Imperfections – deformation and microstructures in polycrystals

Sébastien Merkel
Professor, Physics Department
UMET Laboratory (Unité Matériaux et Transformations)
sebastien.merkel@univ-lille.fr

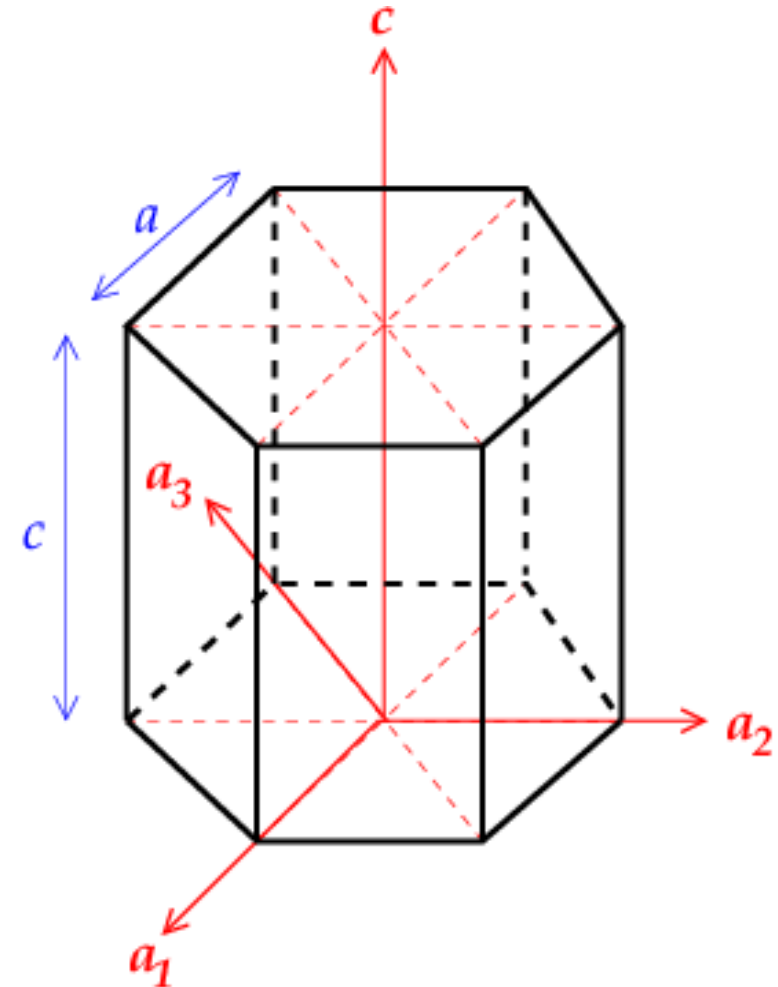# 7- On the hexagonal-close-packed crystal structure

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)
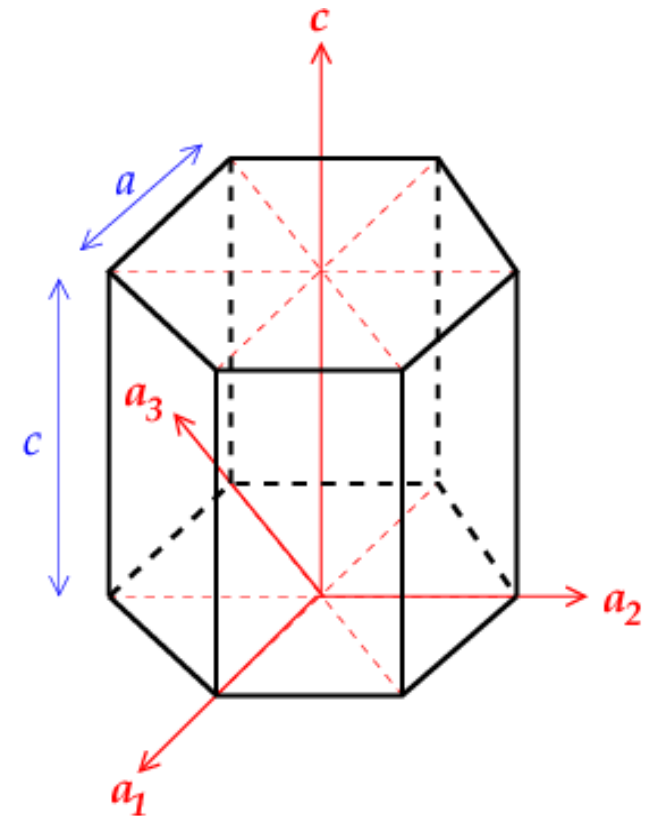- ε–iron: geophysics, Earth's inner core

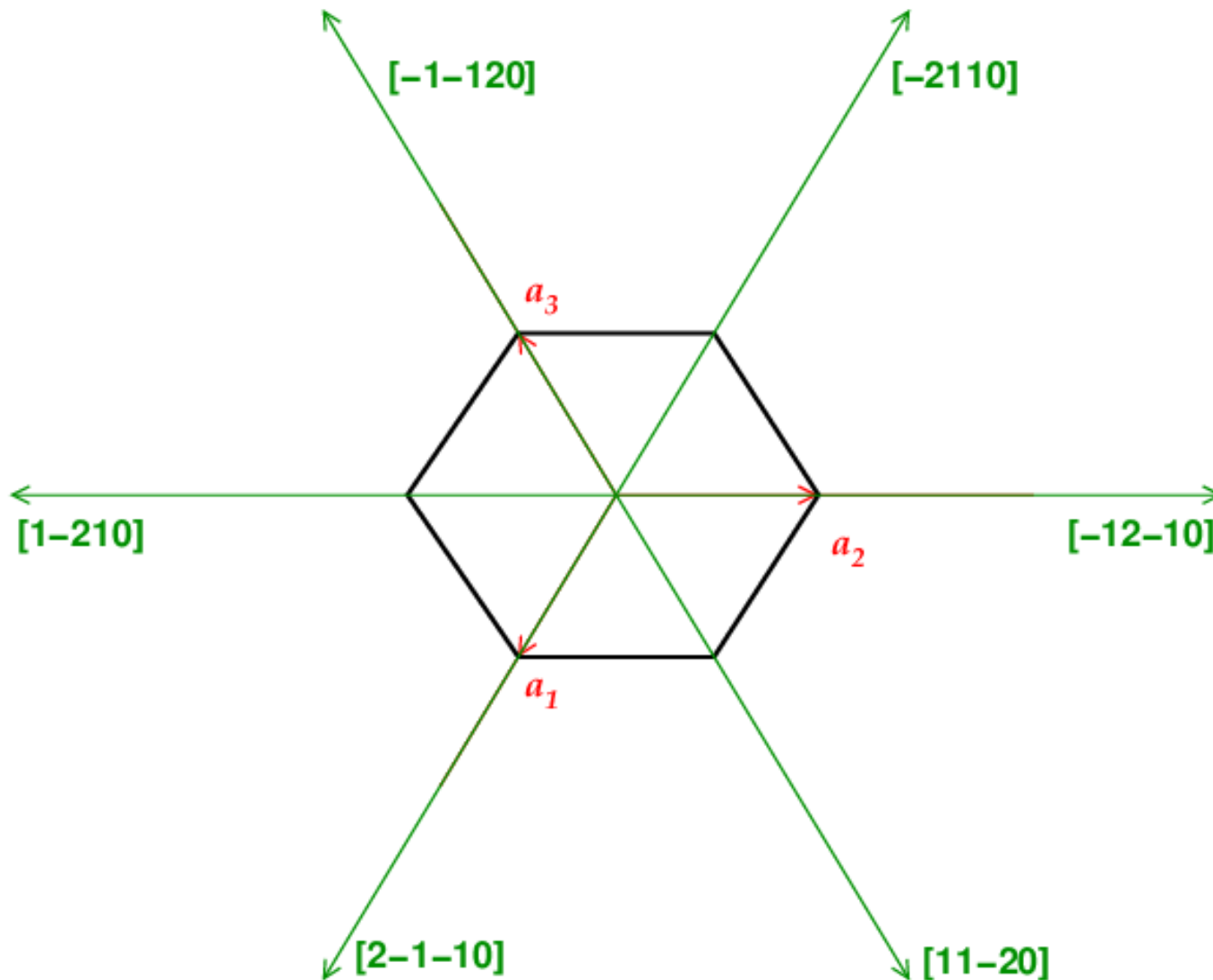Vectors a_1, a_2 and a_3 are equivalent and non-orthogonal to each other
- Definition of Miller indices on 3 non-orthogonal axes (a_1, a_2 et c): can be used but will hide symmetry operations
- Definition of Miller indices on 3 orthogonal axes (a_1, Y et c) can be used but it is easy to use (loss or 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)
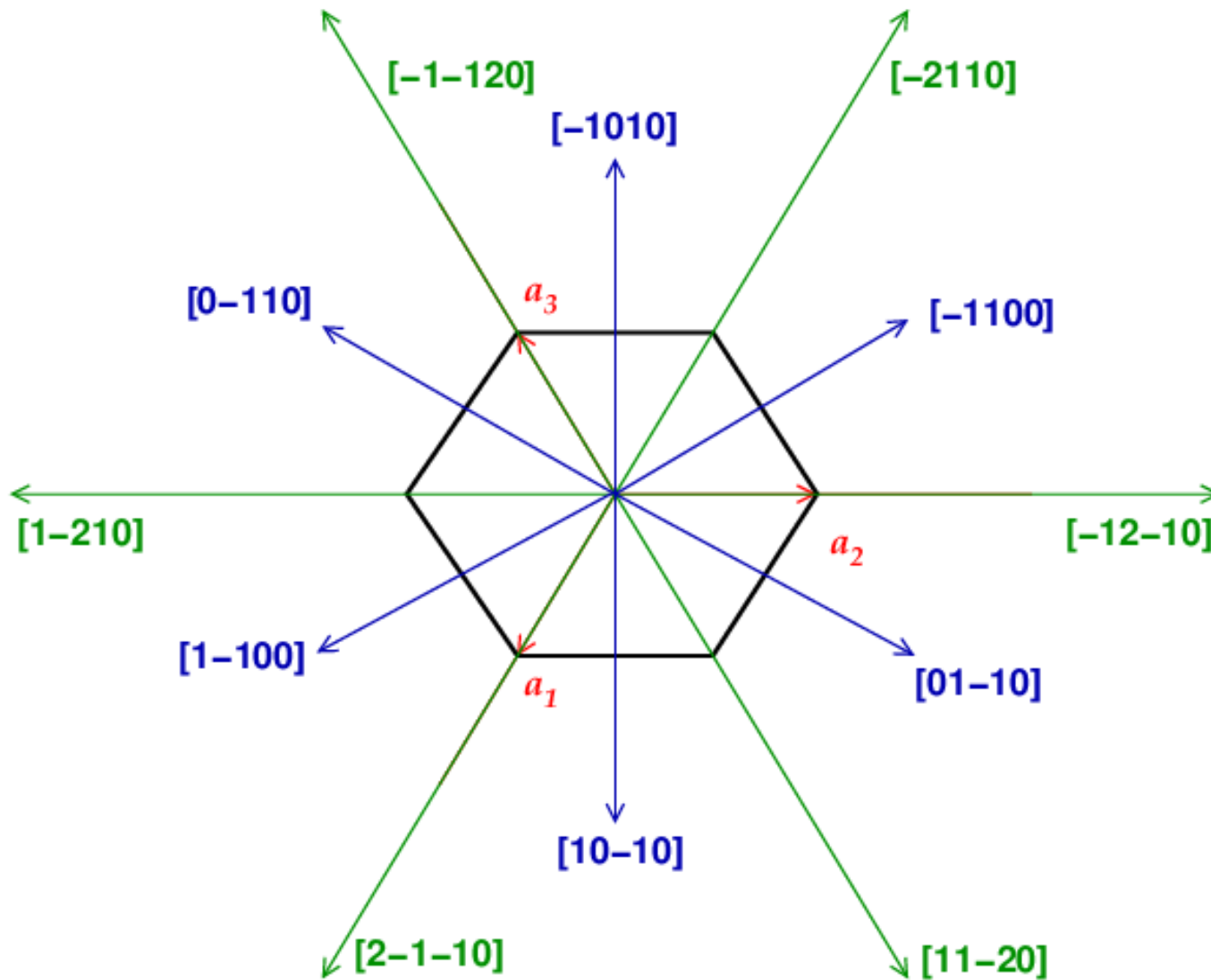 - w = w'
  - [uvtw] with u+v+t=0

Direction examples (1)

Practice:

Pot the $[2\overline{11}0]$ and $[11\overline{2}0]$ directions

Al all other equivalents

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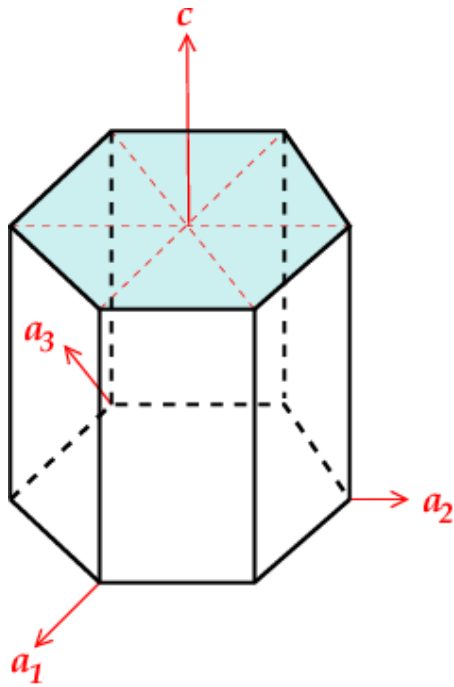
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Direction examples (2)

Practice:

Plot the $[10\overline{1}0]$ and $[01\overline{1}0]$ directions and all other equivalent directions.

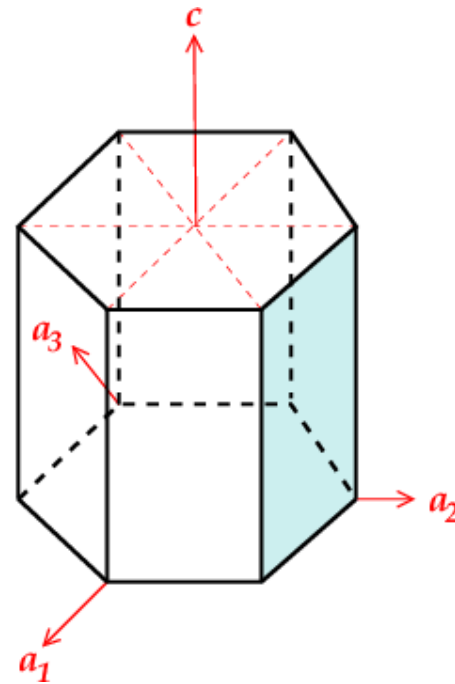Also note
- For directions in the basal plane: [hki0] is orthogonal to the (hki0) plane.
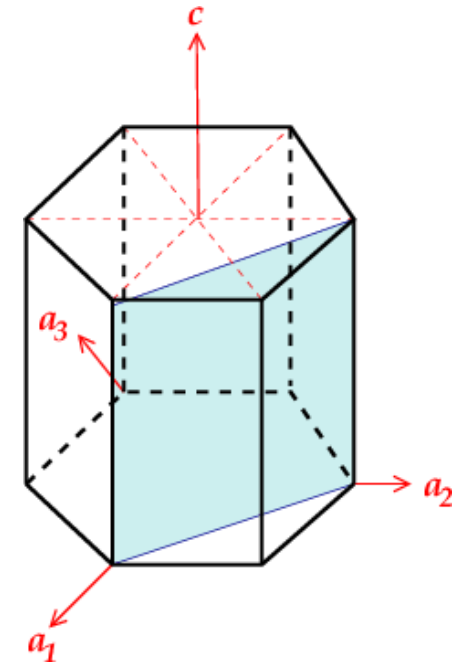- It is not true for (hkil) planes if l ≠ 0.

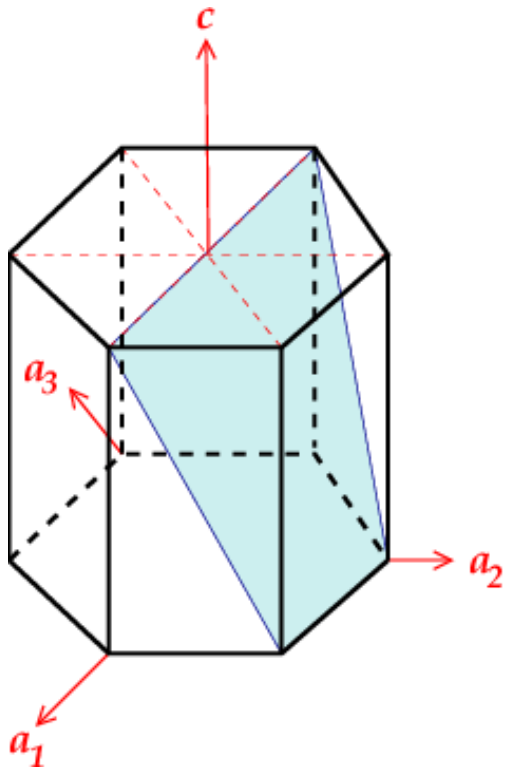# Basal and prismatic planes

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

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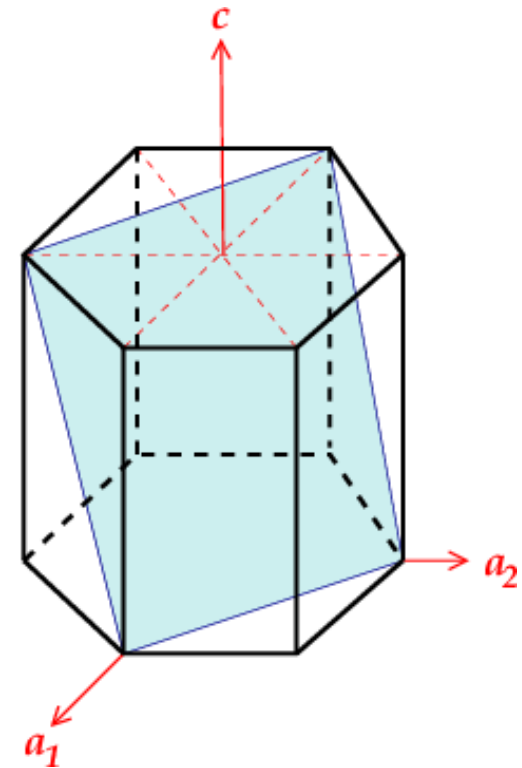$\{01\bar{1}0\}$:
$(01\bar{1}0)$, $(\bar{1}100)$, $(\bar{1}010)$

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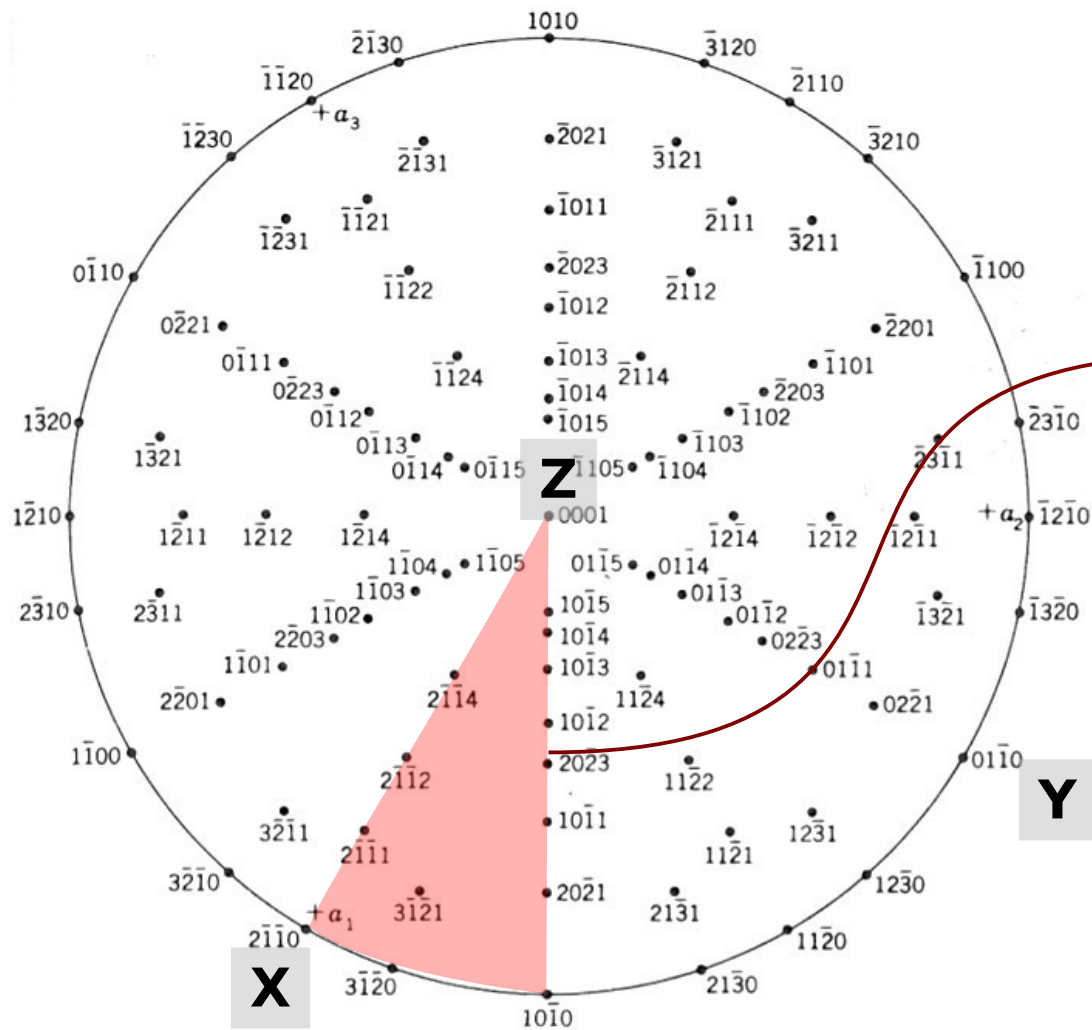No name
$\{11\bar{2}0\}$:
3 equivalents

Pyramidal planes

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

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

Stereographic projection

Fig. 2-10 Standard (0001) projection for zinc (hexagonal, $c/a = 1.86$).

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 ~ 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

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