PMME 2016

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

Sara Fazeli[a], Morteza Vahedpour[a]*, Sayed Khatiboleslam Sadrnezhaad[b]

*a*Department of Chemistry, University of Zanjan, P.O. Box 38791-45371, Zanjan, Iran
*b*Department of Materials Science and Engineering, Sharif University of Technology, P.O. Box 11155-9466, Tehran, Iran

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 insignificantly affects the stress-strain curves curve. The results showed that as the Cu content increased, the Yield Strength and Young's modulus decreased.

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

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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:

$$U_i = F_\alpha\left(\sum_{i\neq j} f_{\alpha\beta}(r_{ij})\right) + \frac{1}{2}\sum_{i\neq j} \emptyset_{\alpha\beta}(r_{ij}) \tag{1}$$

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 GPa for NiTiCu ternary alloy films with increasing Cu content. It can be understood

that the NiTiCu (%Cu=5, 10, 15) are stable and it only exists in the NiTi-Cu (%Cu=20, 25) crystal under tensile loading.
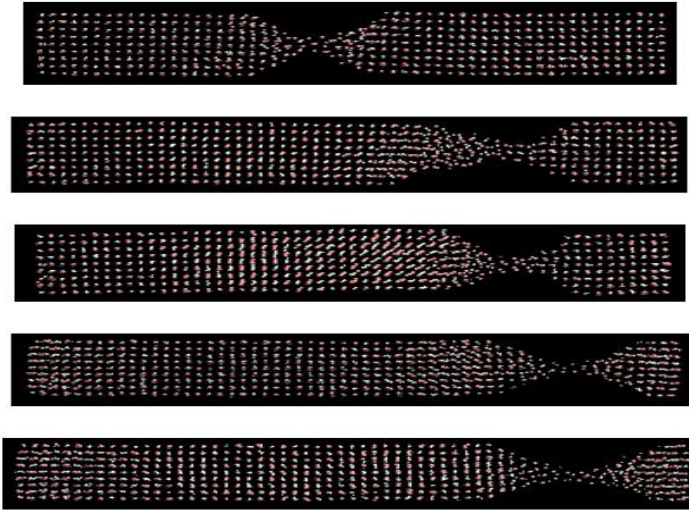

Fig.1 stress-strain curve for the ternary alloy nanowires NiTi-Cu (% Cu= 5, 10, 15, 20, 25)

Table1. Young's modulus and Yield Strength values for the ternary alloy nanowires NiTi-Cu (% Cu= 5, 10, 15, 20, 25)

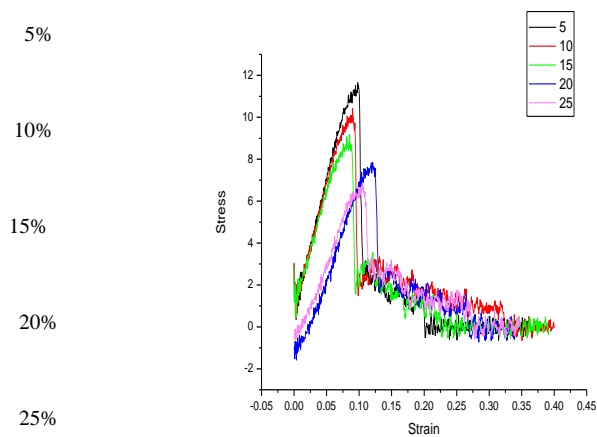| % Cu	5	10	15	20	25
Yield Strength(GPa)	11.43	9.94	8.66	7.64	6.51
Young's Modulu(GPa)	132.14	130.92	125.23	60.33	45.53

Fig.2 VMD snapshots for NiTiCu ternary alloy nanowires with different percent composition of copper

Fig 2. Show the VMD snapshots of the NiTiCu (different content of copper) nanowires, where there are necking zones appearing and developing to failure but the forming mechanisms of necking zones are different in different percent composition of copper. These snapshots demonstrate that most of atoms are also regularly arranged in the cases of NiTi-Cu (%Cu=, 10, 15, 20, 25) but local atomic dislocations cause atomic staking and final necking regions without sharp notch. However, in the case of NiTi-Cu (%Cu=5) most of atoms are irregularly arranged and local atomic dislocations result in atomic stacking, sharp notches and final necking region.

4. Conclusion

In this work, the simulation of NiTiCu with different content of copper is computationally generated using molecular dynamics simulation. The results of stress − strain curves show that the mechanical properties such as Young's modulus and Yield Strength are strongly dependent on the copper composition. However, It can be understood that the NiTiCu (%Cu=5, 10, 15) are stable and it only exists in the NiTi-Cu (%Cu=20, 25) crystal under tensile loading.

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