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Simulations of an Interface Crack Nucleation During Nanoindentaion : Molecular Dynamics and Finite Element Coupling Approach

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ABSTRACT

We carried out the nanoindentation simulations for the Ru (superlayer) / Cu (film) / SiO2 (substrate) system using the finite temperature MD-FEM coupling method. The calculations are performed for the different adhesion energies of Cu/SiO2 ranging from 0.2 to 0.6 J/m^2. During loading, it was found that the interfacial crack nucleation occurs at three to four times the contact radius, driven by the tensile stress acted on the Cu/SiO2 interface. We also show that the asymmetric defect behavior have a great effect on giving birth to the crack nucleation. The observation of our simulation indicates that the mechanism of the crack nucleation strongly depends on the interfacial bonding energy.

INTRODUCTION

Delamination of the thin metallic film on the dielectric substrate is one of the critical issues in the technological applications [1]. Experimentally, much effort has been devoted to measure a quantitative value of the interfacial adhesion energy [2]. One of the common adhesion tests is a superlayer nanoindentation technique recently developed by Kriese et. al [3]. This technique has a great advantage in that it can induce the interfacial crack accurately without the need of the complex sample preparation. However, the critical conditions at which a crack nucleate at the interface and the deformation mechanism involved are still unclear.

Molecular dynamics (MD) is the powerful computational tool to provide a great insight of the defect behavior such as a dislocation motion during indentation loading. But, due to its heavy computational burden, most of the MD simulations have been limited to track the homogeneous dislocation nucleation event which occurs in the early stage of the indentation [4]. The interest of this study is the crack nucleation at interface, which is the further subsequent event during the indentation process. Therefore, we need to incorporate the more sophisticated modeling approach.

The approach we develop here is the coupling method of the molecular dynamics and the continuum calculation based on a finite element method (FEM). In this multiscale framework, the atomistic level description is only applied to the highly deformed inelastic region, which results in the considerable decrease in the degree of the freedom.

We modified the coupling approach originally developed by Kohlhoff [5]. In addition, to consider the dynamic effects of the defect motion, the original static algorithm has been extended to the finite temperature coupling scheme [6]. The above coupling approach is applied to the nanoindentation simulations in the Ru (superlayer) / Cu (film) / SiO2 (substrate) system. In this study, we report the atomistic aspects for the initiation of the interfacial cracking.

MD-FEM COUPLING METHOD

The schematic of the region near the atomistic and continuum interface is shown in Fig. 1. The present coupling method is based on the patch framework presented in Ref. [5]. In this framework, the atomistic and continuum regions are treated as the separated systems. But, to realize the mechanical equilibrium between both systems, the displacement-based couplings are prescribed at the MD-FEM interface as follows. The displacements of the FEM nodes in the region 2 give the atom positions in the region 2 by using the interpolation function, and then the atom positions in region 1 are updated. In the same manner, the displacements of the atoms in the region 2 provide the new boundary conditions for the FEM calculation.

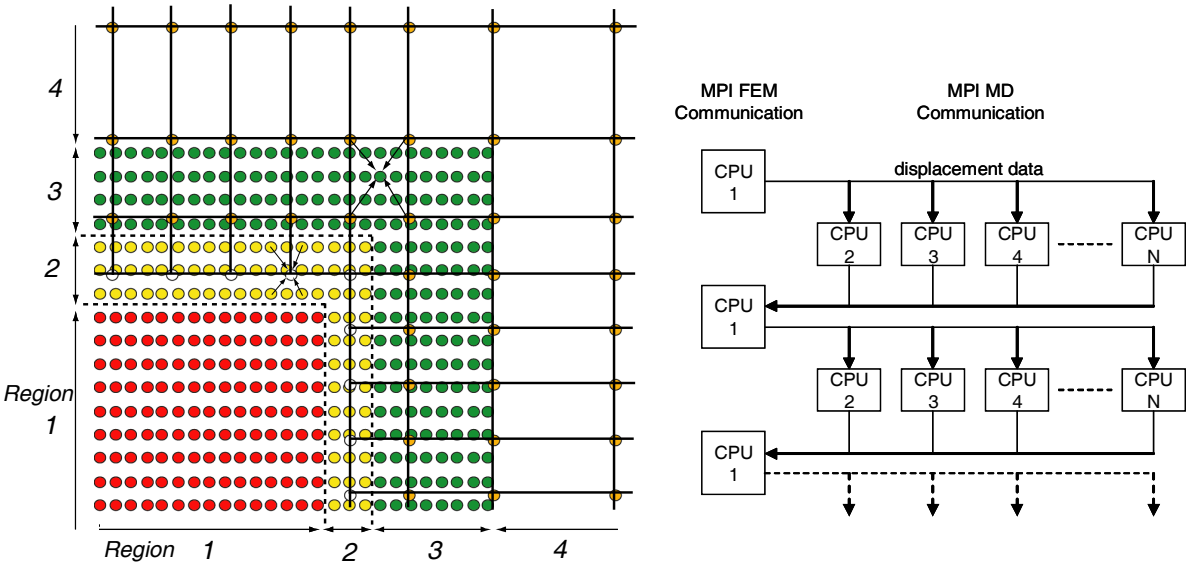

Figure 1. Schematic illustration of: a) the MD/FEM coupling region within a patch framework; b) the parallel computing method applied to the dynamic MD/FEM coupled systems.

While this framework was originally limited to the static computation, we extend the above approach to the finite temperature dynamic systems by using the Qu's scheme that was established for the 2D coupled atomistic discrete dislocation model. As suggested in Ref. [6], a Langevin type thermostat layers are inserted in region 2, which provide an important ability that the high energy wave emitted from atomistic region can absorb without showing the unphysical wave reflection at the MD-FEM interface. In addition, the continuum region is stochastically updated on the time scale comparable to the Debye frequency of the atoms, which results in the proper description of the permanent elastic deformation during simulations.

Moreover, the two efficient techniques are introduced in order to reduce the computational burden. First, we adopt a Watson Sparse Matrix Package (WSMP) developed at the IBM Thomas J. Waston Research Center [7], which is the fast and stable algorithm for solving large systems of linear equations whose coefficient matrices are sparse. Second, we introduce the parallel computation using the Message Passing Interface (MPI) into the coupling

framework. As shown in the schematics of Fig. 1(b), in the total of the N CPUs computation, the only 1 CPU is assigned for the FEM system and the others are for the MD system. For this parallelization in the MD calculation, the spatial decomposition algorithm is used [8].

NANOINDENTATION SIMULATIONS

The model of our nanoindentation simulations is shown in Fig. 2. It consists of the Cu (film) / SiO2 (substrate) layers and the Ru layer is added over the Cu layer as a high-modulus hard superlayer. The interactions of the Ru-Ru, Ru-Cu and Cu-Cu are described by Generalized EAM potential [12,14], which is the extension type of the EAM potential to represent not only the physical properties of a bulk metal (fcc, bcc, hcp metal) but those of the alloy metals with any combinations. For simplicity, the substrate atoms (SiO2) are represented by a simple spring model with fcc lattice structure. Therefore, we assume that the substrate reproduces the elastic solid and the dislocations emitted during indentation cannot penetrate into the substrate. The interaction between Cu and substrate atom is described by Lennard -Jones interatomic potentials [13]. By using the different set of the Lennard-Jones parameters, the calculations are performed for the different adhesion energies W_{ad} of Cu/SiO2 ranging from 0.2 to 0.6 J/m^2. These range correspond to the upper and lower bound of the experimental predictions [9,15]. The *x, y* and *z* axes of the simulation cells are $[10\bar{1}]$, $[1\bar{2}1]$ and [111] direction for the fcc Cu lattice, and $[11\bar{2}0]$, $[\bar{1}100]$ and [0001] direction for the hcp Ru lattice. The interface normal corresponds to the *z* direction. Periodic boundary conditions are applied along the *x* the *y* direction. The dimensions of the whole system are 10.5 nm × 81.5 nm × 102.7 nm, containing about 1,100,000 atoms and 150,000 nodes. In our simulations, the rigid and cylinder shape indenter is assumed. The interaction between the indenter and atoms are modeled through a simple repulsive potential [10]. We performed the indentation of the maximum penetration depth of 10 nm. The indenter velocity is set to at 10 m/s. The thermostat layers are inserted in the substrate region and the temperature of the substrate is kept constant at 10 K in all simulations.

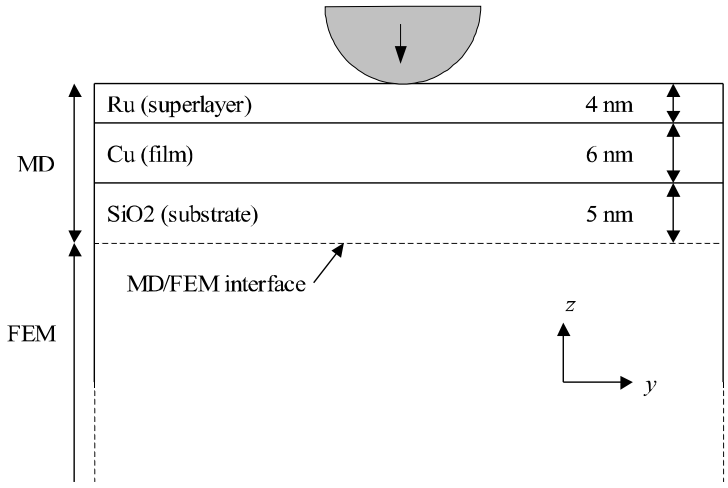

Figure 2. Schematic illustration of the calculation model.

In Fig. 3, the snapshots of the simulation at the various indentation depths of h are shown, where the left figures indicate the result for W_{ad} = 0.2 J/m^2 and the right figures for W_{ad} = 0.6 J/m^2. In these figures, the defect motions are visualized by computing the atoms that do not have 12 first neighbors [11].

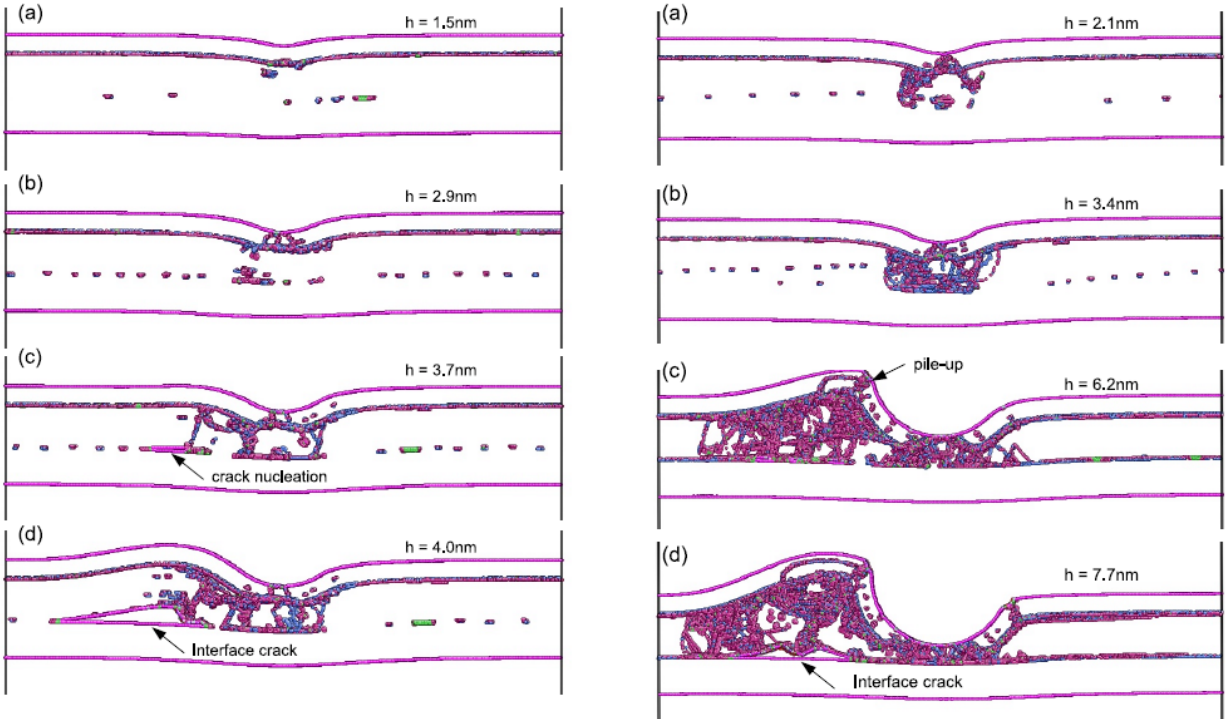

Figure 3. Snapshots of the superlayer nanoindentation simulation at the various indentation depth h. The adhesive energy between Cu and substrate is [Left: (a-d)] 0.2 J/m and [Right: (a-d)] 0.6 J/m, respectively. In these figures, only defect atoms are shown.

Initially, the systems show the almost elastic behavior. At the indentation depth of about 1 nm, the partial dislocations are nucleated from the Ru/Cu interface and evolve into the Cu layer. During the subsequent loading, these dislocations are accumulated on the Cu/substrate interface below the contact region.

For the weaker interface of W_{ad} = 0.2 J/m^2, when the indentation depth is 3.7 nm, it is found that the crack nucleation occurs at the Cu/substrate interface. The nucleation site is displaced from the central axis by about 15 nm, which corresponds to about three times the contact radius. After the initiation, the crack propagates rapidly along the Cu/substrate in the brittle manner. In Fig. 4 (solid line), we shows the σ_{zz} stress distribution along y direction at the Cu/substrate interface just before the crack nucleation. As expected, the large compressive stress is found below the contact region. It is also recognized that the tensile stresses attain a peak value of approximately 2 GPa just outside the contact region. These tensile stresses would be attributed to the suppression of the film bending by the substrate. Clearly, the crack nucleation site is consistent with the generation point of the tensile stress. This indicates that the interfacial normal stress gives the driving force for the crack nucleation. It is also noted that while the tensile stresses generate at nearly symmetric regions with regard to the central axis, the crack nucleation site is asymmetric. This reflects that the dislocations piled-up at the interface provide a role as a trigger of the crack nucleation. In this case, because the slip system for the dislocation emission

in Cu is not symmetric with regard to the central axis, as the result, the dislocation piled-up is achieved at the left side of the contact region prior to the opposite side.

On the other hand, for the stronger interface of W_{ad} = 0.6 J/m^2, the film deformation induced by the dislocation pile-up is observed before crack nucleation at the indentation depth of 6.2 nm. This plastic behavior release the large amount of the stored elastic energy, but the due to constraint by the relatively hard surperlayer, the tensile stresses still attain a peak value of nearly 1 GPa outside the contact region (in Fig.4; dashed line). As a result, at the depth of 7.7 nm, the interfacial crack is initiated through the coalescence process of the several small debondings that appear beneath the dislocation pile-up zone. These results suggest that the mechanism of the crack nucleation strongly depends on the interfacial bond energy.

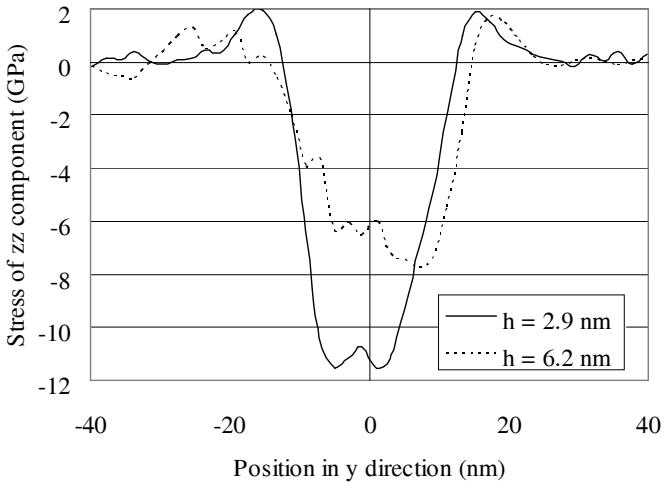

Figure 4. σ_{zz} stress distribution along y direction at the Cu/substrate interface.

CONCLUSIONS

To study the atomistic aspects for the initiation of the interfacial cracking, we have performed the nanoindentation simulations in the Ru (superlayer) / Cu (film) / SiO2 (substrate) system by using the finite temperature MD-FEM coupling method based on the patch framework. The crack nucleation occurs at three to four times the contact radius, driven by the tensile stress acted on the Cu/SiO2 interface during loading. The result of our simulation suggests that the mechanism of the crack nucleation strongly depends on the interfacial bond energy.

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