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

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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: ~ 20 m J / m²) to very high values (Al : ~ 180 m J / m²): 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 |  |
|--------------------|--|---|
| FCC: Face centered cubic close packed, (a) | Hexagonal close packed (a, c) | BCC: Body centered cubic (a) |
| Cu (3.6147) | Be (2.2856, 3.5832) | Fe (2.8664) |
| Ag (4.0857) | Mg (3.2094, 5.2105) | Cr (2.8846) |
| Au (4.0783) | Zn (2.6649, 4.9468) | Mo (3.1469) |
| Al (4.0495) | Cd (2.9788, 5.6167) | W (3.1650) |
| Ni (3.5240) | Ti (2.506, 4.6788) | Ta (3.3026) |
| Pd (3.8907) | Zr (3.312, 5.1477) | Ba (5.019) |
| Pt (3.9239) | Ru (2.7058, 4.2816) |  |
| Pb (4.9502) | Os (2.7353, 4.3191) | Re (2.760, 4.458) |
Crystal structure: BCC

atoms per cell

\[ = (8 \times 1/8) + 1 = 2 \]

coordination number

\[ = 4 + 4 = 8 \]

atomic packaging

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

\[ a = \frac{4}{\sqrt{3}}r \]
[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 = \((8 \times 1/8) + (6 \times \frac{1}{2}) = 4\)

\[
\text{coordination number} = 4 + 4 + 4 = 12
\]

atomic packaging = 0.74

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

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

noncubic symmetry: $a$ and $c$ axes
$c/a \sim 1.633$
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
<table>
<thead>
<tr>
<th>Vectors and Planes</th>
<th>Miller Indices</th>
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<tbody>
<tr>
<td>Mg $T_i$</td>
<td>(1011) 6</td>
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<tr>
<td>Zn $T_i$</td>
<td>(1010) 3</td>
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<tr>
<td>Cd $T_i$</td>
<td>(0001) 1</td>
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<td>Be $T_i$</td>
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<td>Cu $T_i$</td>
<td>[1120] 3</td>
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**Gleichteilung:**
- Cu $T_i$
- Zr $T_i$
- Mg $T_i$
- Zn $T_i$
- Cd $T_i$

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- Cu $T_i$
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Crystal structure: Hexagonal / FCC
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stacking sequence

stacking sequence
Deriving Miller indices: the description of lattice vectors

Intercepts reciprocals

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

Indices

(001)
Deriving Miller indices: the description of lattice vectors

(100) plane
(110) plane
[111] direction

[100] direction
[110] direction
(111) plane

∞ = infinity

\( a, b, c, \\
1, \infty, \infty, \\
\frac{1}{1} \frac{1}{\infty} \frac{1}{\infty} \\
= 1, 0, 0, \)

\( a, b, c, \\
1, 1, \infty, \\
\frac{1}{1} \frac{1}{1} \frac{1}{\infty} \\
= 1, 1, 0, \)

\( a, b, c, \\
1, 1, 1, \\
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= 1, 1, 1, \)
Miller Indices of typical planes and directions in FCC metals

<table>
<thead>
<tr>
<th>Gitter</th>
<th>Beispiel</th>
<th>Gleitebenen G</th>
<th>Gleiträchting g</th>
<th>Gesamtzahl der Gleitsysteme</th>
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### Miller Indices of typical planes and directions in BCC metals

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

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

12E \times 1R = 12
(112) \quad [111]

24E \times 1R = 24
(123) \quad [111]
Miller Indices

\[ <100> = [1,0,0], [\bar{1},0,0], [0,1,0], [0,\bar{1},0], [0,0,1], [0,0,\bar{1}] \]

\[ <110> = [1,1,0], [\bar{1},1,0], [1,\bar{1},0], [\bar{1},\bar{1},0], [1,0,1], [\bar{1},0,\bar{1}] \]......