

Imperfections – deformation and microstructures in polycrystals

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7- On the hexagonal-close-packed crystal structure

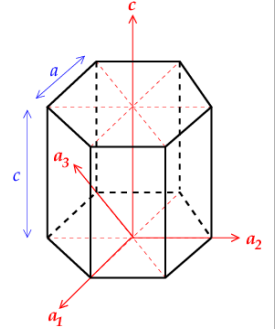
Hexagonal-close-packed (hcp)

Metals with an hcp structure:

- Zirconium, titanium, magnesium, zinc, ϵ -iron ($P > 15$ GPa)

Interest :

- Zirconium alloys (zircalloy) in nuclear industry (fuel rods in nuclear reactors)
- Titanium alloys: airplane engines
- Magnesium: car industry (lighter than steel)
- ϵ -iron: geophysics, Earth's inner core

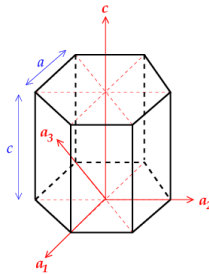


4 indices notation

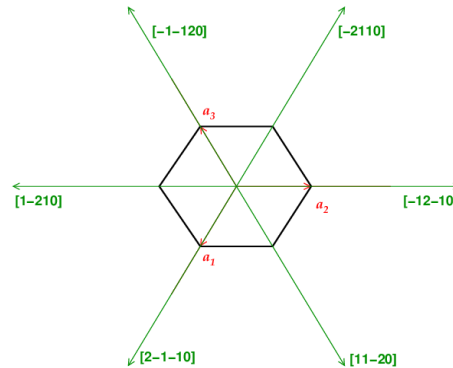
- Vectors a_1 , a_2 and a_3 are equivalent and non-orthogonal to each other
- Definition of Miller indices on 3 non-orthogonal axes (a_1 , a_2 et c): can be used but will hide symmetry operations
 - Definition of Miller indices on 3 orthogonal axes (a_1 , Y et c) can be used but it is easy to use (loss or symmetry elements, difficult to correlate to the crystal structure).

Hence: 4 indices notation:

- For planes: $(hkil)$ avec $h+k+i=0$; h , k , and l are identical to those of the 3 indices notation
- For direction: conversion between 3 and 4 indices is more complex
 - $u = (2u'-v)/3$; $v = (2v'-u)/3$; $t = -(u+v)$
 - $w = w'$
 - $[uvw]$ with $u+v+t=0$



Direction examples (1)

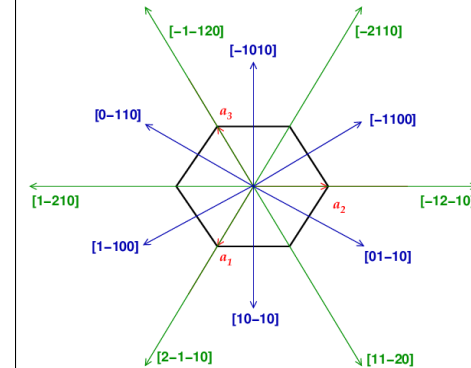


Practice:

Plot the $[2\bar{1}\bar{1}0]$ and $[1\bar{1}\bar{2}0]$ directions

All other equivalents

Direction examples (2)

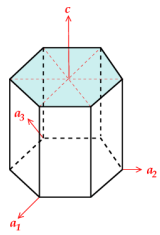


Practice:

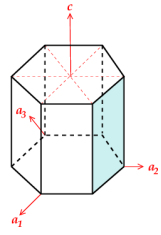
Plot the $[10\bar{1}0]$ and $[0\bar{1}\bar{1}0]$ directions and all other equivalent directions.

- Also note
- For directions in the basal plane: $[hki0]$ is orthogonal to the $(hki0)$ plane.
 - It is not true for $(hkil)$ planes if $l \neq 0$.

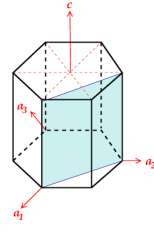
Basal and prismatic planes



(0001)
Basal plane
{0001} : (0001)

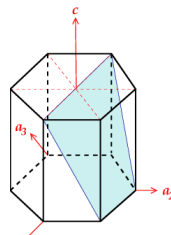


(01 $\bar{1}$ 0)
Prismatic plane
{01 $\bar{1}$ 0} :
(01 $\bar{1}$ 0), ($\bar{1}$ 100), ($\bar{1}$ 010)

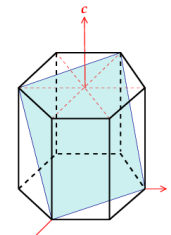


(11 $\bar{2}$ 0)
No name
{11 $\bar{2}$ 0} :
3 equivalents

Pyramidal planes

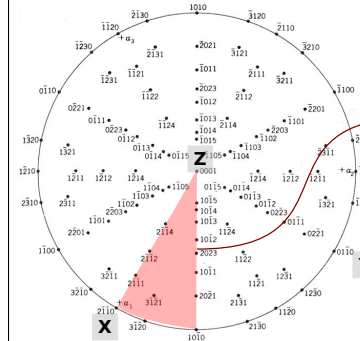


(01 $\bar{1}$ 1)
Pyramidal plane
{01 $\bar{1}$ 1} :
6 equivalents



(11 $\bar{2}$ 1)
Second order pyramidal plane
{11 $\bar{2}$ 1} :
6 equivalents

Stereographic projection



Stereographic projection for hcp-Zn

Hexagonal sector: sufficient for plotting inverse pole figures

Z // [0001], perpendicular to the basal plane
X // [2-1-10], parallel to a1
Y // [01-10], perpendicular to a prismatic plane

Barret & Massalski, *Structure of Metals*, Permagon (1980)

c/a parameter

The c/a parameter is related to the compact nature of the structure

- True compact structure: $c/a = 1.633$
- The c/a parameter has a large influence on plastic deformation in hcp metals

$c/a > 1.633$

$c/a \sim 1.633$

$c/a < 1.633$

| Métal | | c/a |
|-----------|----|-------|
| Cadmium | Cd | 1,886 |
| Zinc | Zn | 1,856 |
| Magnésium | Mg | 1,623 |
| Cobalt | Co | 1,623 |
| Rhénium | Re | 1,615 |
| Zirconium | Zr | 1,592 |
| Osmium | Os | 1,589 |
| Titane | Ti | 1,587 |
| Béryllium | Be | 1,568 |