



20th DISCUSSION MEETING ON THERMODYNAMICS OF ALLOYS
20 - 24 September 2026
BLED - SLOVENIA

Stacking Fault Energy – Bridging the Gaps between DFT, Experiments and Thermodynamic Modelling

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Thermo-Calc Software



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About the Presenter

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Research interests: Modelling of thermodynamic properties, development of 3rd generation CALPHAD descriptions.

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Stacking Fault Energy in Fe-Mn steels

Context and motivation

- Fe-Mn based Twinning Induced Plasticity (TWIP) and Transformation Induced Plasticity (TRIP) steels offer exceptional strength-ductility balance.
- SFE has a central role in determining deformation mechanisms.
- Three challenges in accurately determining SFE in metastable Fcc alloys:
 1. Force balance assumption in experimental methods.
 2. Magnetic states considered in DFT calculations.
 3. Interfacial energy term in thermodynamic modelling.

Apparent SFE from Experimental methods

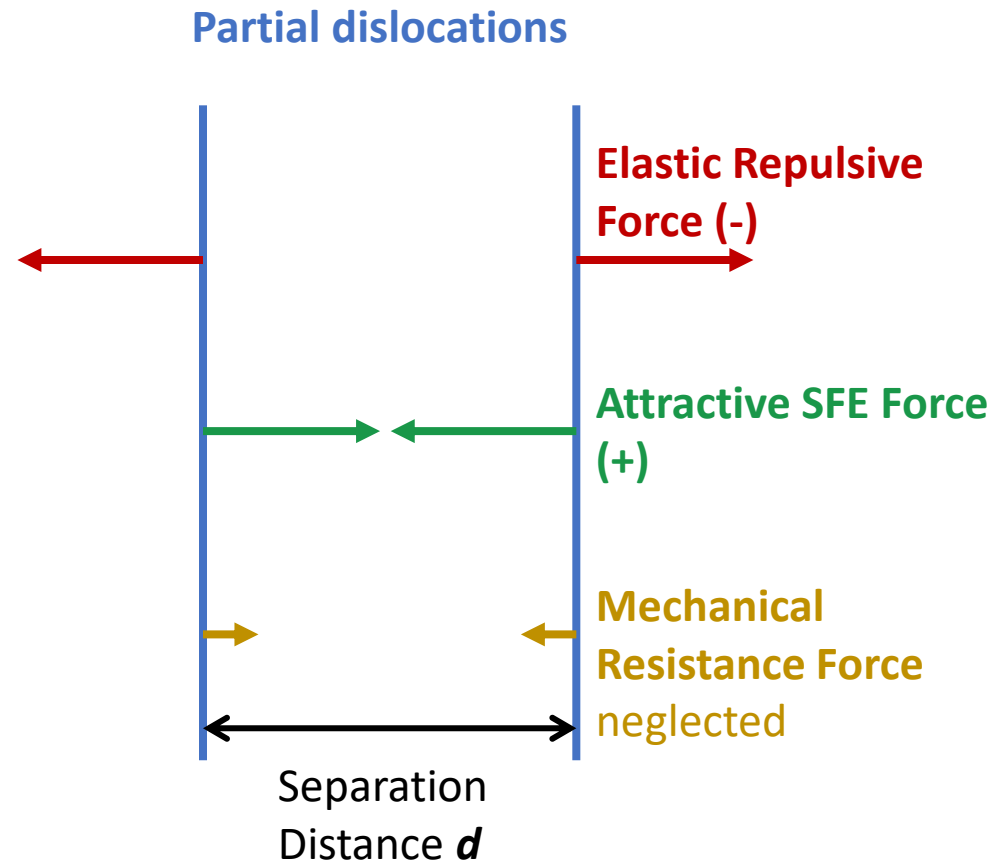
TEM: Measures distance between the leading/trailing partial dislocations.

XRD: Based on the shift and broadening of Bragg peaks.

Experimental SFE is apparent and always **positive** due to the assumed **elastic equilibrium** between the repulsive partial dislocation separation and attractive SFE.

Additional mechanical resistance to partial dislocation separation in alloys are **ignored**.

$$\text{SFE}^{\text{app}} = \frac{\mu b_p^2}{8\pi d} \frac{2-\nu}{1-\nu} \left(1 - \frac{2\nu \cos 2\beta}{2-\nu} \right)$$



DFT Intrinsic SFE

Generalized SFE surface

Explicit Stacking Fault created in austenite supercell.

Direct computation of generalized SFE surface.

Higher computational cost.

$$\text{SFE} = \frac{G^{\text{def}} - G^{\text{ideal}}}{A}$$

A = area of SF in the (111) plane

ANNI model

No explicit Stacking Fault in the simulation.

SFE computed from total energy differences between ideal bulk phases (Hcp vs Fcc).

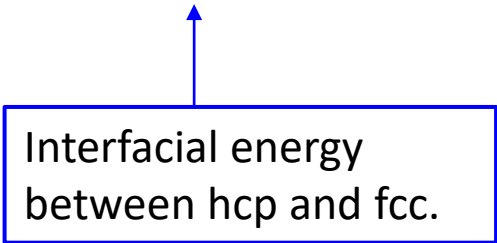
Computationally efficient.

$$\text{SFE} = \frac{2(G^{\text{Hcp}} - G^{\text{Fcc}})}{A}$$

ANNI = Axial Nearest Neighbour Ising

Thermodynamic calculations of SFE

SFE – Olson and Cohen equation

$$\text{SFE} = \frac{2(G^{\text{Hcp}} - G^{\text{Fcc}})}{A} + 2\sigma$$


Interfacial energy
between hcp and fcc.

- Interfacial energy cannot be measured directly.
- Common range: $\sigma \approx 5\text{-}35 \text{ mJ/m}^2$ – artificially large values to fit large positive experimental values.
- This masks the Gibbs energy contributions and explains why thermodynamic models consistently overestimate SFE.

A = area per mole in the (111) plane

Great scatter in SFE

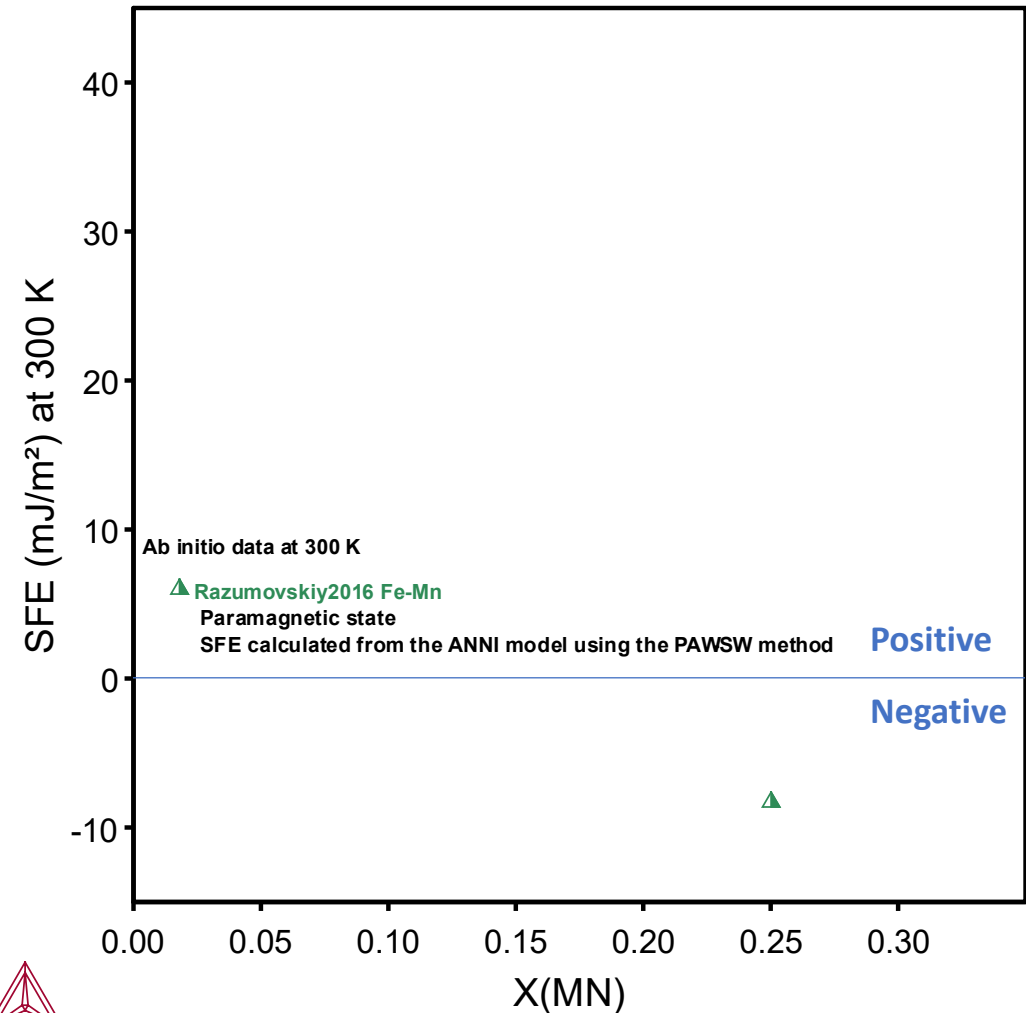
Comparison of previous studies at 300 K

Experiments

- Method
- Composition
- Grain size

Ab initio / DFT-based calculations

- Magnetic and temperature effects
- Paramagnetic

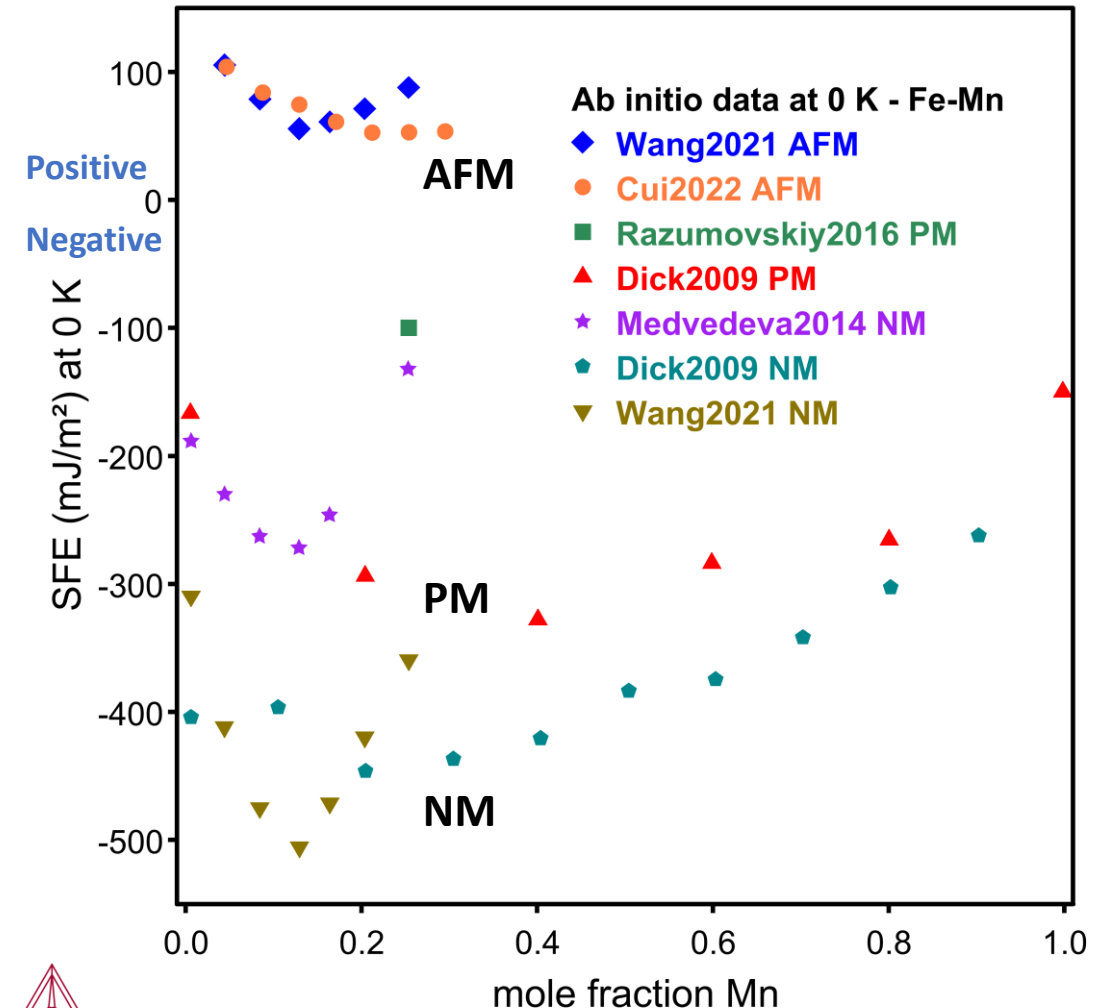


Great scatter in SFE

Comparison of previous studies at 0 K

Ab initio / DFT-based calculations

- SFE values span a wide range.
- Antiferromagnetic (AFM): Positive SFE.
- Paramagnetic (PM): Negative SFE
- Nonmagnetic (NM): Negative SFE.



Role of Magnetism

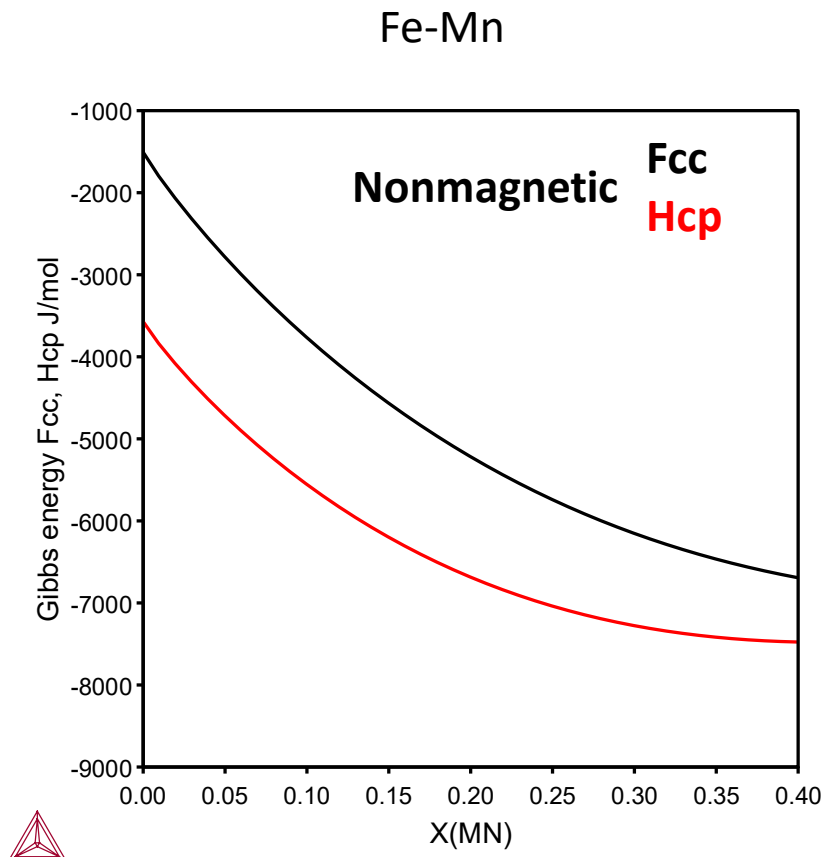
Phase Stability & SFE Connection

- Fe-Mn is **antiferromagnetic** at 0 K.
- Fe-Mn can be **paramagnetic or antiferromagnetic** at elevated temperatures depending on Mn content.

Experimental data on Fe-Mn alloys

- Mn stabilises AFM Fcc
– stabilises Fcc phase.
- Mn destabilises AFM Hcp
– destabilises Hcp phase.
- Phase stability directly governs SFE sign and magnitude

T_N Fcc
 T_N Hcp



Validation of negative SFE

From Apparent to Intrinsic SFE

$$\text{SFE} = \frac{2(G^{\text{Hcp}} - G^{\text{Fcc}})}{A} < 0$$

if Hcp is more stable than Fcc

Negative intrinsic SFE from experiments is possible if the assumed equilibrium **include additional resistance** to partial nucleation and propagation.

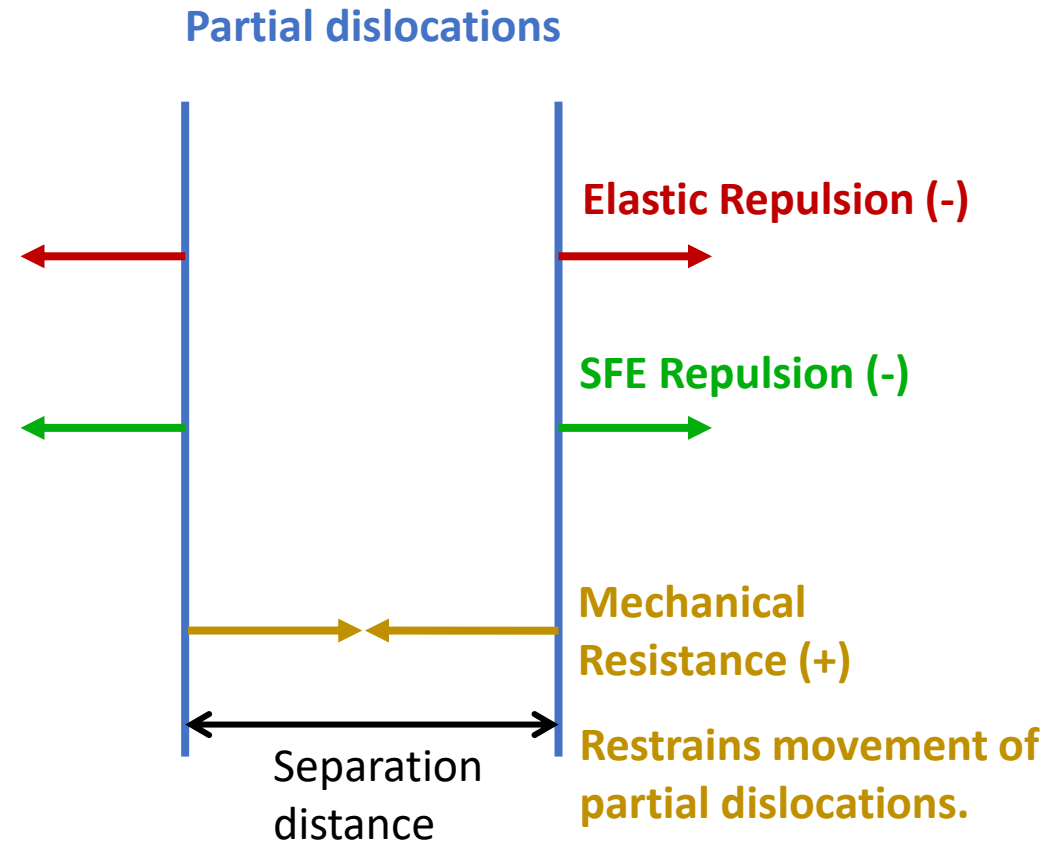
Deformation twinning related to formation of SFs

Critical Resolved Shear Stress (CRSS) for twinning can approximate this resistance:

$$\boxed{\text{Corrected}} \quad \text{SFE}_{\text{intrinsic}} = \boxed{\text{Apparent}} \quad \text{SFE}^{\text{App}} - b_p \left(\tau_{0,\text{twin}} + \frac{K_{\text{twin}}^{\text{HP}}}{\sqrt{D}} \right) \quad \boxed{\text{CRSS}}$$

b_p : Burgers vector of Shockley partials

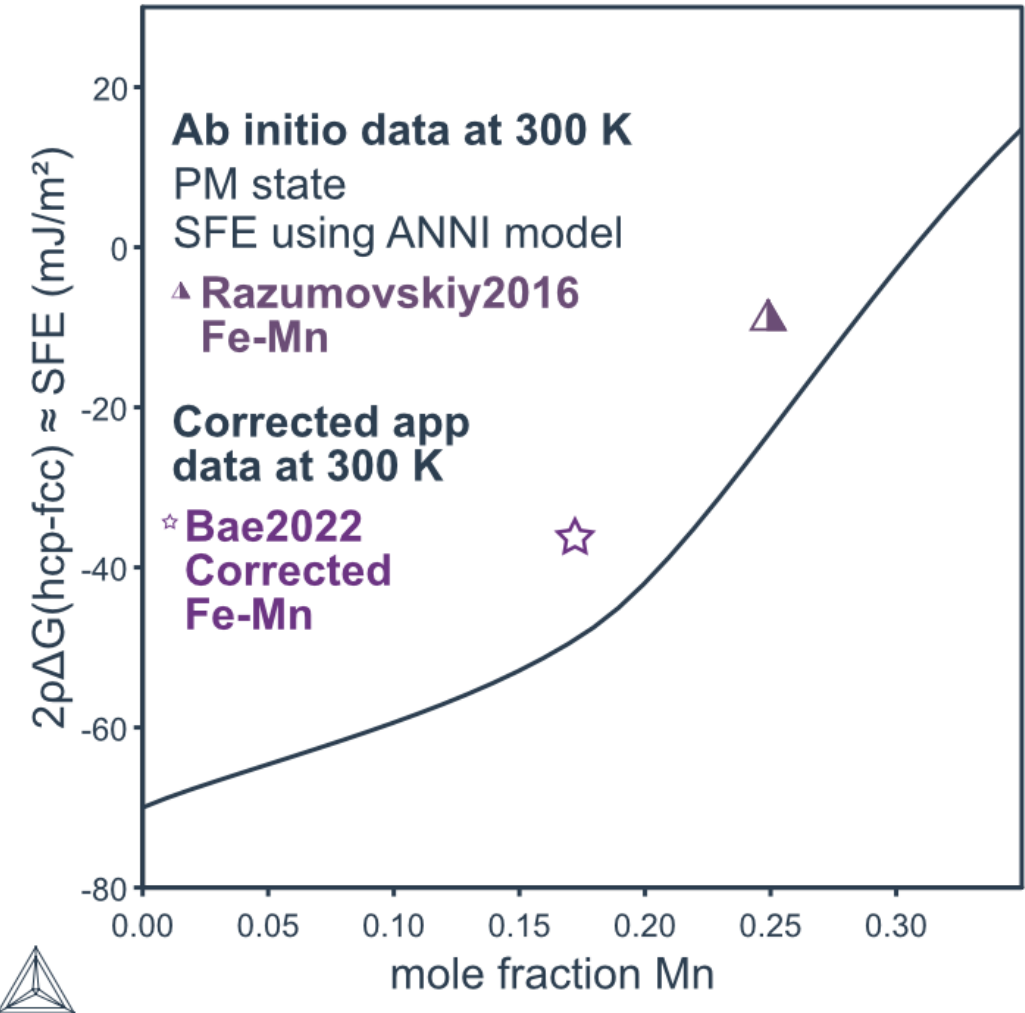
D = grain size





Summary and Conclusions

- **Revise the equilibrium assumption:** include resistance to twinning-partial nucleation and propagation.
- **Use physically grounded interfacial energies:** derive σ from DFT or neglect it rather than fitting to apparent experimental SFE.
- **Avoid fitting σ to apparent SFE:** it can mask Gibbs-energy contributions.
- **Include critical twinning stress** to bridge DFT, experiments, and thermodynamic modelling.



Fe-Mn 3rd generation Calphad description by Kaboli, K., & Bigdeli, S., 2025 at 300 K.



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Thank you for listening!

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