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Effects of grain size on the martensitic phase transformation of nanocrystalline Ni/Al shape memory alloys

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ABSTRACT

Shape memory alloys (SMAs) owe their distinct properties to a diffusion less martensitic phase transformation from a high temperature, high symmetry phase (austenite) to a low temperature (martensite) phase upon cooling or strain. Their shape memory and pseudoelastic properties make SMAs useful as active components in microdevices, medical implants and for vibrational damping. Despite their widespread application, the miniaturization limit of SMAs is not known. In this study, we use large-scale molecular dynamics simulations (up to ~40 million atoms) to characterize the martensitic transformation in nanocrystalline Ni/Al disordered alloys. We quantify how mechanical constraints affect both the transformation temperature and the resulting martensitic domain structure. We find that decreasing the grain size makes the transformation more difficult, and this results in a reduction of the transformed volume fraction at a given temperature. Interestingly, we find a minimum in the transformed fraction as a function of decreasing grain size, with extremely fine-grained samples showing a greater tendency to transform.