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What is the copper thin film thickness effect on thermal properties of NiTi/Cu bi-layer?

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Abstract

Molecular dynamics (MD) simulation was used to study of thermal properties of NiTi/Cu. Embedded atom method (EAM) potentials for describing of inter-atomic interaction and Nose–Hoover thermostat and barostat are employed. The melting of the bi-layers was considered by studying the temperature dependence of the cohesive energy and mean square displacement. To highlight the differences between bi-layers with various copper layer thickness, the effect of copper film thickness on thermal properties containing the cohesive energy, melting point, isobaric heat capacity and latent heat of fusion was estimated. The results show that thermal properties of bi-layer systems are higher than that of their corresponding of pure NiTi. But, these properties of bi-layer systems approximately are independent of copper film thicknesses. The mean square displacement (MSD) results show that, the diffusion coefficients enhance upon increasing of copper film thickness in a linear performance.

1. Introduction

Multilayered shape memory alloy thin films are a novel class of materials that are used for rapid actuation in micro-electro-mechanical systems (MEMS) due to their high surface to volume ratio, in comparison with bulk shape memory alloys (SMAs) [1, 2]. Among all these materials, thin films of NiTi-based alloys are promising candidates for MEMs actuator because of their exceptional properties [3–5]. Among the NiTi-based bi-layer, the NiTi/Cu bi-layer is of exceptional interest due to their excellent electrical and thermal conductivity [6]. It has been widely confirmed that the physical properties (thermal and mechanical) of these bi-layer can be considerably dissimilar from the single crystal. Due to the broad application of thermal properties such as thermal conductivity and diffusivity, these properties are more challenging [7]. So, efficient explorations of the physical properties of these materials can be valuable for better understanding of its applications [8]. Very few experimental data are accessible for the thermal properties of NiTi/Cu bi-layer [9]. Recently, Sanjabi *et al*, have synthesized copper nanowire on NiTi SMA thin films by an electromechanical method [6]. But, the thermal performance of this bi-layer is still not well understood. Hence, the study of this bi-layer is essential for industrial application. Due to limitation in experimental conditions, computer simulation methods are usually used to predict and understand the behavior of materials [10, 11]. The best approaches for the bi-layer thermal properties modeling contain the molecular dynamics simulation (MD). The molecular dynamics simulation technique is relatively appropriate for examination of thermal and mechanical properties of solids or liquids [12]. Such simulations are perfect method for predicting thermal transport properties because no statements about the phonon scattering within the film or at the film boundaries are required [13]. Excellent literatures from MD techniques viewpoint to investigate the thermal properties of multilayered are presented by researchers. MD simulation is used to investigate the dependence of thin film thermal resistance of Ge/Si/Ge and Si/Ge/Si multilayered on film thickness by McGaughey *et al* [13]. Yang *et al*, calculated the thermal properties such as thermal conductivity using the theoretical model, and then the interfacial effect on thermal conductivity is demonstrated [9]. Rodríguez *et al* explained the Effective thermal parameters for a bi-layer and they showed that how to choose the correct solution for the useful thermal parameters, maintaining the physical meaning of the examined thermal property [7].