

PHASE TRANSITIONS IN DISCRETE ONE-DIMENSIONAL CHAINS

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Structural phase transitions such as the martensitic transformations occurring in several metallic alloy systems generally involve microstructural features spanning multiple length and time scales. Any model designed to study these phenomena must incorporate information from the different length and time scales in some consistent manner. Currently, molecular dynamics coupled to continuum mechanics is a preferred means of studying the multiscale problem. However, in addition to the intrinsic difficulties associated with molecular dynamics simulations, fundamental questions concerning the nature of the information required to be transmitted to the continuum scale remain unresolved. For this reason, mesoscale discrete models between atomistic and continuum length scales have been studied and found useful [for e.g., 1,2]. These discrete models are generally of the Frenkel-Kontorova type and the effect of the non-nearest neighbor interactions are subsumed into a substrate potential whereas the nearest neighbor interactions are modelled as either harmonic or anharmonic springs.

The discrete models developed so far have mainly focused on transformations between different variants of martensite (twin boundary motion) at zero or constant finite temperature [1]. In this paper we present a model capable of undergoing temperature dependent transformations between a parent austenite and two variants of the product martensite phase. The model is motivated by the Frenkel-Kontorova model of dislocations in crystals and consists of a chain of discrete particles connected by harmonic springs and placed on a periodic substrate. In contrast to the classical Frenkel-Kontorova model in which the substrate is a sinusoidal potential, the substrate in the current model is a multi-well potential. The periodic images of the three wells representing austenite and two martensite variants are separated by high barriers representing resistance to slip. The interparticle interaction in the model is harmonic in contrast to the model presented in [3]. The central well representing austenite is at a higher energy than the wells corresponding to the martensite variants, reflecting the metastability of austenite at lower temperatures.

The average kinetic energy of the particles represents the temperature of the system in the usual statistical mechanics sense. Our simulations show that at higher temperatures, the austenite phase is stabilized. As the temperature is lowered, the martensitic phase transformation occurs at a critical temperature accompanied by the release of latent heat. The product phase formed is a self-accommodated twinned structure with approximately equal volume fractions of the two variants. The interparticle interaction stiffness plays the role of twin boundary energy and determines the length scale of the thickness of the martensitic twins.

References

- [1] R. Abeyaratne and S. Vedantam, "A lattice-based model of the kinetics of twin boundary motion," *J Mech Phys Solids* **51**, 1675–1700, 2003.
- [2] L. Truskinovsky and A. Vainchtein, "Kinetics of martensitic phase transitions: Lattice model," *SIAM J Appl Math* **66**, 533–553, 2005.
- [3] J. R. Morris and R. J. Gooding, "Exactly solvable heterophase fluctuations at a vibrational-entropy-driven first-order phase transition," *Phys Rev Lett* **65**, 1769–1772, 1990.

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