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The role of strain glass state in the shape memory alloy $Ni_{50+x}Ti_{50-x}$: insight from an atomistic study

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Abstract

Molecular dynamics simulations are performed to study the influence of Ni concentration on the phase transformations in $Ni_{50+x}Ti_{50-x}(0 \leq x \leq 2)$ alloys during thermal cycling between 100 K and 500 K. We successfully reproduce the experimental observations that the martensitic transformation temperature and the thermal hysteresis decrease with increasing Ni concentration when $x \leq 1.5$, and the thermally induced martensitic transformation is prohibited when $x > 1.5$. Three types of martensitic twins are observed; increasing disorder from local distortion in martensitic variants is revealed with increasing Ni concentration at 100 K. Furthermore, a strain glass state with disordered local lattice distortion exists when $x > 1.5$. In addition, it is found that the atomic distributions of the Ni-Ni and Ti-Ni pairs in strain glass can be significantly altered by temperature. Shape memory effect and

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