A2 Ab initio Thermodynamics and Kinetics

Calculation of free energies, stacking fault and grain boundary energies at evaluated temperatures

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Motivation

- Ab initio Thermodynamics
  - Fundamental understanding of materials properties
  - Thermodynamic modelling → A3
- Stacking fault (SF) energies calculations
  - Deformation mechanisms / exp. phenomena
  - Chemical trends, e.g. carbon → A5, A7, B1
- Grain boundaries
  - Twin boundaries → understanding from HR-TEM → C1
  - Obstacles for dislocations movement → A7, A10
- Kinetics, e.g. nanodiffusion near the SF
  - Understanding of TEM experiments→ C10

Methods

- Density functional theory (DFT)
  - Exact MT-orbitals method
  - Projected augmented waves (VASP code)
- Chemical / magnetic disorder
  - Special quasirandom structures (SQS)
  - Coherent potential approximation (CPA)
  - Disordered local moments (DLM) approximation
- Spin space averaging (SSA) method
  - (Generalized) stacking fault / twin energy
  - Explicit supercell approach
  - Axial next nearest neighbour Ising (ANNNI) model
- Kinetics / diffusion barriers
  - Nudged elastic band method

Results

- Influence of local magnetism on thermodynamic properties
- Influence of local magnetism on the GSFE surface in Fe
- Influence of nano-diffusion on the chemical trends of the SFE
- Shift of atomic layers on the twin boundary: local magnetism

Impact

- Impact for the SFB:
  - Important contribution to the multi-scale simulations of deformation mechanisms
  - Understanding of experimental results such as the behaviour of twin boundaries
- Impact for the (worldwide) scientific Community:
  - New methodology (SSA) for the atomic forces calculation at evaluated magnetic temperatures
  - The influence of local effects (chemical composition, pressure, magnetism) on the SFE