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PAPER

Comparison of the mechanical properties of NiTi/Cu bilayer by nanoindentation and tensile test: molecular dynamics simulation

Sara Fazeli[1], **Morteza Vahedpour**[1] **and Sayed Khatiboleslam Sadrnezhaad**[2]

[1] Department of Chemistry, University of Zanjan. PO Box 38791-45371, Zanjan, Iran
[2] Department of Material Science and Engineering, Sharif University of Technology, PO Box 11155-9466, Tehran, Iran

E-mail: vahed@znu.ac.ir

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Abstract

Molecular dynamics simulation was used to study of mechanical properties of NiTi/Cu bilayer by nanoindentation and tensile testing. A comparison has been made among mechanical properties measured and plastic deformation process at different copper thickness during nanoindnetation and tensile test of the samples. Embedded atom method potentials for describing of inter-atomic interaction and Nose–Hoover thermostat and barostat are employed in the simulation at 400 K. The results showed that as the copper film thickness decreased, the maximum load and hardness values increased during nanoindetation. Saha and Nix model is used to describe reduced young's modulus behaviour of the bilayer system through nanoindentation. A good agreement among calculated reduced elastic modulus by nanoindentation test and young's modulus behaviour via tensile test have been obtained. The 'incoherent interface' in both of nanoindentation test and tensile testing is one of the governing factors for the dislocation propagation, which resulted in significant strengthening of the bilayer. It was observed that during tensile test, only copper layers were necked and fractured in all of samples. However, the present study seeks to examine the effect of film thickness on the free energy values that is obtained using Jarzynski's equality during nanoindentation. As the copper film thickness was decreased, the free energy difference increased. According to both techniques, the thin film copper thickness provides lower number of nucleation locations resulting in the higher value of yield strength, hardness and free energy difference during nanoindenation. Mechanical properties of bilayer systems are improved with decreasing of copper film thickness. However, it specifies that strengths of all bilayer systems have prominent increase in young's modulus in compared to the pure NiTi.

Nomenclature

R	Radius of indenter
r	Distance between atoms to the centre of indenter
RDF	Radial distribution function
$P–h$	Load–displacement curve
$P_{\max}$	Maximum load
A	Projected area
h_c	Contact depth of the spherical indentation

h_{max}	Maximum depth of indentation
S_{max}	Slope of the unloading curve at the maximum applied load
h_f	Residual depth of indent
t	Film thickness
E_r	Reduced Young's modulus
E_f	Modulus of the film
V_f	Poisson's ratio of the film
E_s	Modulus of the substrate
V_s	Poisson's ratio of the substrate
k_b	Boltzmann constant
T	Temperature
ΔF	Change of the free energy
W_λ	Nonequilibrium work

1. Introduction

With advances in nanotechnology and nanoscience, multilayered thin films having potential application in various fields of protective coating, magnetic storage, hard disk drives, high—density storage systems, contact surfaces performance and micro/nano-electromechanical devices (MEMS/NEMS) have grown interest [1–3]. Mechanical behaviour of multilayered films is of great importance mainly due to their high elastic modulus and yield strengths predicted by previous researchers [2]. 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 SMAs [4, 5]. Among all these materials, thin films of NiTi-based alloys are promising candidates for MEMs actuator because of their exceptional properties. But, the limited hardness and wear resistance of NiTi make them intricate enough to be used in MEMS applications [6] and their corrosion and wear resistances are not fully acceptable [7, 8]. Among the different methods such as nitrogen ion implantation and laser surface treatment [6, 9–11], metal surface coating and fabrication of the nanoscale multilayer metallic (NMM) techniques have resolved the problems mentioned above [12]. Copper can be introduced as the best metal coating surface, based on its excellent electrical, thermal conductivity and mechanical behaviour [13].

Moreover, it should be noted that NiTi alloys have been used as structural materials for some surgical implants and devices because of their novel properties such as shape memory and superelasticity [14, 15]. Similar to other medical materials, severe implant-related bacterial contamination still encourages possible post-surgical complications [16]. It is widely accepted that the antibacterial activity of copper is appropriate to be NiTi alloys surface modifier and antibacterial coating agent [16, 17].

The contact mechanics of coating-substrate systems is still not fully understood and the associations between the mechanical properties of the coating and substrate are more challenging [18]. In the investigation of mechanical properties it is often essential to know the strengths and failure approaches of the system in consideration [19]. Nanoindentation and tensile test are two kinds of crucial mechanical techniques which can be measure the mechanical properties easily and reliably. Tensile tests have the advantage of uniform stress and strain fields, which can provide information about the mechanical properties at larger scales [20]. Among several methods utilised in nanotechnology, nanoindentation tests are widely used in characterising the nano-mechanical properties of multilayered metal films [1]. This technique has been employed for gathering of the elastic modulus information, indentation hardness and yield strength as well as probing of the early stages of deformation and transition from elasticity to plasticity [21–23]. A lot of factors may influence the plastic behaviour such as size of the substrate, tip geometry of the indenter, penetration depth, time-dependent parameters and strain gradient, and so on. To obtain a deeper insight into the nanoindentation process and the effect of layer's thickness of bilayer system on nanoindentation's results, the examination of thermodynamic quantities such as work and free energy changes released during nanoindentation, can be useful [24]. But there is a lack of studies on this matter. In this research, we have focused on free energy changes computed through