FACULTÉ DES SCIENCES ET TECHNOLOGIES
Département Physique

Université de Lille

Imperfections – deformation and microstructures in polycrystals

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1- Introduction

True material

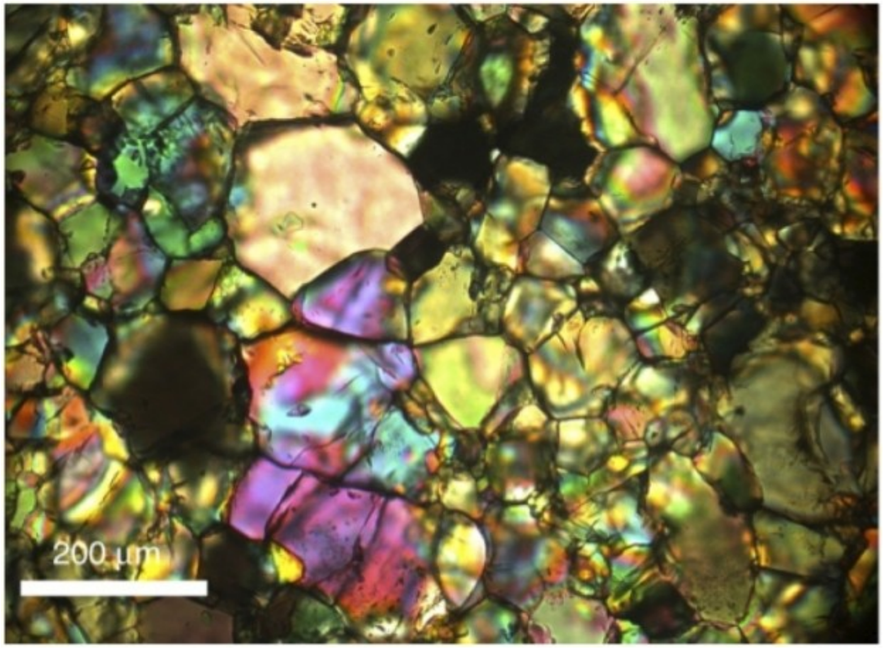
Polycrystal = ensemble of crystallites that form a material

Can be made of a single phase or many crystalline phases

Crystallite = connected volume element having the same crystal structure and orientation

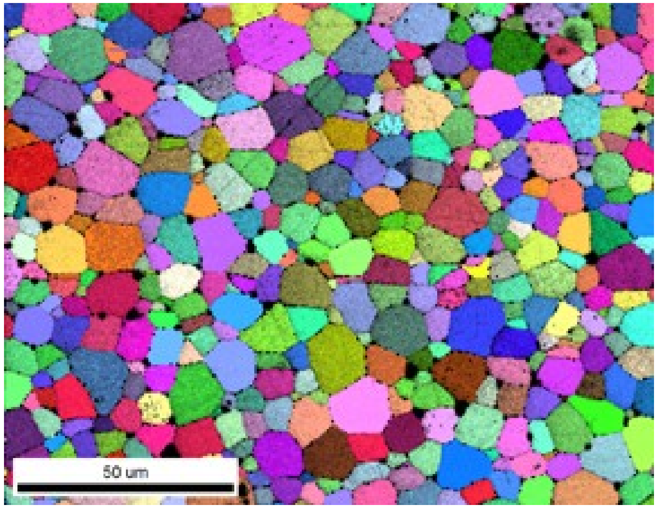
In general, crystallites are attached to each other, through strong chemical liaisons

Definition of a “grain” is not always clear but, sometimes, the word “grain” is used for “crystallite”

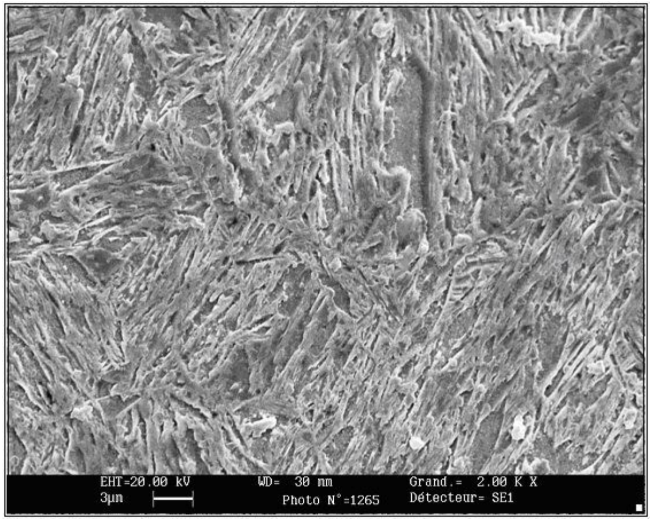


Olivine polycrystal
Image:
S. Demouchy, U. Montpellier

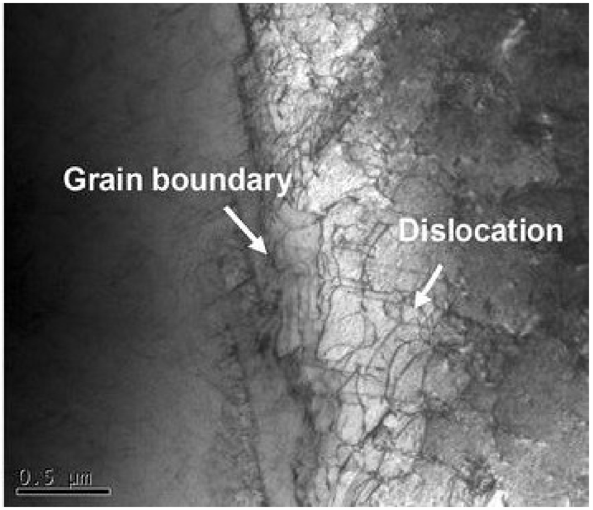
Multi-scale behavior



Zirconium oxide microstructure (grain size ~ 10 µm)
Image EDAX



Steel after chemical treatment (size ~ 1 µm)
Image Arcelor-Mittal



Dislocations and grain boundaries in steel (size ~ 100 nm)
Image Zhao et al, Acta Metall Sin

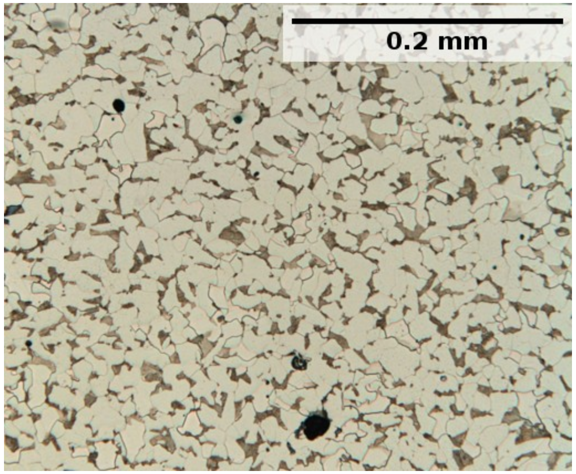
Here : microscopic scale → microstructure

Patrick Cordier, Philippe Carrez : nanoscale → defects

Properties-microstructures relationship

Properties of a material strongly depend on *microstructures*:

- Grain sizes,
- Grain orientations,
- Shape,
- Contrast in physical properties
- etc

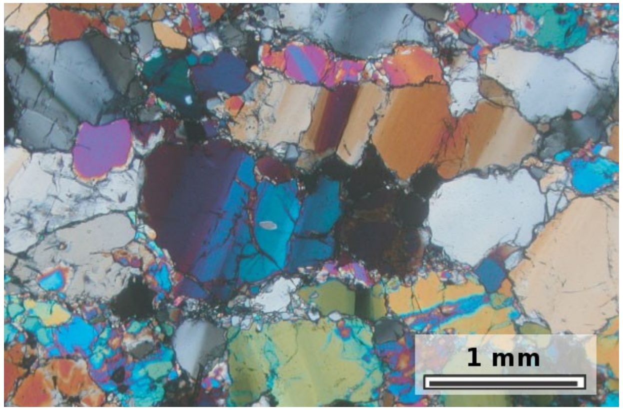


Steel
Touchstone Research Laboratory

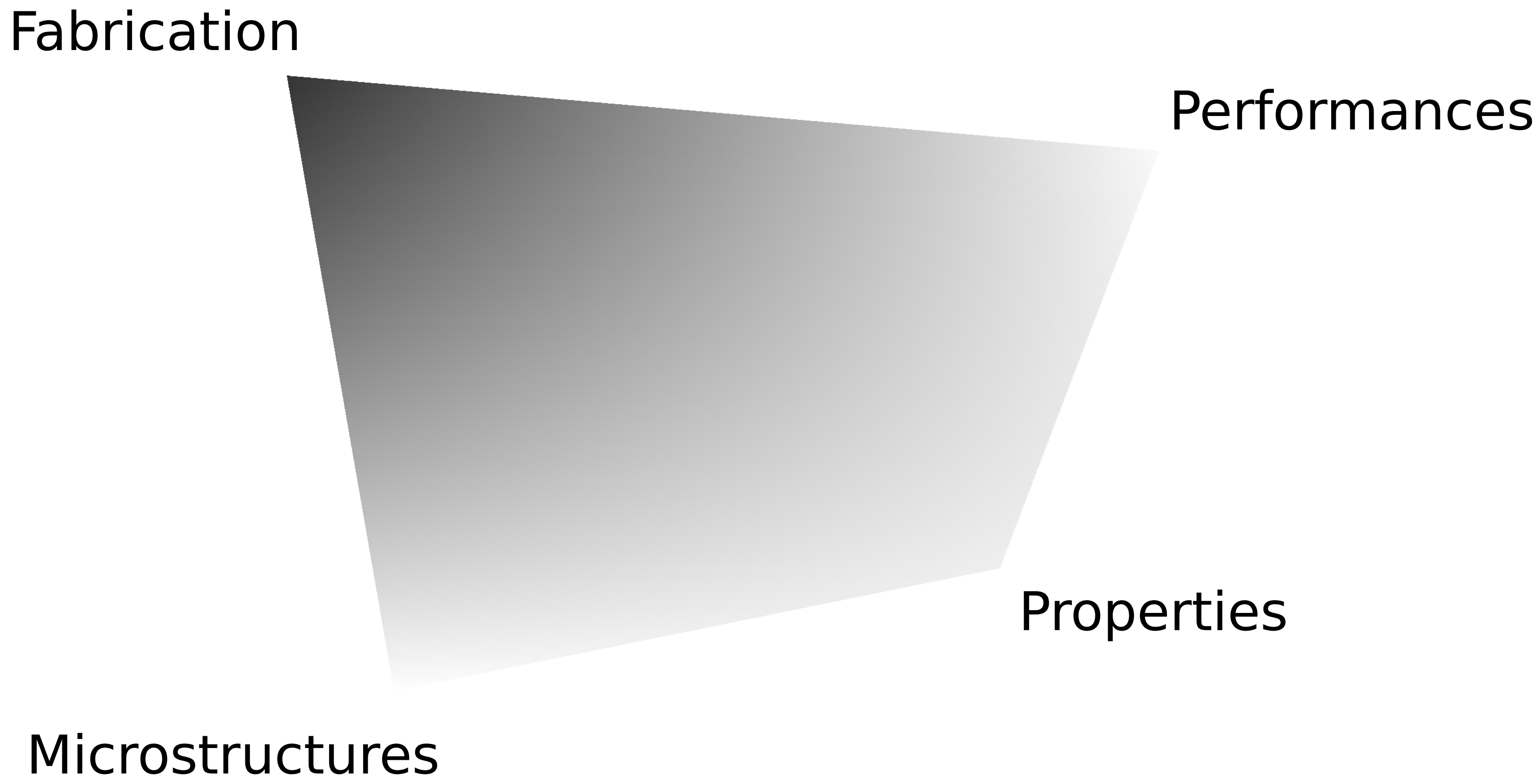
True material, in conditions of use:

- Polycrystal,
- Coherent assemblage of individual grains.

Minerals (olivine)
Ando et al, Nature, 2007



Design of industrial materials



Qualitative approach:

- Describe grain structures, structural phases,
- Describe phase and grain boundaries,
- Analysis using optical microscopy and other tools.

Quantitative approach:

- Grain sizes, aspect ratio, domain sizes, connectivity, etc.
- Quantitative measurements.

Modern quantitative approach:

- Probability calculations,
- Crystal orientations,
- Interfaces analysis,
- Calculation of macroscopic properties based on microstructures.

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Vocabulary

Texture (wikipedia):

- In crystallography and materials science: distribution of crystallographic orientations of a polycrystalline sample
- In geology: physical appearance or character of a rock, such as grain size, shape, arrangement, and other properties, at both the visible and microscopic scale.

Fabrics

- In geology: spatial and geometric configuration of all the elements that make up a rock

Microstructures

- In materials sciences: similar to what geologists call a texture...

Why study textures?

Texture is important in materials science

- To optimize performances
- Because of their (positive or negative) effects on material behavior

Application examples

- Turbines
- Jet engines (titanium or aluminum alloys)
- Nuclear material confinement (zircalloy)
- etc

Fabrication processes can generate texture. They can also be used to optimize textures.

It is quite difficult to predict texture evolution and the associated materials properties.

Texture and materials properties

Crystals have anisotropy in their physical properties.

A material with a sufficient number of randomly orientated crystallites will be isotropic.

Most processes for material fabrication do induce non-random orientations

→ most materials have anisotropic physical properties,

→ those properties depend on crystal properties AND microstructures.

Anisotropy can be good, you can benefit from it in material design.

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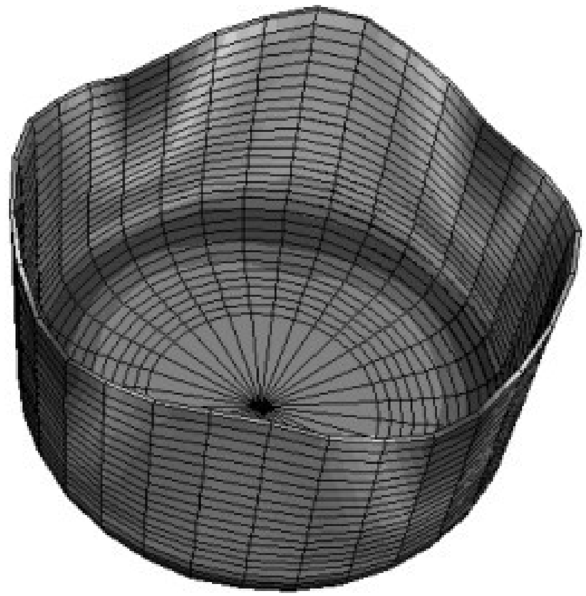
Example: making a beverage can

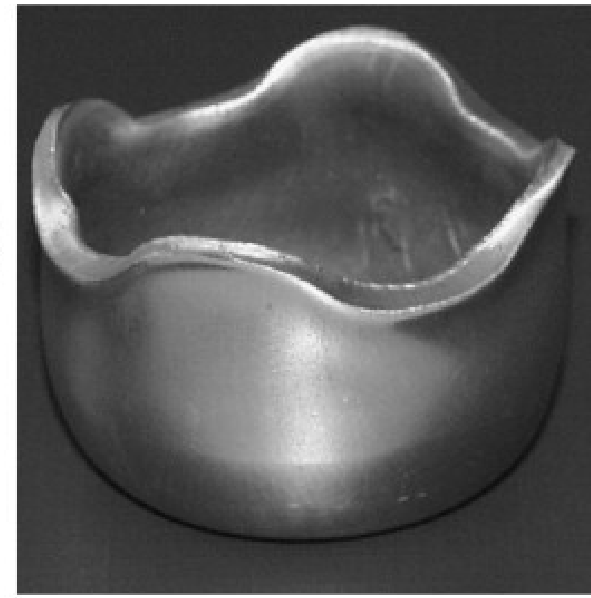
Making of a aluminum can

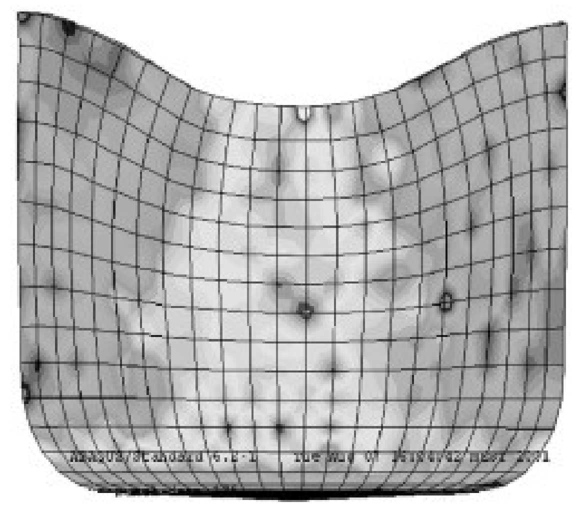
- Left: simulation of a cup drawing test with aluminium The gray scale indicates the sheet thickness.
- Right: experimental result.
- Bottom: local orientation changes during drawing.

Texture generates anisotropy

Pb because on the decreasing sheet thickness







Raabe and Roters, *International Journal of Plasticity* 2004, 20, 339-361

Course outline

1) Grain orientation: mathematical representation using Euler angles, rotation matrices, and graphical representation

2) Orientations in a polycrystal: mathematical description, experimental measurements, and graphical representation

3) Polycrystalline properties calculations: an example on elasticity

4) Underlying plasticity mechanisms: slip systems and grain rotations

5) Microstructure modeling

6) Hexagonal-closed-packed structure

7) Overview of typical textures in metals

Readings

U.F. Kocks, C.N. Tomé, H.R. Wenk, *Texture and Anisotropy*, Cambridge University Press, 1998 (66 €)

H.J. Bunge, *Texture Analysis in Material Science*, Butterworths, 1982 (out of press)

O. Engler, V. Randle, *Introduction to texture analysis*, CRC Press, 2009 (110 €)

Anthony Rollett classes at Carnegie Mellon University:
http://rollett.org/anthony/

MTeX program for plotting textures (and many other things)
http://code.google.com/p/mtex

Software for polycrystalline data modeling
http://maud.radiographema.eu/