Atomistic-continuum Modelling of Defects in Crystal Structures

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The course concerns the modeling of various crystal defects observed in: semiconductor structures, metals and hetero-structures. It concerns extended defects like dislocations, stacking faults, low-angle grain boundaries and the interfacial zones formed during the crystal grown on foreign substrates, e.g. during the growth of wurtzite- and copper-type structures on sapphire. The recent methods of atomistic reconstruction of crystal defects together with the analysis of HRTEM images of defects observed in the nano-scale are discussed. The multi-scale modeling from the viewpoint of the macro-continuum approach as the finite element method (FEM) is found to be, via atomistic modeling, to the computational problems connected with the modeling the optoelectronic properties by the use of the resultant electric potential shift induced by piezoelectric effect.

Main topics:

1. Tensor calculus with elements of crystallography.
2. Extraction of distortion tensor fields from HRTEM images.
3. Mathematical theory of dislocations vs. finite deformation theory.
4. The atomistic reconstruction and modeling of crystal defects.
5. The quantum walls and dots on HRTEM images.
6. FE modeling of residual stresses.
7. FE modeling of the diffusion of chemical elements and point defects in semi-conductor crystals.
8. FE modeling of piezoelectric fields in chemically inhomogeneous crystals:
   - the effect of piezoelectric shift on optoelectronic properties of quantum dots,
   - the effect of dislocations on the stress and electric field distribution.

The total number of lecture hours: 20, laboratory exercises: 20 hours, self-teaching: 60, direct tutoring and consultations: 30 hours.

ECTS Points: 5