P. P., Raabe, D., Parsa, A. B., Kostka, A., Somsen, C., Dlouhy, A., Neuking, K., George, E. P., & Eggeler, G. (2016). On Local Phase Equilibria and the Appearance of Nanoparticles in the Microstructure of Single-Crystal Ni-Base Superalloys. *Advanced Engineering Materials*, 18(9), 1556–1567. <https://doi.org/10.1002/adem.201600237>
- Ye, X., Yan, F., Schäfer, L., Wang, D., Geßwein, H., Wang, W., Chellali, M. R., Stephenson, L. T., Skokov, K., & Gutfleisch, O. (2021). Magnetoelectric Tuning of Pinning-Type Permanent Magnets through Atomic-Scale Engineering of Grain Boundaries. *Advanced Materials*, 33(5), 2006853.
- Yu, Y., Zhang, S., Mio, A. M., Gault, B., Sheskin, A., Scheu, C., Raabe, D., Zu, F., Wuttig, M., Amouyal, Y., & Cojocaru-Mirédin, O. (2018). Ag-Segregation to Dislocations in PbTe-Based Thermoelectric Materials. *ACS Applied Materials and Interfaces*, 10(4), 3609–3615. <https://doi.org/10.1021/acsami.7b17142>
- Yu, Y., Zhou, C., Zhang, S., Zhu, M., Wuttig, M., Scheu, C., Raabe, D., Snyder, G. J., Gault, B., & Cojocaru-Mirédin, O. (2020). Revealing nano-chemistry at lattice defects in thermoelectric materials using atom probe tomography. *Materials Today*, 32(February), 260–274. <https://doi.org/10.1016/j.mattod.2019.11.010>
- Yuan, L., Ponge, D., Wittig, J., Choi, P., Jiménez, J. A., & Raabe, D. (2012). Nanoscale austenite reversion through partitioning, segregation and kinetic freezing: Example of a ductile 2 GPa Fe-Cr-C steel. *Acta Materialia*, 60(6–7), 2790–2804. <https://doi.org/10.1016/j.actamat.2012.01.045>
- Zaafarani, N., Raabe, D., Roters, F., & Zaefferer, S. (2008). On the origin of deformation-induced rotation patterns below nanoindents. *Acta Materialia*, 56(1), 31–42. <https://doi.org/10.1016/j.actamat.2007.09.001>
- Zaafarani, N., Raabe, D., Singh, R. N., Roters, F., & Zaefferer, S. (2006). Three-dimensional investigation of the texture and microstructure below a nanoindent in a Cu single crystal using 3D EBSD and crystal plasticity finite element simulations. *Acta Materialia*, 54(7), 1863–1876. <https://doi.org/10.1016/j.actamat.2005.12.014>
- Zaefferer, S., Kuo, J.-C. C., Zhao, Z., Winning, M., & Raabe, D. (2003). On the influence of the grain boundary misorientation on the plastic deformation of aluminum bicrystals. *Acta Materialia*, 51(16), 4719–4735. [https://doi.org/10.1016/S1359-6454\(03\)00259-3](https://doi.org/10.1016/S1359-6454(03)00259-3)
- Zaefferer, S., Wright, S. I., & Raabe, D. (2008). Three-dimensional orientation microscopy in a focused ion beam-scanning electron microscope: A new dimension of microstructure characterization. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, 39(2), 374–389. <https://doi.org/10.1007/s11661-007-9418-9>

- Zaefferer, S., Wright, S., & Raabe, D. (2007). 3D-orientation microscopy in a FIB SEM: a new dimension of microstructure characterization. *Microscopy and Microanalysis*, *13*(S02), 1508–1509.
- Zahn, D., Tlatlik, H., & Raabe, D. (2009). Modeling of dislocation patterns of small- and high-angle grain boundaries in aluminum. *Computational Materials Science*, *46*(2), 293–296. <https://doi.org/10.1016/j.commatsci.2009.02.036>
- Zambaldi, C., & Raabe, D. (2010). Plastic anisotropy of γ -TiAl revealed by axisymmetric indentation. *Acta Materialia*, *58*(9), 3516–3530. <https://doi.org/10.1016/j.actamat.2010.02.025>
- Zambaldi, C., Roters, F., & Raabe, D. (2011). Analysis of the plastic anisotropy and pre-yielding of (γ/α 2)-phase titanium aluminide microstructures by crystal plasticity simulation. *Intermetallics*, *19*(6), 820–827. <https://doi.org/10.1016/j.intermet.2011.01.012>
- Zambaldi, C., Roters, F., Raabe, D., & Glatzel, U. (2007). Modeling and experiments on the indentation deformation and recrystallization of a single-crystal nickel-base superalloy. *Materials Science and Engineering A*, *454–455*, 433–440. <https://doi.org/10.1016/j.msea.2006.11.068>
- Zambaldi, C., Yang, Y., Bieler, T. R., & Raabe, D. (2012). Orientation informed nanoindentation of α -titanium: Indentation pileup in hexagonal metals deforming by prismatic slip. *Journal of Materials Research*, *27*(1), 356–367. <https://doi.org/10.1557/jmr.2011.334>
- Zambaldi, C., Zehnder, C., & Raabe, D. (2015). Orientation dependent deformation by slip and twinning in magnesium during single crystal indentation. *Acta Materialia*, *91*, 267–288. <https://doi.org/10.1016/j.actamat.2015.01.046>
- Zenk, C. H., Povstugar, I., Li, R., Rinaldi, F., Neumeier, S., Raabe, D., & Göken, M. (2017). A novel type of Co–Ti–Cr-base γ/γ' superalloys with low mass density. *Acta Materialia*, *135*, 244–251. <https://doi.org/10.1016/j.actamat.2017.06.024>
- Zhang, H., Bai, B., & Raabe, D. (2011). Superplastic martensitic Mn–Si–Cr–C steel with 900% elongation. *Acta Materialia*, *59*(14), 5787–5802. <https://doi.org/10.1016/j.actamat.2011.05.055>
- Zhang, H., Bai, B., & Raabe, D. (2011). Superplastic martensitic Mn–Si–Cr–C steel with 900% elongation. *Acta Materialia*, *59*(14), 5787–5802.
- Zhang, H., Diehl, M., Roters, F., & Raabe, D. (2016). A virtual laboratory using high resolution crystal plasticity simulations to determine the initial yield surface for sheet metal forming operations. *International Journal of Plasticity*, *80*, 111–138. <https://doi.org/10.1016/j.ijplas.2016.01.002>
- Zhang, H., Ponge, D., & Raabe, D. (2014). Designing quadplex (four-phase) microstructures in an ultrahigh carbon steel. *Materials Science and Engineering A*, *612*, 46–53. <https://doi.org/10.1016/j.msea.2014.06.023>
- Zhang, H., Ponge, D., & Raabe, D. (2014). Superplastic Mn–Si–Cr–C duplex and triplex steels: Interaction of microstructure and void formation. *Materials Science and Engineering A*, *610*, 355–369. <https://doi.org/10.1016/j.msea.2014.05.061>
- Zhang, H., Pradeep, K. G., Mandal, S., Ponge, D., & Raabe, D. (2014). New insights into the austenitization process of low-alloyed hypereutectoid steels: Nucleation analysis of strain-

- induced austenite formation. *Acta Materialia*, *80*, 296–308.
<https://doi.org/10.1016/j.actamat.2014.07.073>
- Zhang, H., Pradeep, K. G., Mandal, S., Ponge, D., Choi, P., Tasan, C. C., & Raabe, D. (2014). Enhanced superplasticity in an Al-alloyed multicomponent Mn-Si-Cr-C steel. *Acta Materialia*, *63*, 232–244.
<https://doi.org/10.1016/j.actamat.2013.10.034>
- Zhang, H., Pradeep, K. G., Mandal, S., Ponge, D., Springer, H., & Raabe, D. (2015). Dynamic strain-induced transformation: An atomic scale investigation. *Scripta Materialia*, *109*, 23–27.
<https://doi.org/10.1016/j.scriptamat.2015.07.010>
- Zhang, H., Springer, H., Aparicio-Fernández, R., & Raabe, D. (2016). Improving the mechanical properties of Fe–TiB₂ high modulus steels through controlled solidification processes. *Acta Materialia*, *118*, 187–195. <https://doi.org/10.1016/j.actamat.2016.07.056>
- Zhang, J. L., Tasan, C. C., Lai, M. J., Yan, D., & Raabe, D. (2017). Partial recrystallization of gum metal to achieve enhanced strength and ductility. *Acta Materialia*, *135*, 400–410.
<https://doi.org/10.1016/j.actamat.2017.06.051>
- Zhang, J. L., Tasan, C. C., Lai, M. L., Zhang, J., & Raabe, D. (2015). Damage resistance in gum metal through cold work-induced microstructural heterogeneity. *Journal of Materials Science*, *50*(17), 5694–5708. <https://doi.org/10.1007/s10853-015-9105-y>
- Zhang, J. L., Zaefferer, S., & Raabe, D. (2015). A study on the geometry of dislocation patterns in the surrounding of nanoindentations in a TWIP steel using electron channeling contrast imaging and discrete dislocation dynamics simulations. *Materials Science and Engineering A*, *636*, 231–242.
<https://doi.org/10.1016/j.msea.2015.03.078>
- Zhang, J., Raabe, D., & Tasan, C. C. (2017). Designing duplex, ultrafine-grained Fe-Mn-Al-C steels by tuning phase transformation and recrystallization kinetics. *Acta Materialia*, *141*, 374–387.
<https://doi.org/10.1016/j.actamat.2017.09.026>
- Zhang, J., Tasan, C. C., Lai, M. J., Dippel, A. C., & Raabe, D. (2017). Complexion-mediated martensitic phase transformation in Titanium. *Nature Communications*, *8*(May 2016), 1–8.
<https://doi.org/10.1038/ncomms14210>
- Zhang, S., Fang, H., Gramsma, M. E., Kwakernaak, C., Sloof, W. G., Tichelaar, F. D., Kuzmina, M., Herbig, M., Raabe, D., Brück, E., van der Zwaag, S., & van Dijk, N. H. (2016). Autonomous filling of grain-boundary cavities during creep loading in Fe-Mo alloys. *Metallurgical and Materials Transactions A*, *47*(10), 4831–4844. <https://doi.org/10.1007/s11661-016-3642-0>
- Zhang, S., Kwakernaak, C., Tichelaar, F. D., Sloof, W. G., Kuzmina, M., Herbig, M., Raabe, D., Brück, E., van der Zwaag, S., & Van Dijk, N. H. (2015). Autonomous repair mechanism of creep damage in Fe-Au and Fe-Au-BN alloys. *Metallurgical and Materials Transactions A*, *46*(12), 5656–5670.
<https://doi.org/10.1007/s11661-015-3169-9>
- Zhao, H., Chakraborty, P., Ponge, D., Hickel, T., Sun, B., Wu, C.-H., Gault, B., & Raabe, D. (2022). Hydrogen trapping and embrittlement in high-strength Al-alloys. *Nature*, *602*, 437–441.
<https://doi.org/10.1038/s41586-021-04343-z>

- Zhao, H., Chen, Y., Gault, B., Makineni, S. K., Ponge, D., & Raabe, D. (2020). (Al, Zn) 3Zr dispersoids assisted η' precipitation in an Al-Zn-Mg-Cu-Zr alloy. *Materialia*, *10*, 100641.
- Zhao, H., De Geuser, F., Kwiatkowski da Silva, A., Szczepaniak, A., Gault, B., Ponge, D., & Raabe, D. (2018). Segregation assisted grain boundary precipitation in a model Al-Zn-Mg-Cu alloy. *Acta Materialia*, *156*, 318–329. <https://doi.org/10.1016/j.actamat.2018.07.003>
- Zhao, H., Gault, B., Ponge, D., & Raabe, D. (2020). Reversion and re-aging of a peak aged Al-Zn-Mg-Cu alloy. *Scripta Materialia*, *188*, 269–273.
- Zhao, H., Gault, B., Ponge, D., Raabe, D., & De Geuser, F. (2018). Parameter free quantitative analysis of atom probe data by correlation functions: Application to the precipitation in Al-Zn-Mg-Cu. *Scripta Materialia*, *154*, 106–110. <https://doi.org/10.1016/j.scriptamat.2018.05.024>
- Zhao, H., Huber, L., Lu, W., Peter, N. J., An, D., De Geuser, F., Dehm, G., Ponge, D., Neugebauer, J., Gault, B., & Raabe, D. (2020). Interplay of Chemistry and Faceting at Grain Boundaries in a Model Al Alloy. *Physical Review Letters*, *124*(10). <https://doi.org/10.1103/PhysRevLett.124.106102>
- Zhao, Z., Mao, W., Roters, F., & Raabe, D. (2004). A texture optimization study for minimum earing in aluminium by use of a texture component crystal plasticity finite element method. *Acta Materialia*, *52*(4), 1003–1012. <https://doi.org/10.1016/j.actamat.2003.03.001>
- Zhao, Z., Ramesh, M., Raabe, D., Cuitiño, A. M., & Radovitzky, R. (2008). Investigation of three-dimensional aspects of grain-scale plastic surface deformation of an aluminum oligocrystal. *International Journal of Plasticity*, *24*(12), 2278–2297. <https://doi.org/10.1016/j.ijplas.2008.01.002>
- Zheng, C., & Raabe, D. (2013). Interaction between recrystallization and phase transformation during intercritical annealing in a cold-rolled dual-phase steel: A cellular automaton model. *Acta Materialia*, *61*(14), 5504–5517. <https://doi.org/10.1016/j.actamat.2013.05.040>
- Zheng, C., Raabe, D., & Li, D. (2012). Prediction of post-dynamic austenite-to-ferrite transformation and reverse transformation in a low-carbon steel by cellular automaton modeling. *Acta Materialia*, *60*(12), 4768–4779. <https://doi.org/10.1016/j.actamat.2012.06.007>
- Zhou, X., Bai, Y., El-Zoka, A. A., Kim, S.-H., Ma, Y., Liebscher, C. H., Gault, B., Mianroodi, J. R., Dehm, G., & Raabe, D. (2022). Effect of Pore Formation on Redox-Driven Phase Transformation. *Physical Review Letters*, *130*(16), 168001. <https://doi.org/10.1103/PhysRevLett.130.168001>
- Zhou, X., Kamachali, R. D., Boyce, B. L., Clark, B. G., Raabe, D., & Thompson, G. B. (2021). Spinodal Decomposition in Nanocrystalline Alloys. *Acta Materialia*, 117054.
- Zhu, M., Sun, D., Pan, S., Zhang, Q., & Raabe, D. (2014). Modelling of dendritic growth during alloy solidification under natural convection. *Modelling and Simulation in Materials Science and Engineering*, *22*(3), 34006. <https://doi.org/10.1088/0965-0393/22/3/034006>
- Zilnyk, K. D., Almeida Junior, D. R., Sandim, H. R. Z., Rios, P. R., & Raabe, D. (2018). Misorientation distribution between martensite and austenite in Fe-31 wt%Ni-0.01 wt%C. *Acta Materialia*, *143*, 227–236. <https://doi.org/10.1016/j.actamat.2017.10.026>

Zilnyk, K. D., Junior, D. R. A., Sandim, H. R. Z., Rios, P. R., & Raabe, D. (2018). Misorientation distribution between martensite and austenite in Fe-31 wt% Ni-0.01 wt% C. *Acta Materialia*, 143, 227–236.