Ab initio prediction of temperature-dependent stability of heterogeneous B19' phase in TiNi alloy using atomistically informed Eshelby's ellipsoidal inclusion

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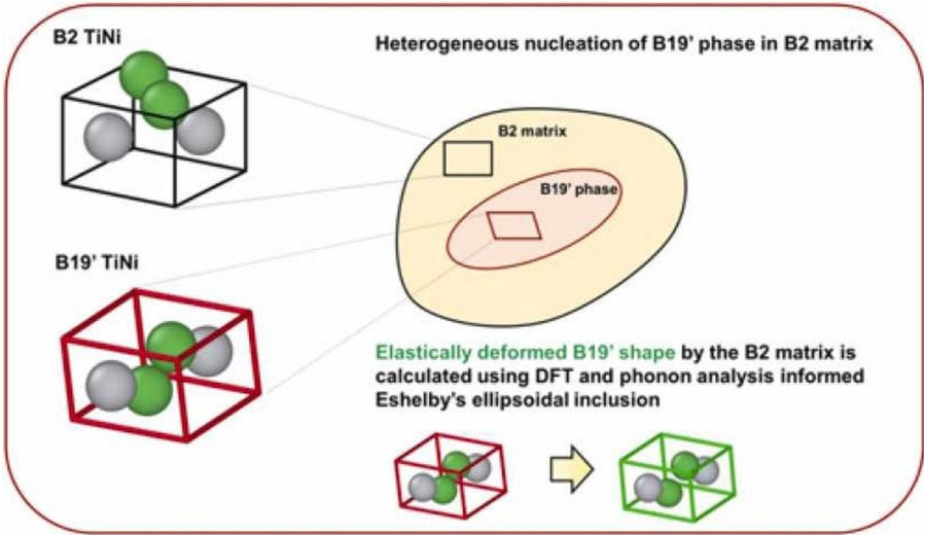
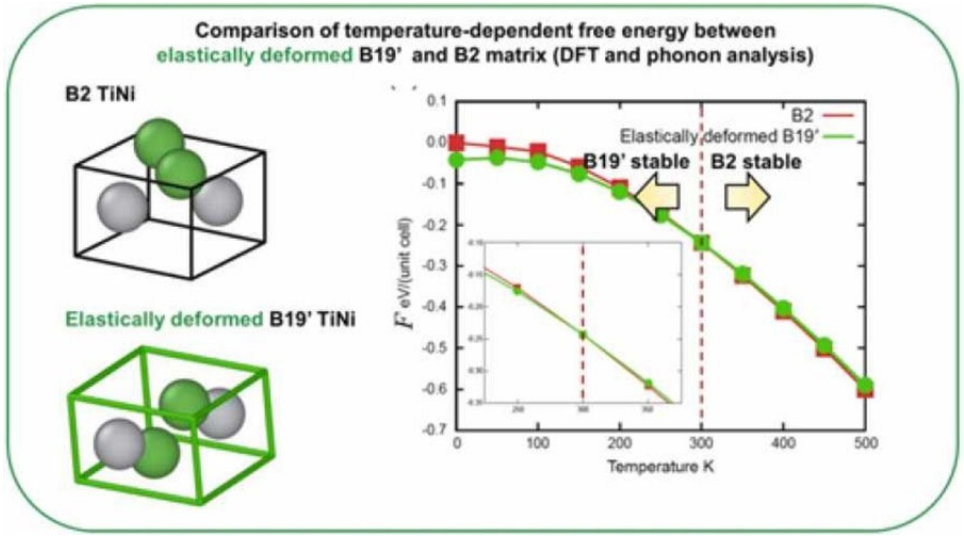
In this study, we energetically predicted the temperature-dependent stability of the heterogeneous B19′ phase in the B2 matrix of TiNi alloys using density functional theory (DFT) and phonon analysis informed Eshelby's ellipsoidal inclusion. The temperature-dependent eigenstrains and elastic constants for Eshelby's ellipsoidal in- clusion were calculated using DFT and phonon analysis under a quasi-harmonic approximation. The stable orientation of the disk-shaped B19′ phase in the B2 matrix and its total strains were evaluated with respect to temperature using Eshelby's ellipsoidal inclusion analysis. Using the total strains, the elastically deformed atomic structure of the heterogeneous B19′ phase in the B2 matrix was determined, and its temperature-dependent free energy was calculated using DFT calculations and phonon analysis. Comparing the temperature-dependent free energies of the B2 and elastically deformed B19′ structures, we successfully predicted that the transformation between the two phases occurs at 300 K, which agrees with experimental observations. Moreover, it is shown that the temperature-dependent difference in the elastic constants between the B19′ phase and B2 matrix in- fluences the phase transformation, which is the origin of the shape-memory effect of TiNi alloy.





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