Phase transformation temperatures and pseudoelasticity behavior ofNiTi-X ternary shape memory alloys: A molecular dynamics simulation study

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Introduction

NiTi alloy stands out as a promising material, particularly in biomedical, aerospace, and heat pump applications, owing to its biocompatibility and distinctive properties, including exceptional shape memory (SME) and pseudoelasticity. These properties arise from the alloy's capacity to undergo phase transformations during heating/cooling and loading/unloading cycles. The specific phase transformation temperatures and pseudoelastic behavior are heavily influenced by the composition of the alloy. The introduction of transition elements such as V, Cr, Mn, Fe, and Co in place of Ni and Ti can lower the martensite start (Ms) temperature, while substitution with Hf, Zr, Ag, and Au for Ni and Sc, Y, Hf, and Zr for Ti can elevate the Ms temperature. Consequently, it is imperative to comprehensively comprehend the effects of third alloying elements on the properties of these alloys from an atomic perspective. Molecular dynamics (MD) simulations, operating at the atomic level, offer a valuable means to explore the impact of various compositions, including the addition of a third element, on the alloy properties, thereby enhancing their performance. However, a significant challenge in MD simulations lies in selecting reliable interatomic potentials between the elements. Developing new potentials poses challenges, prompting the evaluation of existing potentials for ternary systems in this study, which will be compared with experimental results. While several interatomic potentials have been proposed for binary NiTi SMAs [1], limitations arise when extending to tertiary alloys. Existing studies have reported ternary interatomic potentials for NiTiV [2], NiTiNb [3], and NiTiHf [4], but these are insufficient for capturing the phase transformation of these tertiary systems. To address this, a hybrid model will be employed, combining different types of interatomic potentials such as modified embedded atom method (MEAM), embedded atom method (EAM), Lennard-Jones (LJ), and Morse potentials. This approach aims to capture the phase transformation of ternary alloys doped with elements like Cu, Hf, Pd, Pt, Sc, Ta, Mn, Zr, Y, and Au, which can increase transformation temperatures such as the martensite start temperature (Ms), martensite finish temperature (Mf), austenite start temperature (As) and Austenite finish temperature (Af), during cooling and heating processes. These alloys, known as high-temperature shape memory alloys (HT-SMAs), hold significant potential for diverse applications, including actuators, owing to their unique properties and enhanced transformation behaviours.

Results

To determine phase transformation temperatures, we employed the following simulation procedure. Cooling and heating processes were conducted on both NiTi and NiTi-X (where X represents the dopant element) samples with B2 structure (see Fig. 1 (a) for NiTi binary sample). Initially, a B2 structured NiTi atomic model was established at 500 K. Subsequently, the temperature was gradually decreased to 10 K and then increased back to 500 K, employing cooling and heating rates of ±1 K/ps. Throughout this process, periodic boundary conditions were applied in all three dimensions of the samples. The temperature-induced phase transformation was investigated using molecular dynamics (MD) simulations conducted in an isobaric-isothermal (NPT) ensemble at zero-pressure. The variation of atomic volume against temperature for the NiTi sample during the cooling and heating stages is illustrated in Fig. 1 (b and c). Initially, the material maintained the B2 structure. Subsequently, the high-temperature B2 austenite phase transformed into the low-temperature B19' martensite phase at Ms = 255 K during cooling, followed by the transformation of martensite phase back into austenite at As = 290 K during heating. This simulation process is being extended to ternary systems, and the results will be compared with experimental values of phase transformation temperatures to validate the interatomic potential used. Once the potential is validated, the phase

transition behavior of the ternary system under cooling/heating and loading/unloading will be studied with varyingconcentrations of dopant elements (X).

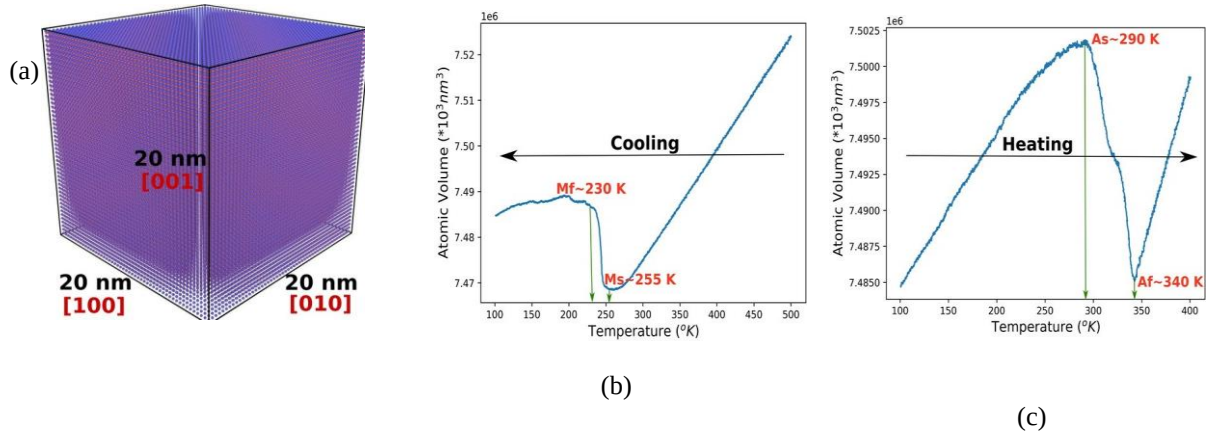

Figure 1: a) the initial simulation box, and variation of atomic volume with temperature duringthe b) cooling and c) heating stages.

Conclusion

In conclusion, molecular dynamics (MD) simulation emerges as a potent tool for investigating the phase transformation behavior of NiTi shape memory alloys. Nonetheless, the reliability of the potential employed in these simulations holds paramount importance. It is crucial that the outcomes obtained from MD simulations at least qualitatively align with experimental observations, recognizing the inherent disparities between length and time scales. By ensuring such consistency, MD simulations can serve as invaluable aids in elucidating the intricate behaviors of NiTi alloys, offering insights that complement experimental findings and enhancing our understanding of these materials at the atomic level.

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