The crystalline structure of metals: why does it matter for crystal plasticity?

Professor Dierk Raabe

Max-Planck-Institut für Eisenforschung GmbH
Düsseldorf, Germany
WWW.MPIE.DE
d.raabe@mpie.de
Multiscale Modeling and Experimentation

Methods: Scientific Fields
Multiscale crystal plasticity FEM

- External boundary conditions
- Mesh
- Elastic tensor
- Phase fractions
- Defect dynamics
- Crystal kinematics
- Orientation
- Homogenization

\[ \dot{\gamma} = \frac{d\gamma}{dt} = \rho_m b \nu \]

\[ L_p = \sum_{\alpha=1}^{12} \dot{\gamma}_\alpha \tilde{b}_\alpha \otimes \tilde{n}_\alpha \]
Why is the crystal lattice relevant for understanding complex dislocation structures?

Body centered cubic (bcc) lattice structure
Why is the crystal lattice relevant for understanding complex dislocation structures?

Densely packed planes: glide planes; densely packed translation shear vectors: Burgers vectors

Twinning systems

Stacking fault energy: cross slip, recovery, annihilation, Suzuki effect, twinning, strain hardening, stair rod dislocations, reactions

Shockley partial dislocations \((b = a/6<112>)\)
Special properties of the 3 main lattice types regarding plasticity defects

FCC: stacking fault energy can vary from very low values (α-Brass- 0 wt% Zn in Cu; TWIP steels: $\approx 20 \text{ m J/m}^2$) to very high values (Al : $\approx 180 \text{ m J/m}^2$): Regarding lattice defects in plasticity FCC is not a ‘homogeneous‘ structure

Hex: hcp or hex?; c/a ratio determines slip systems and twinning: some hex metals are very brittle (Mg) and some are very ductile (Ti)

BCC: non-close packed planes: pencile glide behavior; multiple slip systems: {110}; {112}; {123}; complex core of dislocation; twinnign vs. anti-twinning glide sense
How frequently do certain crystal structures occur in the PSE?
### Lattice parameters

<table>
<thead>
<tr>
<th>FCC: Face centered cubic close packed, (a)</th>
<th>Hexagonal close packed (a, c)</th>
<th>BCC: Body centered cubic (a)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cu (3.6147)</td>
<td>Be (2.2856, 3.5832)</td>
<td>Fe (2.8664)</td>
</tr>
<tr>
<td>Ag (4.0857)</td>
<td>Mg (3.2094, 5.2105)</td>
<td>Cr (2.8846)</td>
</tr>
<tr>
<td>Au (4.0783)</td>
<td>Zn (2.6649, 4.9468)</td>
<td>Mo (3.1469)</td>
</tr>
<tr>
<td>Al (4.0495)</td>
<td>Cd (2.9788, 5.6167)</td>
<td>W (3.1650)</td>
</tr>
<tr>
<td>Ni (3.5240)</td>
<td>Ti (2.506, 4.6788)</td>
<td>Ta (3.3026)</td>
</tr>
<tr>
<td>Pd (3.8907)</td>
<td>Zr (3.312, 5.1477)</td>
<td>Ba (5.019)</td>
</tr>
<tr>
<td>Pt (3.9239)</td>
<td>Ru (2.7058, 4.2816)</td>
<td></td>
</tr>
<tr>
<td>Pb (4.9502)</td>
<td>Os (2.7353, 4.3191)</td>
<td>Re (2.760, 4.458)</td>
</tr>
</tbody>
</table>
Crystal structure: BCC

Atoms per cell

\[ \text{atoms per cell} = (8 \times \frac{1}{8}) + 1 = 2 \]

Coordination number

\[ \text{coordination number} = 4 + 4 = 8 \]

Atomic packaging

\[ 4r = \sqrt{3}a \]

\[ a = \frac{4}{\sqrt[3]{3}}r \]
Glide plane: BCC
[111] stereographic projection showing orientations of all \{110\} and \{112\} planes belonging to the [111] zone.
Glide plane: dislocation core structure in BCC
courtesy of V. Vitek
Crystal structure: FCC

Fe (γ), Al, Cu, Au
Crystal structure: FCC

atoms per cell = \((8 \times 1/8) + (6 \times 1/2)\) = 4

coordination number = 4 + 4 + 4 = 12

atomic packaging = 0.74

\[4r = \sqrt{2}a\]

\[a = 2\sqrt{2}r\]
FCC – stacking sequence of dense (111) planes
FCC – stacking sequence of dense (111) planes
FCC – stacking sequence of dense (111) planes
FCC – stacking sequence of dense (111) planes
FCC – stacking sequence of dense (111) planes
Crystal structure: Hexagonal
3. HCP: hexagonal close-packed

(Mg, Be, Co, Ti, Zn)

noncubic symmetry: \( a \) and \( c \) axes

\( c/a \approx 1.633 \)
Crystal structure: Hexagonal

(a) basal \(<a\>, 3\
(b) prismatic \(<a\>, 3\
(c) pyramidal \(<a\>, 6\
(d) 1st order pyramidal \(<c + a\>, 12\
(e) 2nd order pyramidal \(<c + a\>, 6\)
### Miller Indices

<table>
<thead>
<tr>
<th>Gitter/Beispiel</th>
<th>Gleitebenen ( G )</th>
<th>Gleitrichtung ( g )</th>
<th>Gesamtzahl der Gleitsysteme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Typ ( Z ) abh.</td>
<td>Typ ( Z ) abh.</td>
<td></td>
</tr>
<tr>
<td>Cd, Zn, Mg, ( Ti_\alpha ), Be</td>
<td>(0001) 1</td>
<td>[1120] 3</td>
<td>3</td>
</tr>
<tr>
<td>Cd, Zn, Mg, ( Ti_\alpha ), Be, ( Zr_\alpha )</td>
<td>(1010) 3</td>
<td>[1120] 1</td>
<td>3</td>
</tr>
<tr>
<td>Mg, ( Ti_\alpha )</td>
<td>(1011) 6</td>
<td>[1120] 1</td>
<td>6</td>
</tr>
</tbody>
</table>

**vectors and planes for hexagonal materials**
hexagonal alloy systems: crystal structure and plasticity: examples

Mg - RE

Mg - Li
Crystal structure: Hexagonal / FCC
Crystal structure: Hexagonal / FCC
Crystal structure: Hexagonal / FCC
Crystal structure: Hexagonal / FCC

Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany
Crystal structure: Hexagonal / FCC

stacking sequence

A/CABBC

stacking sequence

ABCABBC
Deriving Miller indices: the description of lattice vectors

Intercepts reciprocals

Indices

\[
\begin{array}{ccc}
\infty & \infty & 1 \\
0 & 0 & 1 \\
\end{array}
\]

\((001)\)
Deriving Miller indices: the description of lattice vectors
Miller Indices of typical planes and directions in FCC metals

<table>
<thead>
<tr>
<th>Gittertyp</th>
<th>Beispiele</th>
<th>Gleiße-</th>
<th>Gleitricht-</th>
<th>Gesamt-</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>nen G</td>
<td>tung g</td>
<td>zahl der</td>
</tr>
<tr>
<td>Typ</td>
<td>Zahl</td>
<td>Typ</td>
<td>Zahl</td>
<td>Gleitsysteme</td>
</tr>
<tr>
<td>kfx</td>
<td>Al, Cu, Ni, Ag, Au</td>
<td>(111) 4</td>
<td>[110] 3</td>
<td>12</td>
</tr>
</tbody>
</table>

\[
\text{kfx} \quad \frac{4E \times 3R}{(111) \quad [110]} = 12
\]
## Miller Indices of typical planes and directions in BCC metals

<table>
<thead>
<tr>
<th>Gitter Beispiel</th>
<th>Gleitebenen G</th>
<th>Gleitrichtung g</th>
<th>Gesamtzahl der Gleitsysteme</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Typ</td>
<td>Zahl</td>
<td>Typ</td>
</tr>
<tr>
<td>( Fe_{αδ} )</td>
<td>(110)</td>
<td>6</td>
<td>[111]</td>
</tr>
<tr>
<td>W</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mo</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nb</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ta</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>( Fe_{αδ} )</td>
<td>(112)</td>
<td>12</td>
<td>[111]</td>
</tr>
<tr>
<td>W</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mo</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Nb</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>krz</td>
<td>(123)</td>
<td>24</td>
<td>[111]</td>
</tr>
<tr>
<td>( Fe_{αδ} )</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>W</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Mo</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ 6E \times 2R = 12 \]

\( (110) \times [111] \)
Miller Indices of typical planes and directions in BCC metals

12E x 1R = 12
(112) [111]

24E x 1R = 24
(123) [111]
\[ <100> = [1,0,0], [1,0,0], [0,1,0], [0,1,0], [0,0,1], [0,0,1] \]

\[ <110> = [1,1,0], [1,1,0], [1,1,0], [1,1,0], [1,0,1], [1,0,1] \]

\[ \text{specific} \]
\[ \text{general} \]

\[ \text{direction} \]
\[ \text{plane} \]

\[ [ \ ] \]
\[ < > \]

\[ ( ) \]
\[ \{ \} \]

vectors and planes
Stacking faults and cross slip