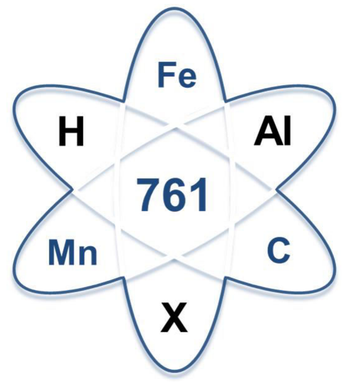
A3 Thermodynamics

Thermodynamics of systems based on Fe-Mn-C



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Goals 3rd period

Content

- Thermodynamic modelling of dual- and multiphase steels with high fraction of κ-phase and ferritic-austenitic medium Mn steels
- Order-disorder modelling of the κ-phase
- Prediction of the austenite stability of single- and multiphase (α+γ, γ+κ) steels

II

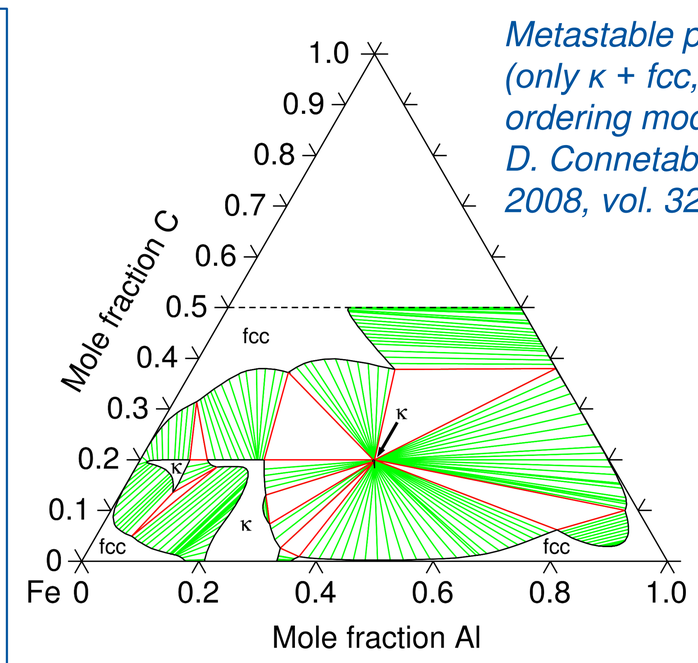
I

Methods

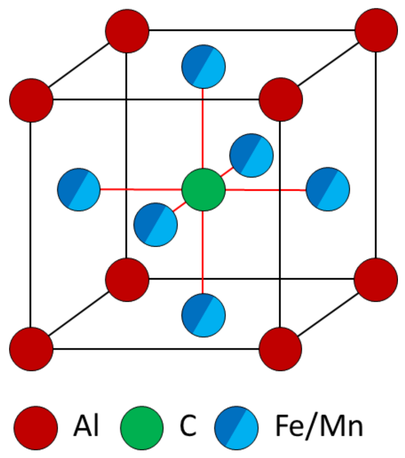
- Thermodynamic evaluation using the Calphad method based on experimental phase diagram data, thermodynamic data and *ab initio* calculations of the phase stabilities
- Evaluation of T_0-lines for the calculation of martensite start temperatures
- Diffusion simulations with DICTRA

Input

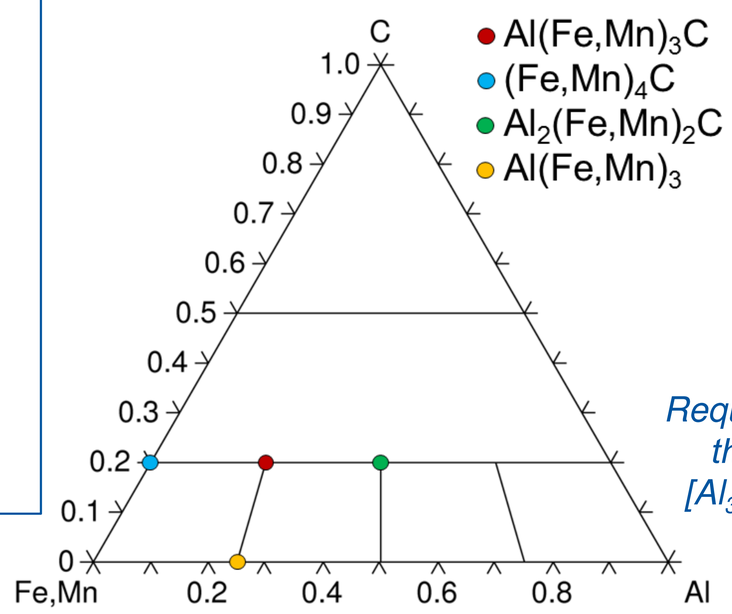
- Formation and defect energies for the κ-phase → **A1**
- Heat capacities, SFE, κ-phase → **A2**
- Experimental liquidus, solidus and distribution coefficients, liquid solubilities of H,N → **B1**
- Experimental microstructure data → **B6**
- Experimental SFE → **C1**
- Stability of the κ-phase → **C3**
- Phase compositions and volume fractions → **C8**
- Experimental austenite stability → **C10**



Metastable phase diagram (only κ + fcc, 600°C) of the ordering modelling from D. Connetable et al: Calphad, 2008, vol. 32, pp. 361–370.



Crystal structure of the κ-phase



Required model compounds for the modelling of the κ-phase [$Al_3(Fe,Mn)C$, $Al_2(Fe,Mn)_2$ and $Al_3(Fe,Mn)$ not shown]

Output

- SFE, κ-phase → **A2**
- SFE, deformation mechanisms, martensite formation → **A5**
- SFE → **A7,B2**
- Peritectic solidification data → **A8**
- Thermodynamic model data for dislocation modelling → **A10**
- Process parameters for solidification → **B1**
- Phase stability and phase formation → **B4**
- Diffusion simulations → **B6**
- SFE, phase equilibria → **C1**
- Thermodynamic calculations → **T2,T3,T4**

Goals/Impact

- Model of the κ-Phase with high accuracy for (phase field) simulations of the κ-phase formation
- Provision of a reliable and tested thermodynamic database for manganese steels (Fe-Mn-Al-C) with particular emphasis on multiphase steels
- Prediction of the austenite stability → $M_s(\varepsilon)$, $M_s(\alpha)$, κ-phase

Work program

WP 1: Thermodynamic modelling
- Model development κ-phase
- Modelling in Fe-Al-C
- Modelling in Mn-Al-C
- Modelling in Fe-Mn-Al-C
- Gas solubility in liquid
- Thermodynamic database

WP 2: Austenite stability
- Modelling of the hcp-phase (ε)
- Calculation of $M_s(\varepsilon)$ and SFE
- Modelling approach for $M_s(\alpha)$

WP 3: Diffusion simulation

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