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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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