Computational Materials Design

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Computational Phase Studies

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Ab-*initio* based study of κ-carbides in Fe-based alloys

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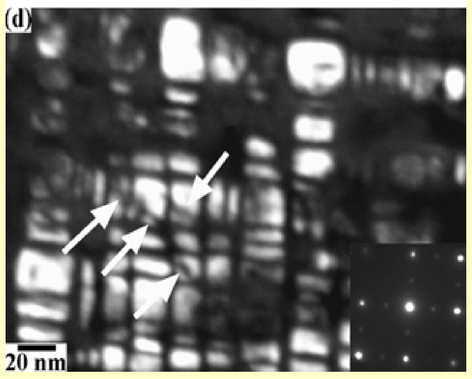
Motivation

- Fe-Mn-Al-C steels exhibit outstanding strength and ductility [1].
- Addition of Al promotes precipitation of nanosized κ–carbides which control mechanical properties in various ways, *e.g.*
  - Strain hardening in alloys [2].
  - Improvement in tensile ductility by specific heat treatment to form γ/κ lamellar microstructure via discontinuous precipitation [3].
- Dispersion of fine precipitates of carbides in the high-strength steels may increase the resistance of these steels to hydrogen embrittlement [4].

Aim

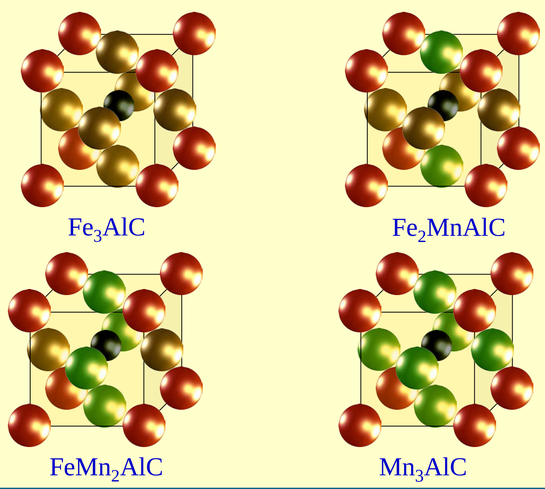
- Ab-*initio* study of κ-carbides as precipitates in austenitic Fe matrix.



Dark-field TEM image of the distribution of κ-carbides in a long annealed Fe-Mn-Al-C sample [2].

Structure and Composition

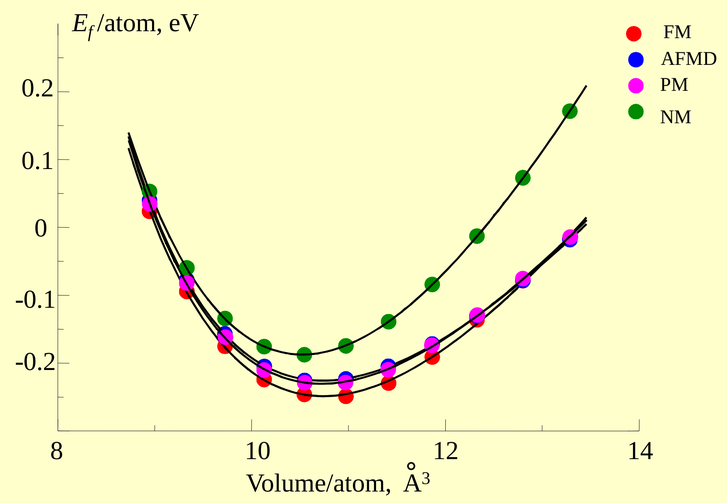
- Crystal structure of κ-carbide is $E2_1$.
- Al atoms sit at the corners of the cube, Fe atoms occupy the face center positions and C is in the octahedral position.
- Mn can replace Fe from its face centered position, eventually giving Mn_3AlC.
- Nominal composition is $(Fe,Mn)_3AlC$.
- APT measurements show deviations from stoichiometry.



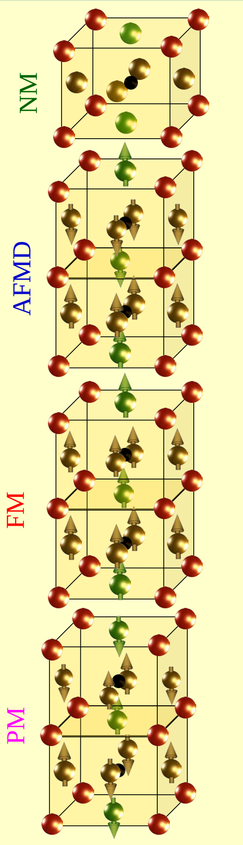
Fe_3AlC Fe_2MnAlC $FeMn_2AlC$ Mn_3AlC

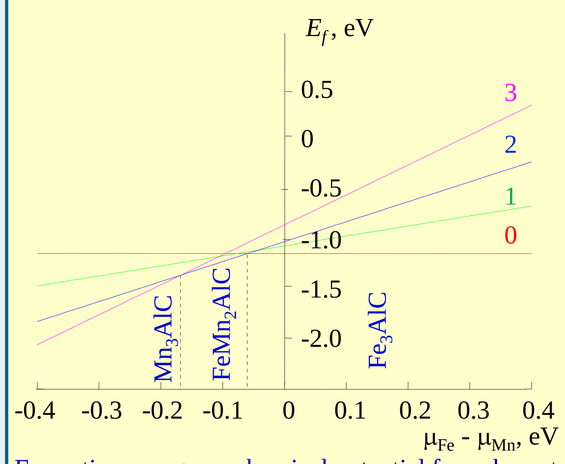
Results: Bulk κ-carbide

Formation energy: $E_f = E(Fe_{3-x}Mn_xAlC) - (3 - x)\,\mu_{Fe} - x\mu_{Mn} - \mu_{Al} - \mu_C$

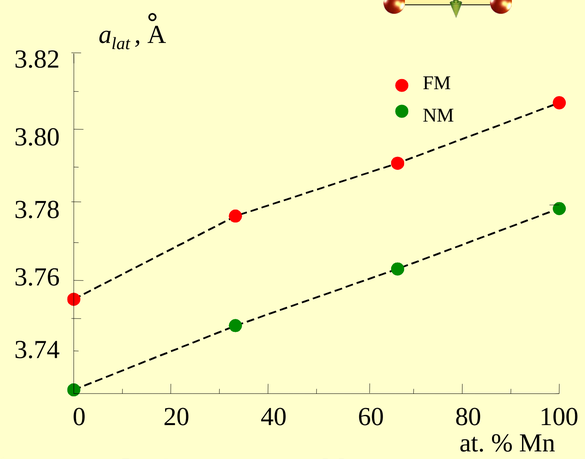


Formation energies vs volume for various magnetic phases of κ-carbide. Here, PM phase is constructed with the aid of special quasi random structure (SQS) scheme.





Formation energy vs chemical potential for coherent precipitates.



Lattice constant vs Mn concentration.

Observations:

- Ferromagnetic phase (FM) is most stable.
- Fe_3AlC is more abundant than Mn containing κ-carbides, as coherent precipitate.
- Lattice mismatch grows with increase in Mn concentration.

References

[1] G. Frommeyer and U. Bruex, Steel Res. Int. **77**, 627 (2006).
[2] I. Gutierrez-Urrutia and D. Raabe, Scripta Materialia **68,** 343 (2013).
[3] Y. Kimura, K. Handa, K. Hayashi and Y. Mishima, Intermetallics **12,** 607 (2004).
[4] J. Takahashi, K. Kawakami and T. Tarui, Scripta Mater. **67**, 213 (2012).

Acknowledgements

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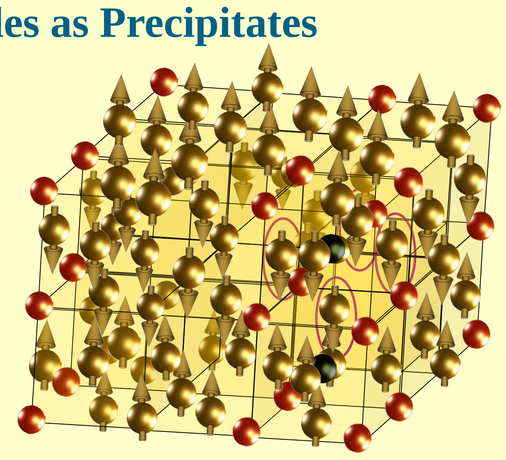
- Work has been performed in collaboration with SZMF.

Results: κ-carbides as Precipitates

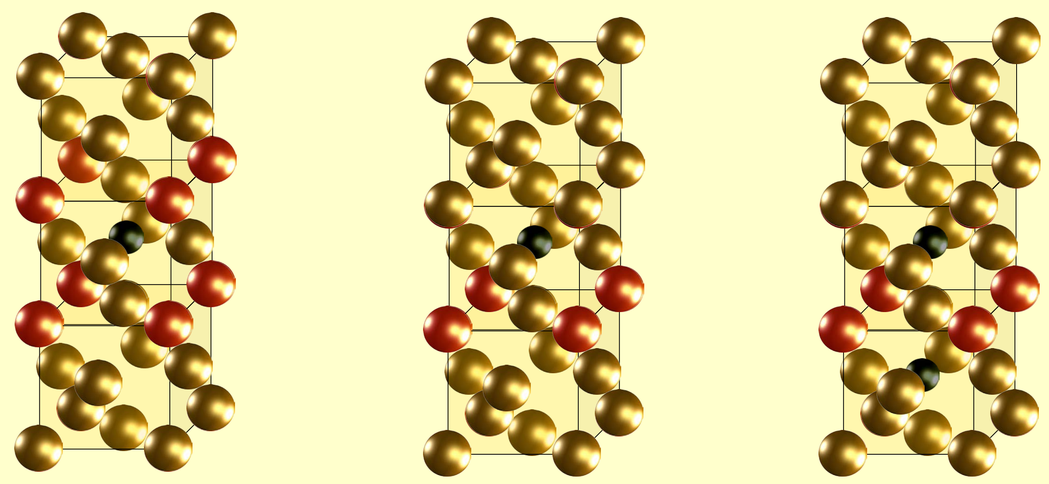


Columnar κ-carbide in AFMD Fe matrix.

Observations:

- AFMD order of Fe matrix influences the magnetic order of the columnar κ-carbide.

Results: Coherent Interface energy



A kind of interface AB kind of interface B kind of interface

$E^{interface} = (E_{tot} - E^{bulk\,Fe} - E^{bulk\,\kappa\text{-}carbide})/2$

$(E^{tot} - E^{bulk\,Fe}) = n_\kappa E_\kappa + 2E^{interface}$

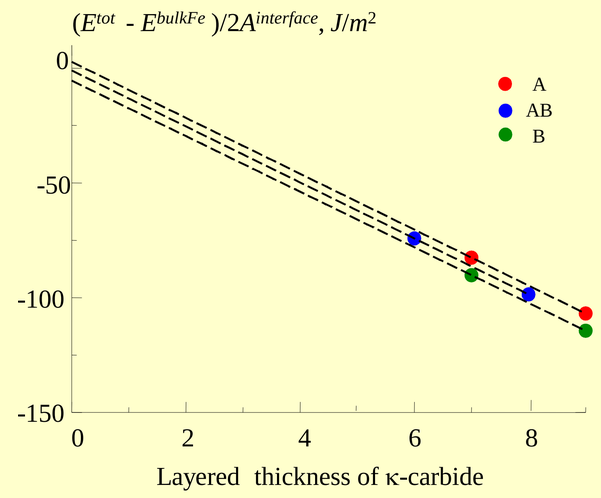
n_κ: Layered thickness of κ-carbide

Interface energy: $\gamma_{coh} = E^{interface}/A^{interface}$

γ_{coh} = 2.7 J/m^2 (A kind of interface)

γ_{coh} = -1.0 J/m^2 (AB kind of interface)

γ_{coh} = -5.4 J/m^2 (B kind of interface)



Interface energy vs thickness for 1x1x8 supercell of Fe and κ-carbide at constraint lattice constant of Fe.

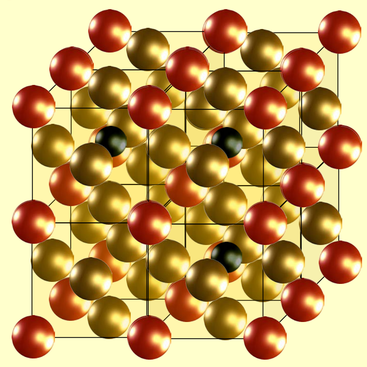
Observations:

- B kind of interface is energetically most favourable.
- Negative interface energies for AB and B kind of interfaces between κ-carbides and Fe matrix.
- Coherent interface energies computed, indicate towards spinodal decomposition which can be probably related to the experimental findings.

Results: Vacancies in κ-carbide

Vacancy formation energy: $E_F(Vacancy) = E(\kappa\ with\ vacancy) + \mu_C - E(bulk\ \kappa\text{–}carbide)$

Lattice constant (Å)	Vacancy formation energy (eV)
3.75 (of κ)	0.75
3.60 (Intermediate)	0.04
3.45 (of Fe)	-2.12



Vacancy at C-site in 2x2x2 SC

Observations:

- Increase in strain energy (by growing misfit) is compensated by lowering of vacancy formation energy.
- Explains deviation from stoichiometry as observed in experiments.

Outlook

- To explore the role played by κ-carbide precipitates in influencing the sensitivity of the host matrix to hydrogen embrittlement e.g. interplay of vacancies and hydrogen.
- Deeper understanding of the kinetics involved in the κ-carbide formation.