**A2 Ab initio Thermodynamics and Kinetics**

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

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**Content**

- Ab initio study of selected, experimentally observed key phenomena in Fe-Mn-Al-C system
- Ab initio simulations of extended defects and temperature dependences of relevant parameters
- Dislocations simulations
- Further thermodynamic methodology development
- Kinetic processes modelling

**Methods**

- Density functional theory
- Exact MT-orbitals method
- Projected augmented waves (VASP code)
- Chemical / magnetic disorder
- SQS, Cluster-Expansion
- DLM, SSA
- Dislocations: Lattice Green’s function
- Kinetics: Kinetic Monte-Carlo

**Goals of the 3rd phase**

- Obtain an ab initio understanding of thermodynamics and kinetics of processes induced by boundary surfaces:
  - Phase stability near grain boundaries
  - Phase stability on the phase boundaries crucial for microstructure formation
  - Further thermodynamic methodology development
  - Explicit simulations of dislocation properties and their splitting

**Goals/Impact**

- Thermodynamic description of bulk phases: phase transformations, alloying, vacancies, κ-carbide
- Stacking faults and dislocations: energy barriers, atomic structure of dislocation cores, Peierls barrier
- Grain boundaries: Mn-induced ferrite embrittlement
- Phase boundaries: phase stability in the vicinity of αγ boundary, boundary segregation, misfit-dislocations

**Input**

**General:** gaining the crucial parameters (exp. difficult to access) required for atomic level understanding of material properties

- A1: Structure and local chemistry on the κ-γ boundary
- A7: α-γ boundary
- C1: Atomic positions on twin, grain, and phase boundaries
- C6: Role of Mn on the grain boundary embrittlement in ferrite

**Output**

- A3: TD stability of κ-phase
- A7: α-γ boundary
- A8: Enthalpies, GB-energies, T-depend. elast. constants,
- A9: T-dependence for key parameters of H-embrittlement
- A10: Spatial atomic rearrangements in dislocation core
- C1: Atomic positions
- C3, A10: Structure of α-γ and κ-γ boundaries
- C6: Role of Mn in grain boundary embrittlement in ferrite
- C8: APB energy of κ-carbide
- T4: Boundaries

**Work packages**

**Lattice Green’s Function approach for key parameters of dislocations**

**Figure from:** http://dtrinkle.matse.illinois.edu