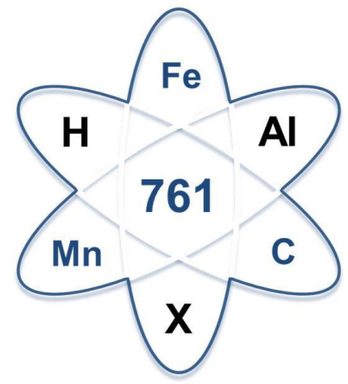
A2 *Ab initio* Thermodynamics and Kinetics

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



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Goals of the 3rd phase

Content

I II

- *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

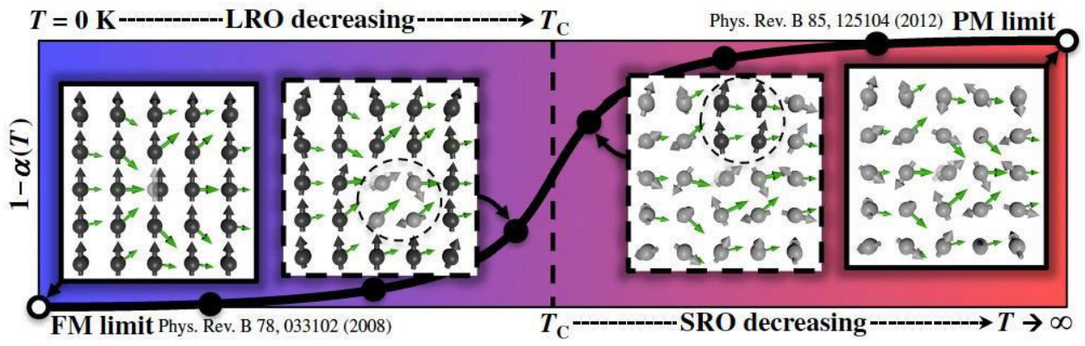
Methods

- 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

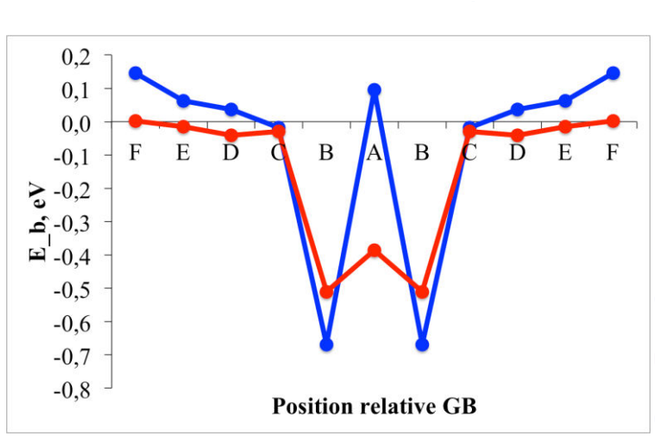
Input

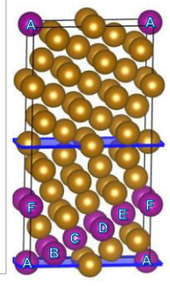
General: gaining the crucial parameters (exp. difficult to access) required for atomic level understanding of material properties

→**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

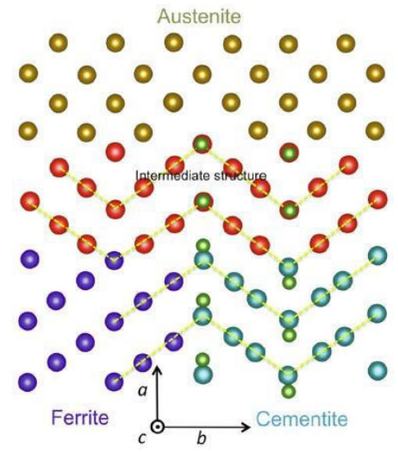


Recently developed methodology to describe the temperature dependent magnon-phonon coupling

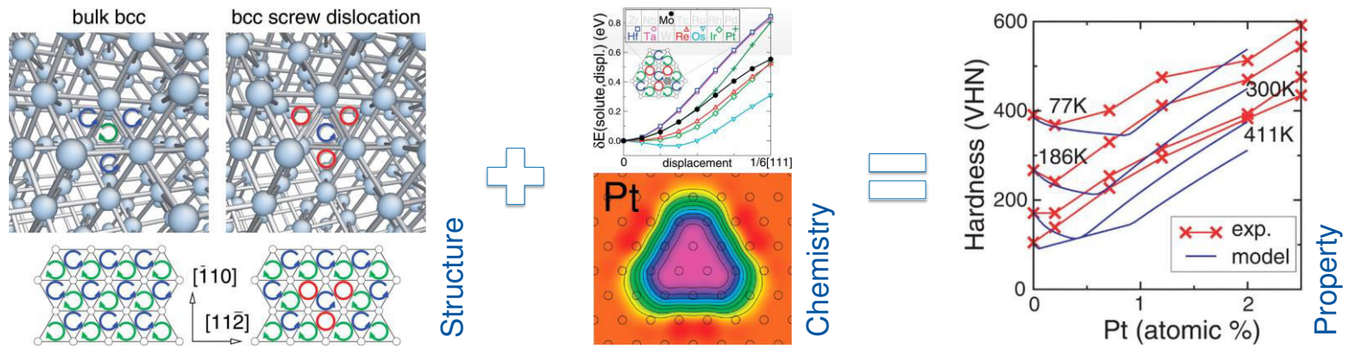




Energy of Mn atom in the vicinity of Σ5 (013) grain boundary in bcc Fe



New concept for ferrite-ausenite boundary surface



Lattice Green's Function approach for key parameters of dislocations

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

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

Goals/Impact

- 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

Work packages

- 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 α|γ boundary, boundary segregation, misfit-dislocations*

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