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Effect of copper content on tensile mechanical properties of ternary NiTiCu alloy nanowire: Molecular dynamics simulation

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Abstract

Molecular dynamics (MD) simulation was used to study of mechanical properties of NiTiCu with different content of copper. It was shown that the percent composition of copper are significantly affects the stress-strain curves curve. The results showed that as the Cu content increased, the Yield Strength and Young's modulus decreased.

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1. Introduction

Equi-atomic NiTi compounds are extensively used in medical and engineering applications, due to their strong recovery force, large recovery strain, and biocompatibility [1, 2]. Recently, fabrication of Cu-containing NiTi shape memory alloys has attracted much attention [3]. Due to their suitable thermo-mechanical properties, NiTiCu alloys are a preferred choice mainly for cyclical applications [4]. Many properties (such as thermomechanical properties) are considerably changed by a composition deviation and can be noticeably enhanced by the addition of a third element (such as Cu) to the binary compound [1]. The advantages of Cu substitution for Ni are resulting in narrowing the transformation hysteresis, reducing the chemical composition dependency of transformation temperatures, and improving the ability to respond and corrosion resistance, etc., when compared to a binary Cu-free NiTi alloy [3]. Recent studies have found that substituting copper (<25 at %) for nickel in NiTi extensively reduce the compositional sensitivity [5]. So, the NiTiCu alloy is can be a better candidate for technical interest, such as

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Nomenclature

ϕ	pair-interaction term
β	neighbor atom type
α	central atom type

sensors or actuators [4]. Due to limitation in experimental conditions, computer simulation methods are usually adopted to predict and understand the behavior of materials. These include molecular dynamics (MD), Monte Carlo method and discreteness simulation [6]. MD seems to be an efficient tool to study deformation behavior of strain hardened metallic nano laminates and been confirmed the best suit for analyzing mechanical properties [7]. In this work, molecular dynamics method was used to study stress−strain curves and microscopic deformations of the ternary alloy nanowires (NiTiCu) with different composition of copper and the main purposes of this work is to investigate the effect of the third element on their mechanical properties.

2. Computational Section

LAMMPS coding has been performed to simulate tensile mechanical behaviors of the NiTiCu nanowire alloy with different composition of copper and resulting models and structures have been analyzed and processed using VMD visualization program. The NiTiCu nanowire is modeled with (10 x 100) {diameter Å x height Å} size in crystalline form. Periodic boundary conditions are imposed in three directions and uniaxial tensile deformation of nanowires applied along x-direction under controlled temperatures conditions (400K). The MD simulations were conducted in the NVT ensemble, where a Nose-Hoover thermostat was employed and timestep is 0.002 ps. Atomic pair interactions, including Cu-Ni, Cu-Ti and Ni-Ti are modeled using embedded atom method (EAM) potentials. The EAM is a many-body interatomic potential consisting of a pair function and a many-body interaction term. In the Finnis-Sinclair of the embedded atom method, the energy of a single atom is computed as:

$$U_i = F_\alpha(\sum_{i\neq j} f_{\alpha\beta}(r_{ij})) + {}^1/_2 \sum_{i\neq j} \emptyset_{\alpha\beta}(r_{ij}) \quad (1)$$

where the sum is over all atoms less than a cutoff distance apart. The key features of this formula are a pair-interaction term, ϕ, and an embedding function, F, that depend non-linearly on the contributions from the neighboring atoms to the local electron density, f. in this form, the pair-interaction and electron density functions are different for each combination of central atom type (α) and neighbor type (β), whereas the embedding functions are specific to the species of each neighbor, β, and central atom, α, respectively [8].

3. Results and discussion

According to the literatures, Cu has been shown to dissolve in the B2 (austenite) phase in a concentration up to 30 at%. However, NiTi-Cu solid solutions containing more than 10at% are characterized by poor formability so that alloys of technical interest usually contain Cu in the range from 5 to 10 at% [9]. So, five percent compositions of copper are selected and their mechanical properties are investigated. Fig.1 shows stress−strain curves of the NiTiCu nanowires with different copper content. Elastic modulus of the ternary alloy nanowires can be obtained by numerical fitting of the linear segment of stress-strain curve. However, Yield Strength is the maximum stress that can be applied without exceeding a specified value of permanent strain. As can be seen from Fig.1, the mechanical properties of nanowires are powerfully dependent on the copper composition. However, the effect of percent composition of copper on Young's modulus and Yield Strength are presented in Table 1. The Yield Strength decreases from ~11 GPa to ~6