Atomistic Simulations of Mn-based Magnetic Shape Memory Alloys

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Introduction

- Magnetic shape memory alloys (MSMAs) are a class of smart materials that can produce large strains under external magnetic fields.
- Intelligent alloy design and the need for novel energy-harvesting technologies motivate studies on the fundamental physics of MSMAs.
- We present atomistic calculations of magnetic structure and anisotropy energies (MAE) of Ni_2MnIn MSMA.
- We also use the quasiharmonic theory of lattice dynamics to evaluate phase stability between the austenite and martensite phases of stoichiometric Ni_2MnIn.

Computational Methodology

- Total energies and interatomic forces for each phase are calculated with Density Functional Theory.[1-3]
- Magnetic structures and MAE are calculated with the spin arrangements shown in Fig. 1.

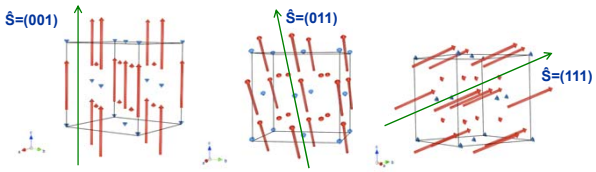

Figure 1. Model for calculating MAE. Atomic spins are oriented along different crystallographic directions.

- Vibrational modes and frequencies are calculated by diagonalization of the dynamical matrix.
- Free energy of each phase is the sum of electronic and vibrational energies:

$$F(V,T) = E(V) + F_{\text{vib}}(V,T)$$

- Helmholtz vibrational free energy: $F_{\text{vib}} = -k_B T \ln Z_{\text{vib}}$
- Vibrational partition function (harmonic approximation):

$$Z_{\text{vib}} = \exp(-\varphi / k_B T) \prod_{\mathbf{k},\nu} \frac{\exp(-\text{h}\omega(\mathbf{k},\nu)/2k_B T)}{1-\exp(-\text{h}\omega(\mathbf{k},\nu)/k_B T)}$$

- Free energy surfaces are generated using the quasiharmonic approximation (Fig. 2).

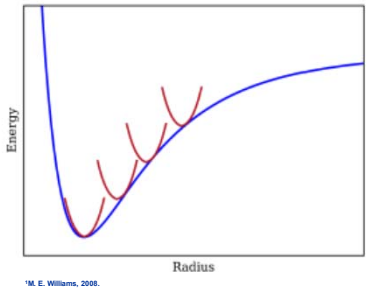

Figure 2. Schematic of the harmonic approximation extended to different points on the PES.

[1] M. E. Williams, 2008.

Results: Magnetic & Elastic Properties

- Ferromagnetic (positive) exchange occurs between Mn-Mn and Mn-Ni pairs (Fig. 3).
- Most of the magnetic moment resides on the Mn ions, but the *d* electrons of Ni mediate the interaction.
- Noncollinear magnetic calculations show that MAE is insignificant in the $L2_1$ structure of Ni-Mn-In, with average values less than 1 meV/atom.

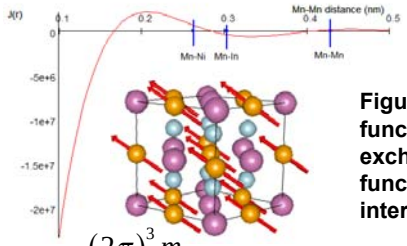

Figure 3. Plot of RKKY function for magnetic exchange, $J(\mathbf{r})$ in Ni_2MnIn as a function of Mn-Mn interatomic distance.

$$J(r) = \frac{(2\pi)^3 m_e}{4\hbar^2 r^4}\left[2k_F r\cos(2k_F r) - \sin(2k_F r)\right],$$

Results: Phase Stability & Free Energy Surfaces

- Imaginary phonon frequencies in the lowest acoustic mode indicate vibrational instability of $L2_1$ structure (Fig. 4).[4]
- We find no instability for the tetragonal structure. Similar to conclusions for Ni_2MnGa system.[5]
- Contrary to Ni_2MnGa, there is no phase transformation driven by vibrational instability in Ni_2MnIn (Fig. 5).

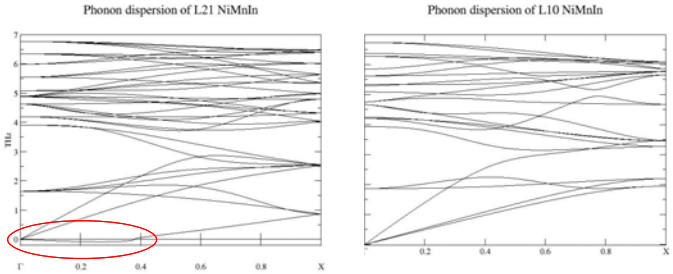

Figure 4. Phonon dispersions of austenite $L2_1$ and martensite $L1_0$ phases of Ni_2MnIn.

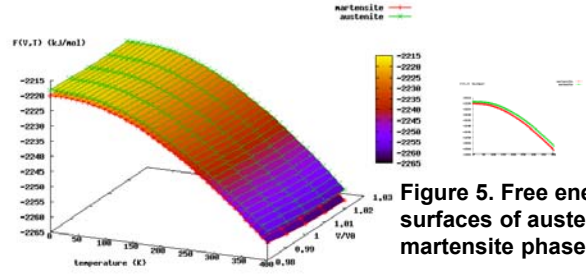

Figure 5. Free energy surfaces of austenite and martensite phases of Ni_2MnIn.

Conclusions

- Atomistic simulations can be used to predict real materials behavior, such as magnetic ordering and phase stability.
- Imaginary phonon frequencies show instability in vibrational modes of $L2_1$ austenite of Ni_2MnIn.
- Free energy calculations find no phase transformation between austenite and martensite at the stoichiometric composition.

References

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