Bachelor /Master /Mini thesis

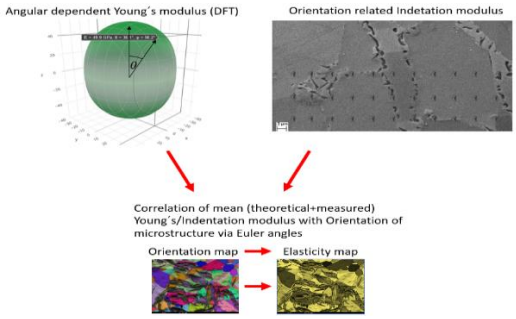
Correlation of the DFT-based Young's modulus calculation with orientation-dependent indentation moduli to determine a total elastic characteristic

Institute for Physical Metallurgy and Materials Physics

RWTH Aachen University

28. May 2021

Motivation:



In the field of material characterisation, new material systems are constantly being investigated, which are becoming more and more relevant and have to meet increasingly complex requirement profiles. Hence, the physical properties of intermetallic systems like Sm-Co and Fe-Ta are being studied at the IMM.

In the context of computational materials science, ab initio DFT (density functional theory) calculations enable the prediction of material behaviour based on quantum mechanical principles. In this process, the electronic structure is evaluated with a potential, that consists of the elementary composition or the structure of the system and interelectronic interactions and acts on the electrons of the system. These calculations result, for example, in material system-specific quantities, such as elastic constants. From these, among other things, the Young's modulus can be determined.

Combining EBSD measurements and nanoindentation tests, an orientation-dependent indentation modulus can be determined for the material systems. By correlating this parameter with the Young's moduli resulting from the DFT simulations, the overall elastic behaviour of the material system can be derived as a function of the microstructure orientation, from which an orientation-dependent elasticity distribution can finally be created.

Task:

Determination of elastic constants by DFT simulations and EBSD or indentation measurements in order to determine material system-specific parameters.

What we offer:

- Experience in combining simulative work and material science analysis methodology
- Collaboration with a young, motivated team.

The ideal candidates have:

- A high level of motivation for familiarisation with DFT simulation.
- Interest in generation, processing, preparation and measurement of alloy systems.
- Programming skills (Python/Matlab, shell script).
- A technical, physical or mathematical background with corresponding interests and skills.

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