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Investigation of Crack Growth in Deposited and Perfect Titanium/Titanium Nitride Structure by Molecular Dynamic Simulation

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ABSTRACT: The crack propagation behavior in the deposited titanium/titanium nitride bilayer is compared with the perfect structure using the molecular dynamics method. For this purpose, titanium nitride was deposited on the titanium substrate, then crack growth was investigated in the two structures. The titanium nitride film growth on the titanium substrate was an island, and the structure has defects and residual stress. The results showed that both the biaxial and normal stresses in the substrate and film are tensile and compressive, respectively. The cohesive energy of the interface was calculated by energy difference along with the atomic layers. In the following, a crack was considered perpendicular to the titanium/titanium nitride interface in both models, with an initial length of 15 Å. Due to the brittle behavior of the ceramic layer, the crack propagates rapidly until interface. The plastic deformation of the titanium layer and the structure of the interface blunt the tip of the crack and prevent it to fail. Also, the critical stress for crack growth in a perfect structure is found to 2.5 times its value in the deposited structure because of defects and residual stress.

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1. INTRODUCTION[1]

In some applications such as gas turbine compressor blade, the Ti/TiN multilayer coatings which are deposited by the Physical Vapor Deposition (PVD) on the compressor blade, prevent it from damaging. Depending on working conditions such as the corrosive environment, wear and erosion due to the sands and other particles ingested by the engines primary cracks are formed in multilayer coatings. Different deposition parameters such as partial pressure of the gas, substrate temperature, the energy of incident atoms and flux ratio affect the growth and properties of multilayer coatings [1]. Mechanical behavior of thin films such as strength and adhesion has a significant role in their performance. Iwasaki [2] presented a method based on Molecular Dynamics (MD) simulation for calculating the adhesion strength of the Al/Cu bilayer. Zientarski and Chocyk [3] investigated the deposition and stress evolution in Cu/Au and Fe/Au systems using MD. In both systems, in the early stage of growth one observes compressive stress. Next, the Cu/Au system has compressive stress, while tensile stress is observed in Fe/Au.

The continuum mechanics and fracture mechanics are used to study crack propagation at the macro scale, though it occurs widely at the micro-scale. Therefore, MD has been used to explore the mechanical properties and mechanisms of nanoscale material fracture. As the thickness of the layers decreases to the nanoscale, the preferred crystalline orientation and plane for the layers to grow on each other have an important effect on the mechanical characteristics and the crack growth. Zhou et al. [4] reported four different mechanisms for crack growth in the Al/SiC interface considered eight different orientations by MD simulation. These four mechanisms demonstrated that crack growth behavior is dependent on the crystalline orientation in the interface. The purpose of this study was to investigate the crack growth in deposited and perfect Ti/TiN structures and the effect of defects and residual stress caused by the deposition process on it. First, the deposition of TiN on Ti substrate was carried out. Then, crack growth in both deposited and perfect structures analyzed and compared.

2. SIMULATION METHOD

2-1- Deposition

The 3D model of the deposition process is shown in Fig. 1. The substrate consists of 4000 Ti atoms with hcp structure with dimensions of $5a\times10a\times20a$ (lattice constant of Ti is a=2.95 Å) in the x, y, and z, respectively. The crystal orientation for the structure is x(100), y(010) and z(001). The substrate atoms are divided into three groups: 1) Two atomic layers at the bottom of the substrate are fixed to prevent the substrate from moving due to the incident of Ti and N atoms. 2) Eight layers of intermediate atomic layers are defined as isothermal layers, using the Canonical Ensemble (NVT) ensemble. 3) The other upper layers are free to absorb the energy of the deposited atoms. The initial substrate temperature is

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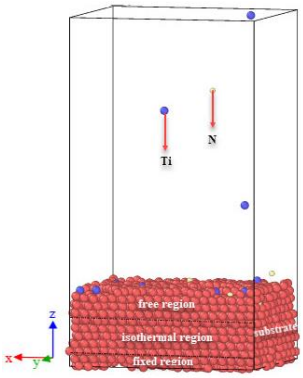

Fig. 1. Deposition of Ti and TiN on Ti substrate

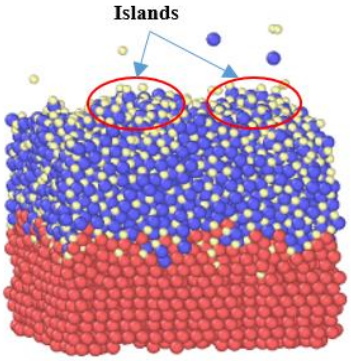

Fig. 3. Snapshot of the deposition process at 3466 ps

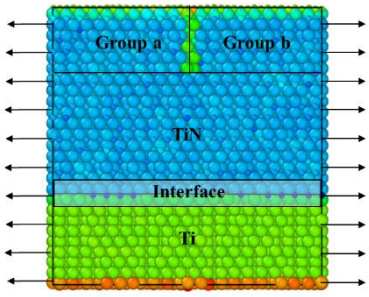

Fig. 2. Schematic of Ti/TiN perfect structure after equilibrium. Atoms are colored based on energy per atom.

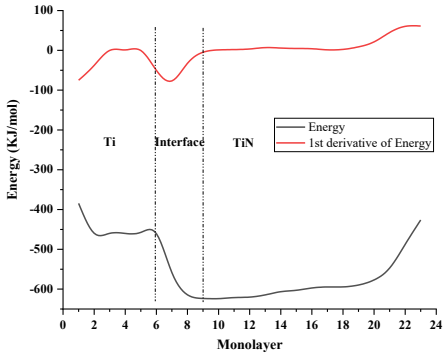

Fig. 4. The cohesive energy between Ti and TiN layers in the deposited Ti/TiN structure

600 K and the periodic boundary conditions are applied in both *x* and *y* directions. The deposition was performed by inserting 10,000 Ti and N atoms along *z* direction with 10 atoms/ps rate from an area 24-fold-lattice height toward the substrate surface. The kinetic energy of the incident atoms is 0.1 eV. After the deposition was completed, an equilibrium process was carried out for 200 ps until the system was fully equilibrated at 300 K.

In Fig. 2, the 3D model of Ti/TiN perfect structure has been shown, in which crystal plane Ti(0001)||TiN(111) is considered in the interface. The *x*-*y* plane is the interface between the layers and the *z*-axis is normal to the interface. Periodic boundary conditions were applied in both the *x* and *y* directions and shrink in the *z*-direction. Due to the difference in lattice constants of Ti and TiN, the mismatch in both *x* and *y* directions is 1.68%. The simulation dimensions were chosen according to the deposition model. The equilibrium of the structure was reached at 300 K and zero bar with the Isothermal-Isobaric Ensemble (NPT) ensemble for 50 ps. According to Fig. 2, the initial crack with 15 Å length is located in the TiN layer by excluding the atomic interaction between a and b groups.

After deposition, an initial crack was created in deposited structure by removing atoms. Then, the structure was equilibrated for 20 ps. Next, both deposited and perfect Ti/TiN bilayer with a constant strain rate 0.5×10^{8} s^{-1} at 300 K is subjected to tensile loading parallel to the interface. To observe the plastic deformation during loading and crack growth, the Microcanonical Ensemble (NVE) ensemble is implied. The time step in all simulations is 1 fs. The second nearest neighbor modified embedded-atom-method (2NN-MEAM) interatomic potential was used [5] to describe interactions between atoms [1]. Atomic modeling has been done using the Lammps [6] code. Ovito [7] was used to visualize results.

3. RESULT AND DISCUSSION

Fig. 3 shows the deposition of the TiN film on the Ti substrate. In the TiN layer growth, islands are formed. The penetration of N atoms increases adhesion between film and substrate. The deposited structure has some defects, which is similar to what is happed in PVD process. In this study, the mean biaxial $(\sigma_{xx}^{ave}+\sigma_{yy}^{ave})/2$ and normal stresses σ_{zz}^{ave} were used to investigate the residual stress of the layers [8]. Both biaxial and normal stresses of the substrate are tensile converted to compressive stresses in the interface. In this region, the biaxial stress is higher than normal stress. Also, in TiN film stresses are compressive.

To calculate the cohesive energy between the film and substrate, the potential energy of each atomic layer was calculated and plotted in Fig. 4, in which energy drop in the interface is defined as the cohesive energy.

As shown in Fig. 5, at low strains, both metal, and ceramic layers are under elastic deformation and the crack opening is still unclear. Young's modulus of Ti/TiN is obtained 274.436 GPa. With increasing strain, the stress reaches the critical value and the crack begins to grow. Due to the brittle behavior of the TiN, the crack grows rapidly through its thickness.

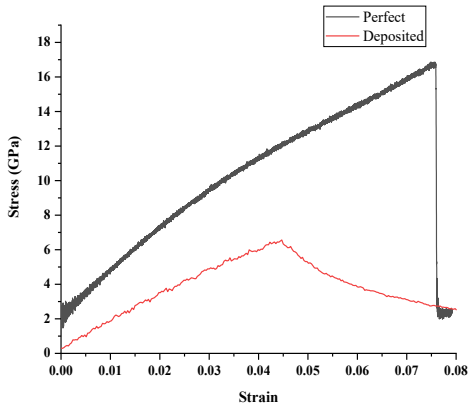

Fig. 5. Comparison of Strain-stress response of the Ti/TiN deposited and perfect structure

Because of crack growth, the stress decreases from the critical value to 2.44 GPa. The crack with a sharp tip travels to the Ti/TiN interface, then it is blunted by the interface. Comparison of the two stress-strain curves in Fig. 5 shows that the critical stresses for crack growth in the perfect and deposited structure are 16.72 GPa and 6.54 GPa, respectively. These results indicate that the perfect structure has a higher resistance to crack growth than the deposited structure. Also, the strain associated with critical stress for the perfect Ti/TiN structure is 0.075. However, this value for the deposited structure is 0.045. Based on the Griffith criterion [9], critical stress intensity factor (K_{IC}) and released energy rate (G_{IC}) of crack growth in the perfect structure were calculated 1.028 MPa.m$^{1/2}$ and 3.357 J/m^2, respectively.

4. CONCLUSIONS

In this study, the deposition of TiN on Ti substrate was performed by MD method. Then crack growth in the perfect and deposited structure was compared. The deposition results show that the penetration of N atoms in the upper layers of the Ti substrate was observed, which increased the adhesion between the layers. Due to the difference between the lattice structure of the substrate and the coating (hcp/fcc) and the penetration of the N atoms, the coating has an amorphous structure. The results illustrate that both biaxial and normal stresses for the substrate and TiN layer are tensile and compressive, respectively. The critical stress for crack growth was obtained 16.72 GPa for perfect structure and 6.54 GPa for deposited structure. Also, crack growth for the perfect structure occurs at 0.075 strain, while for the deposited structure is 0.045. The reason for the low critical stress and strain of crack growth in the deposited structure is due to residual stresses and defects.

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