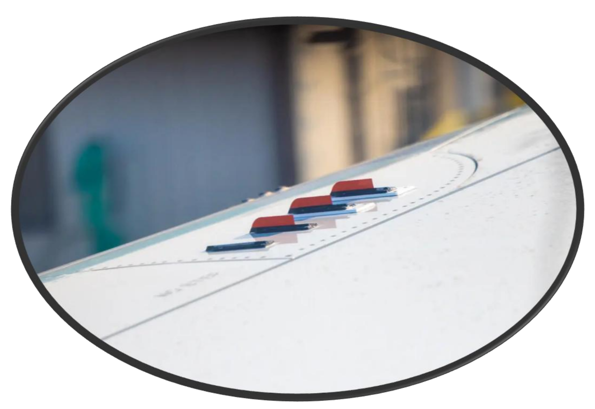
Atomic Scale Modeling of Microstructural Features and Defects in Shape Memory Alloys

Gabriel Plummer, Mikhail I. Mendelev, John W. Lawson
NASA Ames Research Center

Diverse SMA Applications at NASA

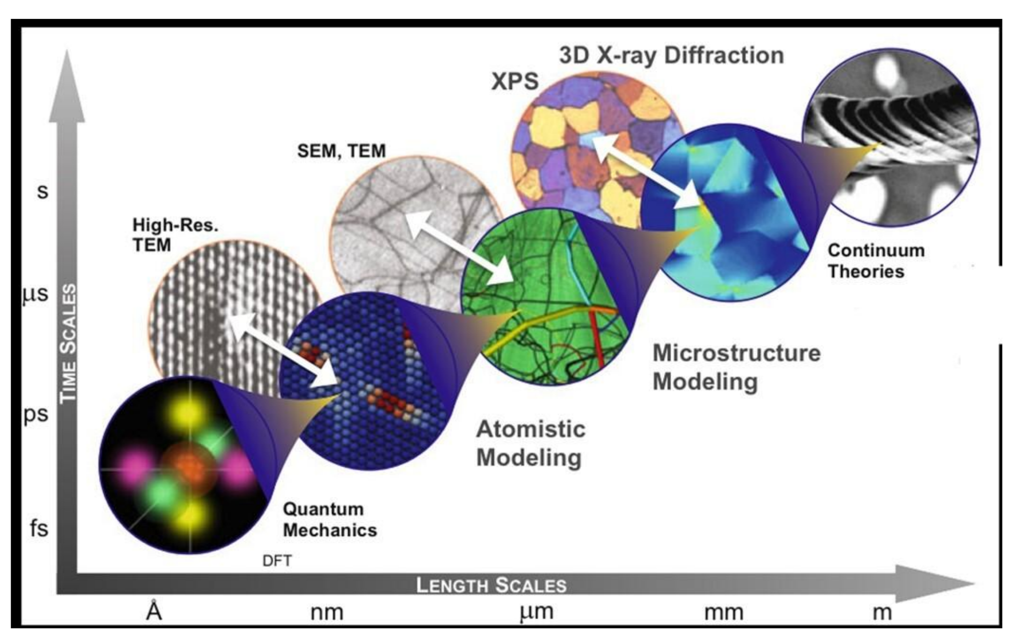
Actuators on aircraft: morphing airframes, vortex generators

Superelastic components for extreme environments: lunar rover tires, bearings



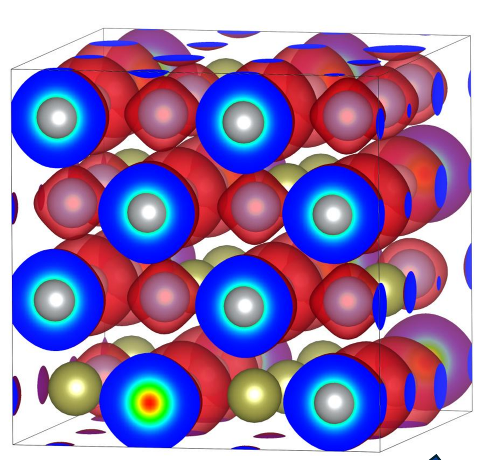
Wide-ranging property needs – computational techniques can be leveraged for accelerated alloy development

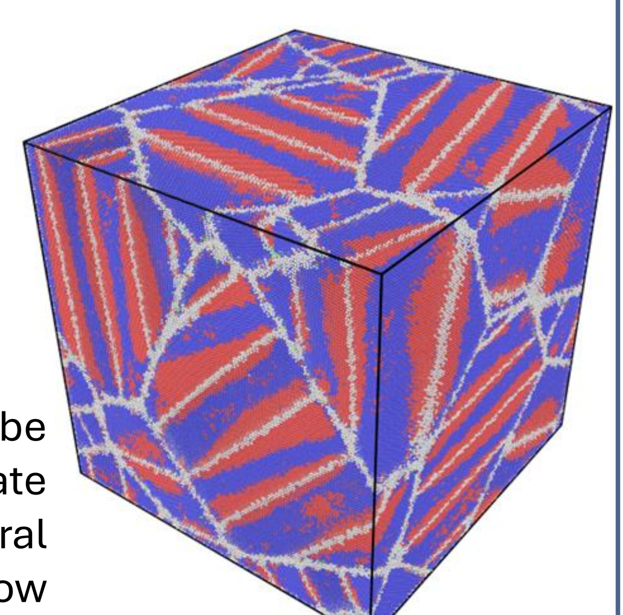
Atomistic Modeling Approach



Materials modeling is a multi-scale endeavor involving numerous different techniques. Continuum scale modeling is regularly applied to SMAs. Atomic scale modeling has lagged behind but has potential to be a powerful design tool.

Ab initio techniques invoke quantum mechanics and can be used to screen SMAs for favorable bulk properties.



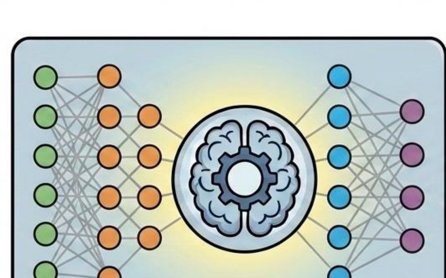


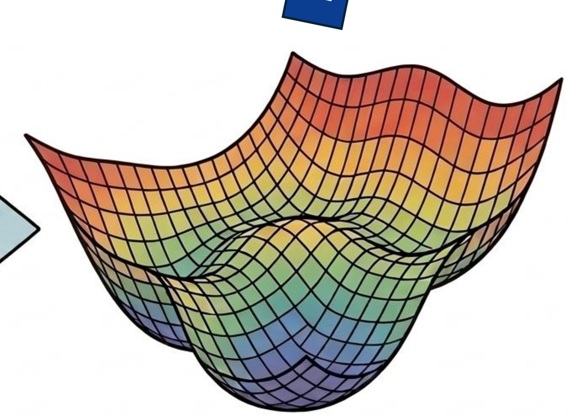
These models can be used to simulate complex microstructural features/defects and how they influence SMA properties.

Data in

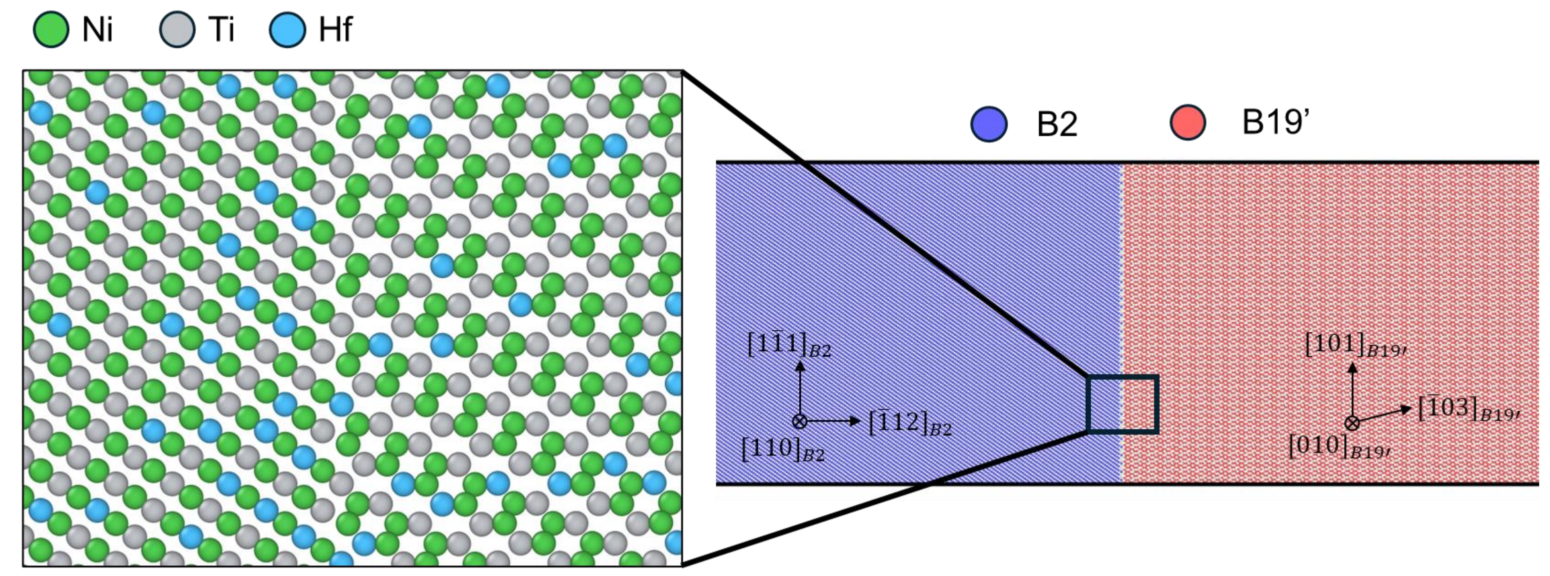
Model out

They are too expensive for larger systems, so we train cheaper machine learning or physics-based models.

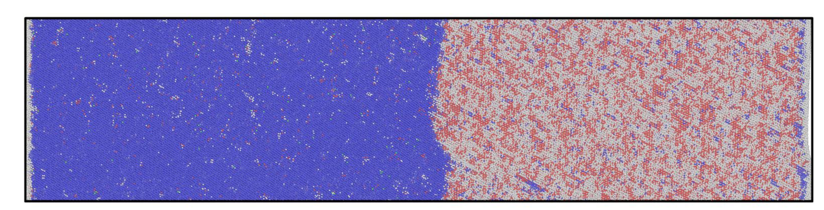




Austenite-Martensite Interface Kinetics



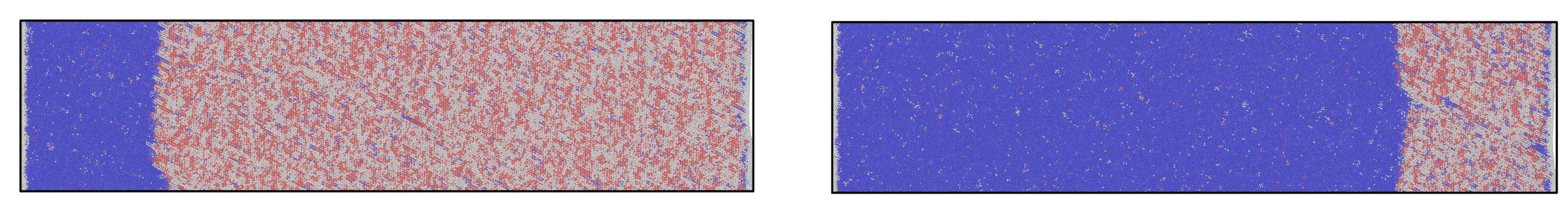
Interfaces with atomic scale detail can be constructed to investigate kinetic aspects of the martensitic transformation.

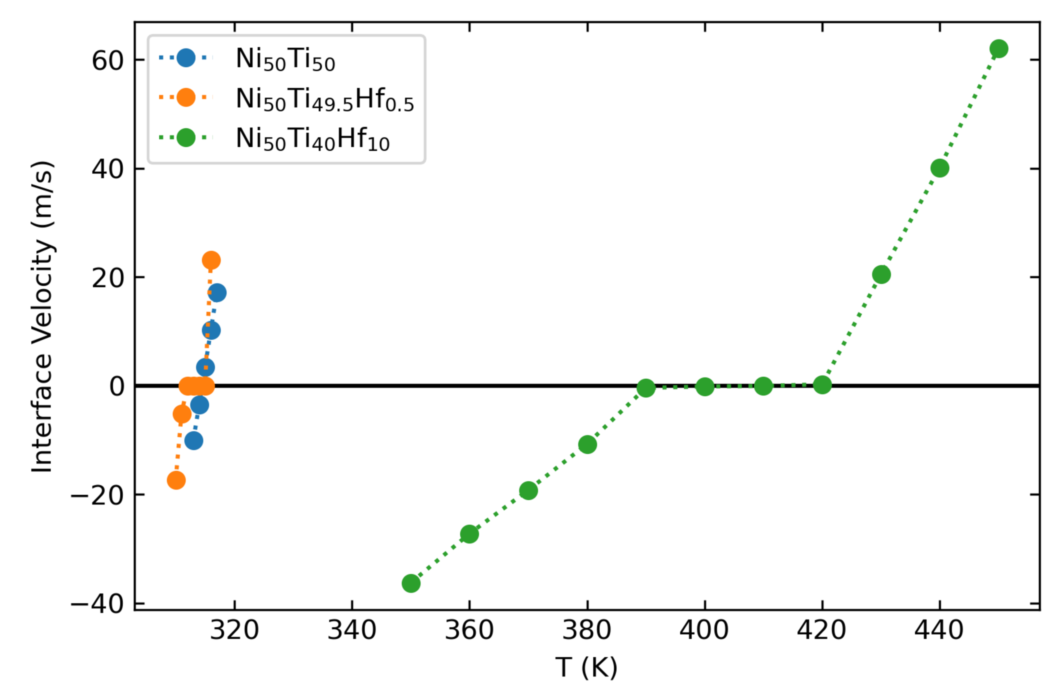


T < MTT

Growth of austenite or martensite phase depending on temperature

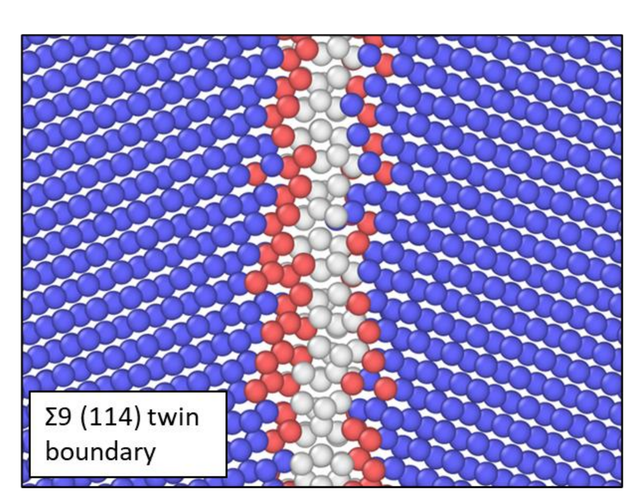
T > MTT

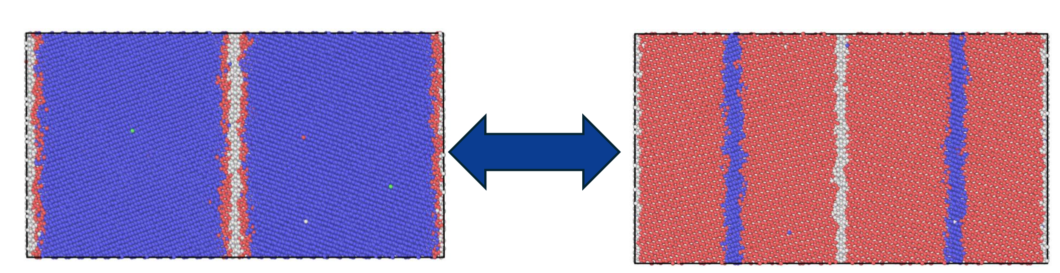




Interface velocity can be measured as a function of temperature. Some alloys exhibit sluggish kinetics close to the MTT due to frictional effects resulting from lattice distortions. This can be a contributing factor to hysteresis, likely becoming important in low temperature and high entropy SMAs.

Defects Promoting Transformations

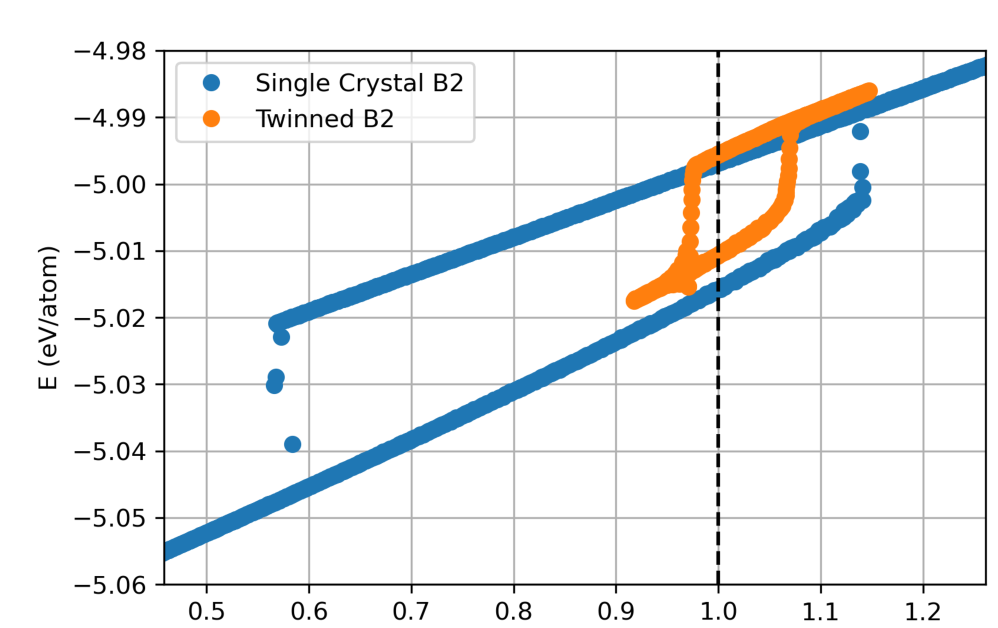




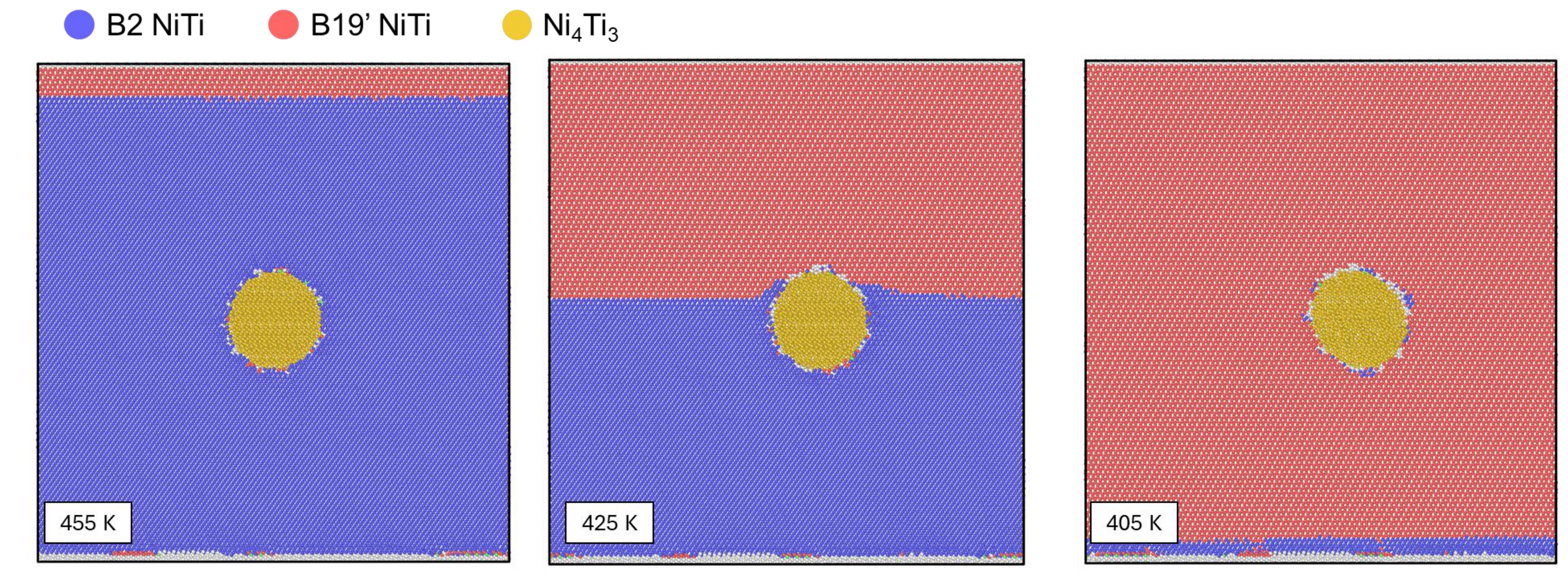
High temperature

Low temperature

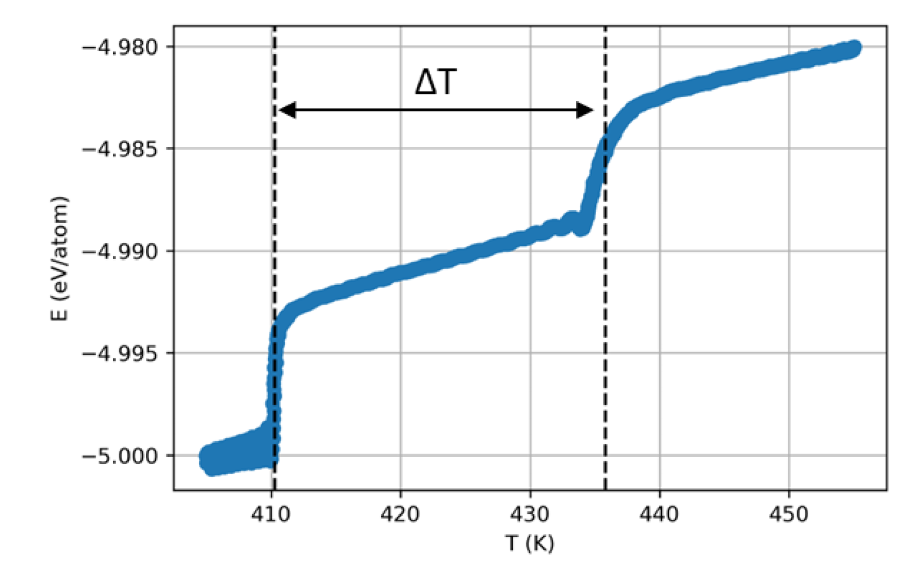
Specific defects can serve as preferential nucleation sites for martensite – for example, this twin boundary in NiTi forms a thin layer at its core. Such reductions to the nucleation barrier can significantly impact hysteresis, creating options for microstructural engineering.



Precipitate-Interface Interactions

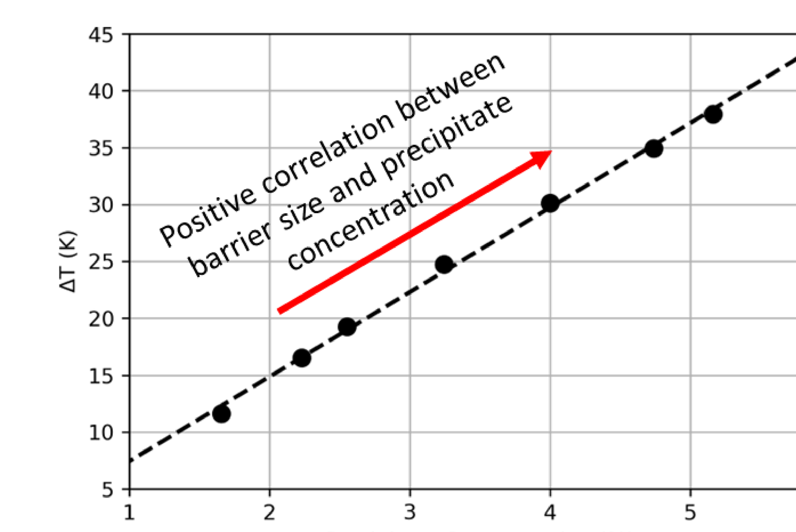


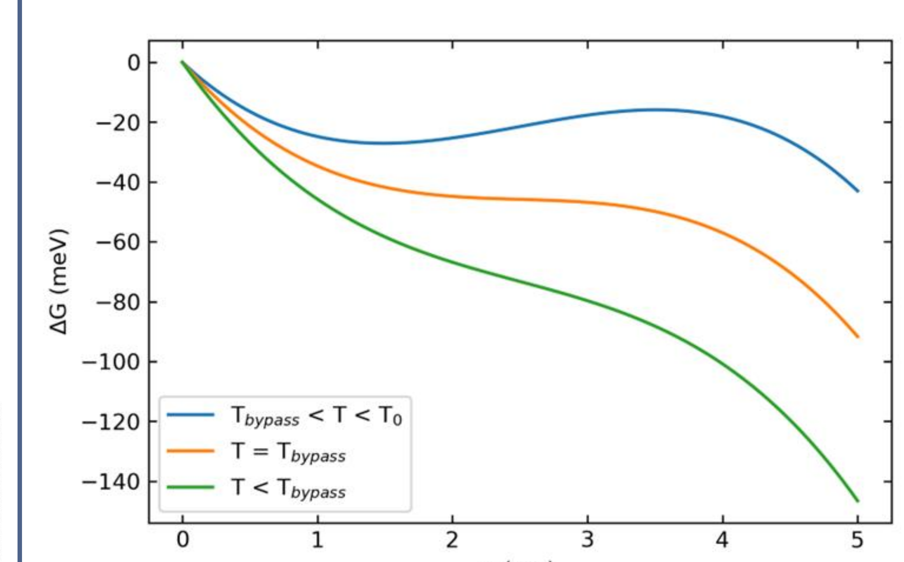
Precipitates provide an energetic barrier to interface motion



Non-transforming precipitates must be strained when the surrounding matrix transforms. This sets up a thermoelastic balance which governs progression of the phase transformation. We can measure this in simulations in the form of an undercooling required for interface propagation.

The measured undercooling increases with precipitate concentration as the thermoelastic balance shifts in the direction of elastic strain.





Such data derived from atomic scale simulations can be used to parametrize higher order models, e.g. mesoscale models like phase field which can capture microstructural evolution. This type of scale-bridging is a key use of atomic scale modeling.

For additional information on atomic scale modeling of SMAs, see the following:
- *Physical Review Materials* 6, 123601 (2022)
- *Journal of Physics: Condensed Matter* 35, 495404 (2023)
- *International Journal of Plasticity* 184, 104203 (2025)
- *JOM* 77, 2844-2851 (2025)
- *Scripta Materialia* 271, 117040 (2026)

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