The Analysis of Transformation Temperature and Microstructural Evolution in Ni-Ti Based Shape Memory Alloys by Molecular Dynamics

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Abstract: Shape memory alloys has been widely applied on actuators and medical devices. The transformation temperature and microstructural evolution play the crucial factors and dominate the behavior of shape memory alloys. In order to understand the influence of the composition of the Ni-Ti on the two factors, molecular dynamics (MD) is adopted to simulate the temperature-induced phase transformation in the current study. In addition, the results are post-processed by the martensite variant identification method. The method allows to reveal the detailed microstructural evolution and the volume fraction of each variant/phase in each case of the composition of Ni-Ti. Many features that have good agreement with those reported in the literature are found, such as the well-known herringbone structures; the higher concentration of nickel, the lower transformation temperature. In addition, some new features also discovered. For example, the transformation temperature changes more dramatically in the case of high concentration of nickel; the microstructure adopts different paths during the phase transition, giving complex interface movement. The results generated in the current study are expected to provide the design guidelines for the shape memory alloys applications.

Keywords: Shape memory effect; transformation temperature; molecular dynamics; crystal variants