MSE-651

Crystallography of structural phase transformations

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Cursus	Sem.	Type
Materials Science and Engineering		Obl.

Language of teaching	English
Credits	1
Session	
Exam	Written
Workload	30h
Hours	**14**
Courses	14
Number of positions	**20**

Frequency

Every year

Summary

The microstructure of many alloys and ceramics are constituted of very fine intricate domains (variants) created by diffusive or displacive phase transformations. The course introduces the crystallographic tools required to define, calculate and predict the different configurations of variants.

Content

Many alloys, ceramics and nanomaterials are constituted of a fine microstructure created by structural phase transformations: nano-precipitates in aluminium or other alloys, laths of martensitic steels, basket-weave morphologies in titanium or zirconium alloys, twinned martensite in shape memory alloys, oriented domains in ferroelectrics, multiple twins in some metallic or silicon nanowires etc. The small size and complex intricacy of the domains give to the materials their unique mechanical and physical properties. A branch of materials science aims at improving these properties by studying the influence of some element additions and some modifications of elaboration process parameters. For these studies, a good understanding of the formation of the crystallographic domains is required: How can the domains be mathematically defined and computed? Why do they adopt such complex fine morphologies? Is it possible to extract information on the parent phase from a completely transformed material?

The aim of the course is to give the main elements of response:

- The course will start by a global overview of the different microstructures resulting from a phase transformation in its broad meaning; which includes precipitation, order-disorder, twinning etc.
- Simple notions of crystallography will be recalled: The crystal systems, the point and space groups, and the notions of holohedry will be shortly explained (or reminded).
- Matrix calculations in direct and reciprocal space will be explained: structure, metric, correspondence and other transformation matrices will be detailed. The notion of coincidence site latice (CSL) and special grain boundries will be treated.
- The geometrical notions of global/local symmetries and the related algebraic concepts of groups and actions of groups will be introduced with simple geometric examples. It will be shown that a generalized structure derived from groups, called groupoid, can catch the fascinating complexity of the variants.
- Some characteristics such as hysteresis, reversibility, transformation plasticity will be considered in direct link with some crystallographic properties such as group/subgroup relation, lattice compatibilities etc.
- These theoretical concepts will be applied to specific materials (precipitation in aluminium, martensite in steels, multiple twinning in copper) correlated to industrial problems. It will be shown how groupoids can be used to reconstruct the prior parent grains and quantify variant selection mechanisms.
- Finally, brief examples will be taken from literature to show that groupoids are well adapted to treat many symmetry-related problems in physics, chemistry and biology.

This course is intended for students or researchers in materials science. Chemists and biologists working on problems involving symmetries can also be interested in the general concepts.

Keywords

Symmetries, variants, domains, phase transformations/transitions, coordinate transformation matrices, correspondence matrices, group theory, groupoids.

Learning Prerequisites

Recommended courses

The course does not require specific knowledge, except a basic background on linear algebra.

Resources

Websites

- https://www.researchgate.net/profile/Cyril_Cayron