



Role of atomic variability and mechanical constraints on the martensitic phase transformation of a model disordered shape memory alloy via molecular dynamics

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Abstract

We use molecular dynamics (MD) with an embedded atom model potential parameterized for NiAl to study martensitic phase transformations in a disordered shape memory alloy. We focus on the role of intrinsic atomic-level variability and mechanical constraints on the martensite and austenite transformation temperatures and on the martensite microstructure for specimens with varying size. We find that periodic system size has a weak effect on transformation temperature all the way to the nanometer scale, with the entropy-stabilized austenite phase slightly penalized with decreasing size. Atomic-level variability in these random alloys leads to significant sample-to-sample variability in transformation temperature. The uncertainty in the austenite transformation temperature increases with decreasing size, reaching $\sim 10\%$ of the mean value for samples 10 nm on the side. Interestingly, the variability of the high-temperature martensite transition shows little size dependence. We find that a critical size of ~ 40 nm is required to develop multidomain martensite microstructures, and mechanical constraints reduce this critical size to ~ 7 nm, while significantly affecting the transformation temperatures. These results contribute to the understanding of martensitic transformation in nanocrystalline samples and of the fundamental limits of miniaturization of these alloys.

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1. Introduction

Shape memory alloys (SMAs) are used in a wide variety of applications, including medical implants, microactuators and for mechanical damping [1,2]. The unique properties of these materials, shape memory and superelasticity, originate from a solid-to-solid martensite transformation, and the microstructure development during the transformation plays an important role in their performance. Martensitic transformations are diffusionless, solid-to-solid transitions between a high-symmetry, high-temperature

phase called austenite (and stabilized by entropy) and a low-temperature phase called martensite, which has lower symmetry than the austenite [3]. For example, in $\text{Ni}_x\text{Al}_{1-x}$ disordered alloys that exhibit shape memory for x between 62 and 64% [4], the martensite transformation is between a B2-based austenite and monoclinic martensite [5,6]. In these alloys shape memory is observed if the samples are quenched to room temperature to avoid the occurrence of the Ni_5Al_3 phase, which is stable below 700 °C [4]. During the transformation from austenite, the martensite phase develops a multiple-domain (or multivariant) structure in order to accommodate the elastic strain and retain the original shape of the sample. Plastic deformation in the martensite phase occurs via domain wall motion rather

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than dislocation glide; thus, every atom retains its nearest neighbors. As a result, upon heating and transforming back to austenite, the material will have the same atomic configuration, resulting in shape memory [7]. Our understanding of the development of the martensite microstructure is incomplete; this is particularly true regarding the role of size and mechanical constraints that dominate the properties in nanostructured or nanocrystalline samples. These challenges are compounded in disordered SMAs, such as NiAl, where the intrinsic atomic variability can affect the behavior of nanoscale specimens.

The martensitic transformation involves significant multiaxial strain that causes complex internal stress distributions in polycrystalline samples which are expected to affect transformation temperature or stress and the development of multidomain microstructures. Experimental work is beginning to shed light on the details of the transformation process in polycrystalline samples and size effects. Under stress, the transformation originates in grains that are favorably oriented; these occur randomly throughout the material and lead to a homogeneous transformation macroscopically, but significant heterogeneities at length scales comparable to those of the grains. Furthermore, grains that attempt to transform become physically constrained by neighboring ones, resulting in the need for increasingly larger stress or degree of undercooling to complete the transformation [2]. Another important aspect is the release of latent heat upon transformation, which increases the local temperature of the material and further restricts the transformation [2,8]. Recent experimental work on sheets of NiTi SMAs under uniaxial loading has characterized the propagation of the martensitic transformation through the sample at the microscale; the authors characterized the strain distribution of the transformed material as well as the effect of texture on the transformation [9,10]. Experimental work on NiTiCu nanocrystals ranging from 10 to 50 nm in diameter and dispersed in a Ni₅₀Ti₂₅Cu₂₅ matrix revealed size-dependent transformation temperatures. All nanocrystals >25 nm showed complete martensitic transformation upon cooling to room temperature, while nanocrystals between 15 and 25 nm showed partial transformation [11], whereas other work [12] reported nanograins of NiTi not transforming to martensite below 50 nm. Interestingly, no significant size effects were observed in In–21 at.% Ti nanowires with diameters between 10 and 650 nm [13]. Experimental work has also shed light on how the shape memory effect works in NiTi [14], and how deformation of the martensite stabilizes the structure, and changes the austenite transformation temperature [15].

Molecular dynamics (MD) simulations are also contributing to our understanding of these phenomena. Rahman and Parrinello [16] pioneered work on solid–solid phase transformations using MD and even warned of the limitations of using small system sizes with periodic boundary conditions. The limited size of MD simulation cells had a strong effect on early MD work on martensitic

transformations [17,18]. More recent work [19] showed only two martensite variants during the body-centered cubic (bcc)–hexagonal close-packed (hcp) transition in Zr for systems with 40,000 atoms, indicating strong size effects at these sizes. Boundary conditions and shape also affect size effects in martensitic transformations. MD was used to characterize size effects on the martensitic microstructure of Zr and Fe nanowires [20,21], revealing that the size and shape of nanoscale specimens have a strong effect on microstructure and transition temperature, and that metastable phases are often present, minimizing the overall strain and domain wall energy. Ackland and collaborators [22,23] used MD simulations to produce realistic NiAl martensitic microstructures in 2-D systems consisting of parallel microtwins with opposite shear and characterized their formation. Such simulations are contributing to a deeper understanding of martensitic transformations [19,24–33], martensite nanostructures [19,24,25,27,30,32,33], size effects on mechanical behavior and hysteresis [26], surface effects on the transformation [31,34] and the effects of grain size [30]. Recent MD simulations [19,33] revealed how martensite nucleation and growth works in Zr. Martensite nucleates within the crystal upon cooling and imposes strain on the lattice. Different variants of martensite will then nucleate to compensate for this strain. Studies of the B2 to B19 phase transition in SMAs [33] revealed a twinning hierarchy. Microtwins formed within the martensite variants, in addition to the macrotwinning along the bar that is responsible for shape memory by responding to shear and propagating the domain wall. Despite such progress, several aspects of the martensite transformation remain poorly understood; among these are the effects of size and mechanical constraints on transformation temperature and on the resulting microstructure. The present paper focuses on the role of specimen size and mechanical constraints on sample-to-sample variability of the properties and microstructure of disordered SMAs modeled after a Ni₆₃Al₃₇ system.

The remainder of the paper is organized as follows. Section 2 describes the details of our simulations. Section 3 discusses size effects on the austenite and martensite transformation. Section 4 illustrates size effects on the martensitic microstructure. Section 5 describes the effects of mechanical constraints on the martensite structure and transformation. Finally, conclusions are drawn in Section 6.

2. Simulation details

The initial atomistic structures of the Ni₆₃Al₃₇ alloys were created by replicating a two-atom cubic B2 NiAl unit cell in all directions until the desired size was reached. We studied systems ranging in size from 6,750 atoms (which corresponds to a simulation cell length of 4.29 nm at 600 K), to 5,971,968 atoms (corresponding to a simulation cell length of 41.99 nm at 600 K). The simulations used periodic boundary conditions and the size refers to the length of the periodic cell.

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