Provided for non-commercial research and education use. Not for reproduction, distribution or commercial use.



This article appeared in a journal published by Elsevier. The attached copy is furnished to the author for internal non-commercial research and education use, including for instruction at the authors institution and sharing with colleagues.

Other uses, including reproduction and distribution, or selling or licensing copies, or posting to personal, institutional or third party websites are prohibited.

In most cases authors are permitted to post their version of the article (e.g. in Word or Tex form) to their personal website or institutional repository. Authors requiring further information regarding Elsevier's archiving and manuscript policies are encouraged to visit:

http://www.elsevier.com/copyright



Available online at www.sciencedirect.com



Acta Materialia 57 (2009) 4209-4216



www.elsevier.com/locate/actamat

Multiscale analysis on the onset of nanoindentation-induced delamination: Effect of high-modulus Ru overlayer

S. Hara*, T. Kumagai, S. Izumi, S. Sakai

The University of Tokyo, School of Engineering, Department of Mechanical Engineering, 7-3-1, Bunkyo-ku, Hongo, Tokyo, Japan

Received 23 March 2009; received in revised form 13 May 2009; accepted 15 May 2009 Available online 11 June 2009

Abstract

This paper provides atomistic level findings regarding interfacial crack nucleation and propagation processes. To see the Cu/SiO_2 cracking, we carried out nanoindentations in the $Ru/Cu/SiO_2$ system using an atomistic/continuum coupling method. We found that interfacial crack nucleation is triggered by heterogeneous dislocation nucleation. The resulting buckling delamination mode is qualitatively similar to that observed experimentally. In addition, comparison with the nanoindentation in the Cu/SiO_2 system demonstrates that nanoindentation testing utilizing the high-modulus Ru overlayer is an effective probe for evaluating Cu film delamination. In the system with the Ru overlayer, the crack propagates along the interface in a brittle manner once the crack nucleates. On the other hand, without the Ru overlayer, crack propagation is significantly retarded and less driven, which is attributed to a large number of plastic events in the Cu film during loading. These results would provide a clear physical picture for explaining the experimental results. © 2009 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

Keywords: Nanoindentation; Delamination; Interfaces; Molecular dynamics simulations; Finite element modeling

1. Introduction

Ductile Cu film of nanoscale thickness bonded to a SiO_2 substrate is an important structure in electronic devices. The delamination of such an interface is known as one of the critical failure modes that is strongly related to device reliability [1–3]. Among a considerable number of experimental methods for measuring delamination strength, nano-indentation-induced delamination is the most common technique and has the unique advantage of simplicity of sample preparation and applicability to small-scale materials [4].

In general, nanoindentation is not always suitable for delaminating a ductile film due to its considerable plastic deformation during loading [5]. To address this issue, Kriese et al. [6] developed a nanoindentation test utilizing a high-modulus overlayer and demonstrated that the method is capable of promoting delamination of Cu film with a wide range of thickness. However, even if delamination

* Corresponding author. *E-mail address:* hara.shotaro@fml.t.u-tokyo.ac.jp (S. Hara). can be successfully achieved, accurately determining the value of interfacial toughness Γ is a crucial task. Based on a linear fracture mechanics concept, Γ is defined as the value of the critical stain energy release rate G_{crit} when the interface crack starts to grow. In indentation testing, the value of G_{crit} is estimated using the Marshall and Evans mechanics model [7]. Although this model has been widely applicable, it is actually premised on a simple assumption about the complex plastic deformation of ductile film induced by the indenter [4]. Since the detailed mechanisms involved are still unclear, it is essential to understand the relationship between the defect evolutions during loading and the interfacial cracking process.

Our objective is to use atomistic-based multiscale modeling to gain knowledge about how dislocation behavior in nanoscale ductile film on an elastic substrate affects the onset of interfacial cracking. For the same situation of ductile film on an elastic substrate system, several numerical studies using the finite element method (FEM) have previously been performed [8,9], mainly devoted to investigating the effect of the interfacial adhesive properties on the

^{1359-6454/\$36.00} \odot 2009 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved. doi:10.1016/j.actamat.2009.05.018

delamination process. On the other hand, while an atomistically based approach is a powerful computational probe for providing insight into the defect behavior at fully atomistic resolution, few works have addressed crack initiation in the above system. The previous atomistic simulations have been limited to tackling the incipient plasticity event (such as dislocation nucleation) during indentation [10,11].

The approach we develop here involves coupling molecular dynamics (MD) and the continuum calculation based on a FEM. Our approach was applied to nanoindentation simulations in the Ru/Cu/SiO₂ system. The choice of Ru as an overlayer was motivated by: (i) its high bulk modulus K_{Ru} , compared to that of Cu ($K_{Ru}/K_{Cu} = 2.3$) and (ii) its promise as a diffusion barrier material in recent Cu interconnects [12]. In this study, we report several atomic-level findings regarding the mechanism of interfacial cracking. In addition, to investigate the effect of the high-modulus overlayer on the cracking mechanism, the results are compared with nanoindentation in the Cu/SiO₂ system.

2. MD-FEM coupling model

A two-dimensional (2D) schematic of the MD–FEM coupling model is shown in Fig. 1. The model consists of a 6 nm thick Cu layer, capped by a 4 nm thick Ru layer, on a 84 nm thick glass (SiO₂) substrate. The Ru, Cu and a part of the glass substrate region are treated by MD. Since the SiO₂ is separate from the indenter, the region should behave as an elastic solid. This permits us to treat the large part of the substrate within a linear elastic approximation in FEM, except near the Cu/SiO₂ interface, where a crack would nucleate. For the present case, the substrate region, 5 nm from the Cu/SiO₂ interface, is considered as a continuum. For the MD region, the periodic boundary conditions are applied along the x and y direction, while the top surface of Ru is traction free. The sys-



Fig. 1. 2D schematic of the nanoindentation model using a coupled MD–FEM framework.

tem contains about 1.1 million atoms and the cell sizes are $10 \text{ nm} \times 100 \text{ nm} \times 94 \text{ nm}$. The length of the x axis is large enough to capture the 3D feature of dislocation behavior.

We use the generalized embedded atom method potential [13] to describe the Ru-Ru, Ru-Cu and Cu-Cu interactions. Since the parameter sets for Ru are lacking, new sets are separately developed according to the fitting procedure given in Refs. [14,15]. The crystallographic directions along the cell are $x = [11\overline{2}0], y = [\overline{1}100]$ and z = [0001] for the hexagonal close-packed (hcp) Ru lattice, and $x = [10\overline{1}],$ $y = [\overline{1}2\overline{1}]$ and z = [111] for the face-centered cubic (fcc) Cu lattice. For both materials, the number of unit lattices involved along the x, y axes in the cell was chosen so as to minimize the residual misfit strain (below 0.01%) [16]. Thus, the Ru/Cu interface is semicoherent and includes misfit dislocations.

To simplify the modeling, the substrate atoms are described as a spring model with a fcc lattice structure. Here, the spring constant is given to reproduce a bulk modulus of 100 GPa and the lattice constant is identical to that of Cu. In fact, the real oxide glass has a complicated amorphous structure. However, as several experiments and FEM simulations have already demonstrated [9,17,18], the glass substrate never yields until the indenter penetrates the substrate due to the yield stress of glass being significantly higher than that of ductile film. Thus, the above substrate modeling is reasonable. It should be noted that the Cu/SiO₂ interface is atomistically coherent, but dislocations emitted during indentation cannot penetrate into the substrate.

Currently, the structural and physical properties of the Cu/SiO_2 interface are still unclear [19], and it is not a straightforward task to represent the bonding properties of the Cu/SiO_2 interface in an empirical manner. From this perspective, the interactions between Cu atoms and glass atoms are modeled using the Lennard-Jones-type potential function. The parameter sets are defined to reproduce the intrinsic adhesion energy (thermodynamic work of adhesion) W_{ad} between Cu and SiO₂. The W_{ad} value has been measured using various methods. From density functional theory (DFT) calculation, Nagao et al. [19] directly determined the W_{ad} of 0.331 J m⁻² between Cu and SiO₂ terminated with hydroxyls. Kriese et al. [20] estimated the W_{ad} of 0.2 J m⁻² based on contact angle theory. They also experimentally predicted the Wad using a nanoindentaioninduced delamination testing. While the measured values have a large scatter, the maximum of their distribution is within the range of $0.2-0.3 \text{ Jm}^{-2}$ (see Fig. 6b in Ref. [20]). Thus, the W_{ad} of 0.2 J m⁻² is used here. Further discussion about the dependence of the crack nucleation mechanism on W_{ad} is given in Ref. [21]. Nevertheless, compared to the intrinsic adhesion energy of 4.6 Jm^{-2} for the Ru/Cu interface, Cu/SiO₂ is regarded as a considerably weaker interface in the present system.

Several techniques to couple the MD and FEM region have been developed. The advantages and disadvantages

of each technique were described in a recent review paper [22]. For the present study, we use the patch approach presented in Ref. [23]. Only a brief description is given here; more details have been provided elsewhere [21]. In this approach, the atomistic and continuum regions are treated as separate systems, while the displacement of the atoms or nodes at the MD/FEM transition region is prescribed through the displacement-interpolation algorithm. Through the energy minimization calculation, the mechanical equilibrium of entire systems is realized. Here, since the original version is limited to the static method, we extend the method to the finite-temperature dynamic framework by introducing Qu's scheme [24]. The Langevin-type thermostat layers are inserted in the substrate region to a thickness of 4 nm. For the FEM part, 13,000 eight-node hexahedron elements are used and the Watson Sparse Matrix Package (WSMP) [25] is employed as an efficient solver for a linear sparse matrix. Calculation were performed using parallel computing with 16 processors.

For indenting, the rigid and cylindrical shape indenter along the x axis with a radius R of 10 nm is employed. The interaction between the indenter and atoms is described using a simple repulsive potential [26]. The indentation normal to the Ru(0001) surface is performed up to the penetration depth of 5 nm with a constant rate of 10 m s^{-1} . The temperature of the thermostat region was kept constant at 1 K during the simulations. In this study, the loading rate and temperature effects are also considered using different conditions (1 m s⁻¹ and 300 K), and the corresponding results are briefly shown in the following section.

3. Results

In Fig. 2, we show the load-displacement (P-h) curve during indentation. The overall system response can be roughly divided into three different stages (I, II, III), corresponding to the considerable changes in the deformation process under the indenter. In the following, we provide the detailed atomistic mechanisms observed at each stage.

3.1. Stage I: elastic response

The *P*-*h* curve during stage I in Fig. 2 shows that the system responds almost elastically. However, the inelastic events, which cannot be detected from the *P*-*h* response, have already taken place during this stage. We show the atomic displacement distributions of u_y (Fig. 3a) and u_z (Fig. 3b) normal to the x = 0 plane when the indentation depth *h* reaches 0.64 nm (point (A) in Fig. 2). In Fig. 3a, obvious discontinuities of the displacement u_y on the Ru/Cu interface and Cu/SiO₂ interface are found, while the u_z displacement field in Fig. 3b is completely continuous. The discontinuities at the Ru/Cu interface are attributed to interfacial sliding mediated by misfit dislocation. On the other hand, the discontinuity on the Cu/SiO₂ interface results from the creation of the misfit dislocation. These



Fig. 2. Load-displacement (P-h) curve during indentation. Stages I–III correspond to the typical changes in the deformation process under an indenter. Atomistic views of points (A)–(E) are described in the text.

inelastic events mainly occur at the region within 10 nm from the z axis, where the shear stress acting on both interfaces is relatively high.

3.2. Stage II: dislocation nucleation under the indenter

The typical deformation mechanism observed in stage II is a heterogeneous dislocation nucleation below the contact area. Snapshots at indentation depths of h = 1.92 nm(Fig. 4a) and of h = 2.20 nm (Fig. 4b) are shown. For clarification, the surface, interface, hcp Cu and fcc Ru atoms are presented in these figures. The local structure (fcc or hcp) of each atom is defined through the CNA analysis [27]. The first load drop at point B in Fig. 2 corresponds to the heterogeneous nucleation of the Shockley partial dislocation in Cu from the Cu/SiO₂ interface, as denoted by (i) in Fig. 4a. The second load drop at point C in Fig. 2 is a signal for heterogeneous nucleation of the dislocation from the Ru/Cu interface. At the second drop, the Shockley partial dislocations on the $\{111\}$ slip plane in the Cu nucleate from the Ru/Cu interface (see arrow (ii) in Fig. 4b). At almost the same time, the perfect dislocations on the $\{1010\}$ slip plane of Ru also nucleate from the same interface (see arrow (iii) in Fig. 4b).

3.3. Stage III: onset of the cracking at the Cu/SiO₂ interface

As shown in Fig. 2, at the indentation depth h of 4.14 nm, the *P*-h curve reaches its maximum value $P_{\rm crit}$, followed by a rapid drop in the load *P*. The remarkable point at the stage III is the interfacial cracking induced by the heterogeneous dislocation nucleation. The sequences of the MD snapshots during the interfacial cracking are

S. Hara et al. | Acta Materialia 57 (2009) 4209-4216



Fig. 3. Cross-section views of the MD region below the cylindrical indenter. Atomic displacement distributions of (a) u_y and (b) u_z normal to the x = 0 plane, at the indentation depth h = 0.64 nm, are illustrated.

displayed in Fig. 5a–d. Prior to the load drop $P = 0.87P_{crit}$, when the indentation depth is 3.95 nm (point D in Fig. 2), the leading partial dislocation of the Burgers vector $\mathbf{b} = a_0/6[121](\overline{1}1\overline{1})$ nucleates from the Cu/SiO₂ interface heterogeneously (Fig. 5a), where the $a_0 = 3.615$ Å is the lattice constant of Cu. The nucleation site is 2.75a (16.3 nm) away from the central axis, where a is the contact radius defined by $a = \sqrt{2Rh - h^2}$. We see that this slip triggers a small cracking zone, as denoted in Fig. 5a. Subsequently, the following nucleation of the trailing partial dislocation of $\mathbf{b} = a_0/6[21\overline{1}](\overline{1}1\overline{1})$ on the same slip plane enhances the extent of the cracking, as shown in Fig. 5b. The load then reaches a maximum $(P = P_{crit}, point E in$ Fig. 2) when the length of the interfacial crack becomes about 7 nm (Fig. 5c). For further loading, the crack propagates rapidly toward the -y direction along the Cu/SiO₂ interface in a brittle manner (Fig. 5c and d). Plastic events in the Ru layer and at the crack tip are not observed during crack propagation (Fig. 5d). During the indentation of 5 nm, cracking occurs only at the left side with respect to the z axis (y < 0 region). We find that the buckling failure mode shown in Fig. 5d is qualitatively similar to recent observations during adhesion testing [1,4].

Here, the results for a different loading rate (1 m s^{-1}) and temperature (300 K) are mentioned briefly. In both cases, the underlying deformation mechanisms until interfacial cracking occurs are analogous to that reported in this section. For the simulation with a rate of 1 m s^{-1} , the *P*-*h* curve reaches its maximum value P_{crit} at an indentation depth h_{crit} of 4.07 nm, which is close to that for 10 m s⁻¹ case. On the other hand, for the simulation at 300 K, the obtained indentation depth h_{crit} is 3.75 nm, which is about 10% lower than that for 10 m s⁻¹ case. The reduction in indentation depth at 300 K indicates that the heterogeneous dislocation nucleation event illustrated in Fig. 5 is thermally activated.

4. Discussions

4.1. Crack nucleation mechanism based on heterogeneous dislocation nucleation

One of the striking results of our simulation is that interfacial crack nucleation takes place through the mediation of the slip event. In this section, we investigate the local stress state near the Cu/SiO_2 interface in order to provide



Fig. 4. Atomistic views of the MD region below the cylindrical indenter. Structures of heterogeneously nucleated dislocation at the indentation depths of (a) 1.92 nm and (b) 2.20 nm are presented. The hcp Cu atoms (red) and fcc Ru atoms (light blue) are displayed as defect atoms. Surface and interface atoms of Ru (purple), interface atoms of Cu (yellow), and interface atoms of SiO₂ (green) are also shown. Each arrow represent (i) Shockley partial dislocations in Cu emitted from Cu/SiO_2 interface; (ii) Shockley partial dislocations in Cu emitted from Ru/Cu interface. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

S. Hara et al. | Acta Materialia 57 (2009) 4209-4216



Fig. 5. Atomistic views of interfacial cracking process in the $Ru/Cu/SiO_2$ system. The left side with respect to the *z* axis within MD region are shown. Each view is at the indentation depths of (a) 3.95 nm, (b) 4.01 nm, (c) 4.14 nm, and (d) 4.53 nm. The colors of the snapshots are the same as those in Fig. 4.

further understanding of this complex mechanism. In Fig. 6 we show the stress distributions of the σ_v and σ_z components along the -y direction on the Cu/SiO₂ interface just before the heterogeneous nucleation of the leading partial dislocation. Each point represents an averaged value of the atomic stress in Cu within 2.0 nm from the interface. As expected, a high compressive stress of σ_z is found below the contact region. It is also recognized that the tensile stress of σ_z gives a peak value of approximately 1.6 GPa outside the contact region. The tensile stress is caused by the resistance of the substrate against the film bending [28,29]. On the other hand, the indenter also provides the compressive σ_{v} stress over a wide range along the y axis. Based on these stress components, the resolved shear stress τ_{rss} for the leading partial dislocation of $\mathbf{b} = a_0/6[1\,2\,1](\bar{1}\,1\,\bar{1})$ is computed (Fig. 6). Clearly, at the crack nucleation site, which



Fig. 6. Stress distributions of the σ_y and σ_z components along the -y direction at the Cu/SiO₂ interface (*a* is the contact radius) just before the heterogeneous nucleation of the leading partial dislocation of $\mathbf{b} = a_0/6$ [121]($\bar{1}1\bar{1}$). Resolved shear stress τ_{rss} with respect to the [121]($\bar{1}1\bar{1}$) slip system is also shown.

is about 2.75*a* apart from the central *z* axis, the τ_{rss} distribution reaches its maximum value of 3.0 GPa. This value of τ_{rss} is close to the theoretical shear strength of 2.0 GPa for this empirical potential. Thus, it is reasonable to suppose that the cracking site is a preferable site for heterogeneous dislocation nucleation.

It is also important to discuss the possibility that the interfacial separation at this site occurs prior to dislocation nucleation. Here, we investigated the ideal interfacial tensile strength for Cu/SiO₂ using a simple MD simulation. We observed the failure at the Cu/SiO_2 interface when a 1.65% tensile strain normal to the interface is imposed. An interfacial tensile strength of about 2.2 GPa is obtained, which is higher than the interfacial normal stress of 1.6 GPa acting on the cracking site. To check the effect of the other stress components (particularly the high compressive stress in y direction) on the interfacial tensile strength, we have carried out the loading test, in which the σ_v of -7.5 GPa is kept constant. The resulting interfacial tensile strength of 1.9 GPa is still higher than 1.6 GPa. These clearly demonstrate how the dislocation nucleation event triggers interfacial crack nucleation.

We consider the above mechanism to be characteristic of nanoscale film samples since a heterogeneous dislocation nucleation is likely to be a dominant process for the plastic deformation in small-volume samples due to dislocation source starvation in the bulk [30]. As O'Day has demonstrated [29], if film thickness reaches the submicron scale, crack nucleation may be driven by collective dislocation motion activated by Frank–Read sources in the bulk.

4.2. Effect of high-modulus Ru overlayer on crack propagation process

To discuss the effect of the high-modulus Ru overlayer on the crack propagation process, we performed a nanoindentation simulation of the Cu/SiO₂ system and compared it with the result for the Ru/Cu/SiO₂ system. First, the time evolution of the crack propagation distance is shown in Fig. 7. As mentioned in the previous section, in the Ru/Cu/SiO₂ case, the crack advances along the interface in a brittle manner with a speed of about 370 m s⁻¹ once the crack nucleates. On the other hand, in the Cu/SiO₂ case, the crack propagation is significantly retarded and less driven (Fig. 7). This difference infers that the use of the high-modulus overlayer tends to facilitate the delamination of the Cu film, and the tendency is consistent with the experimental result [1,4,6].

Here, an atomic-level interpretation is given through MD snapshots during indentation (Fig. 8a-d). One of the unique features in the Cu/SiO₂ system is that the Cu free surface plays an important role as a preferred dislocation source ((i) in Fig. 8a). At the indentation depth of about 3 nm, multiple dislocation nucleation on the $(\overline{1}1\overline{1})$ slip plane takes place continuously from the left contact edge of the indenter ((ii) in Fig. 8b), and these dislocations trigger crack nucleation at the Cu/SiO₂ interface ((iii) in Fig. 8b). During subsequent loading, as shown in Fig. 8c, we observe complicated defect behavior in the system. Accompanied by slow crack extension, a large amount of dislocation is emitted from the upper crack surface. Some of these dislocations behave as threading-type dislocations which propagate above the crack in the -y direction ((iv) in Fig. 8c). Others travel toward the surface and form the pile-up region on the Cu surface ((v) in Fig. 8c). In addition, several dislocations newly nucleate from the Cu surface ((vi) in Fig. 8c), which result in subcrack generation ahead of the main crack ((vii) in Fig. 8c). These subcracks



Fig. 7. Time evolution of the crack propagation distance during indentation into the $Ru/Cu/SiO_2$ system and the Cu/SiO_2 system, respectively.



Fig. 8. Atomistic representations of interfacial cracking process in the Cu/SiO₂ system. The left side with respect to the *z* axis within the MD region is shown. Each view corresponds to indentation depths of (a) 2.54 nm, (b) 3.06 nm, (c) 3.97 nm, and (d) 4.62 nm. The colors of the snapshots are the same as those in Fig. 4. Each arrow represents (i) Shockley partial dislocation nucleation from the left contact edge of the indenter, (ii) multiple dislocation nucleation at the Cu/SiO₂ interface, (iv) threading-type dislocations propagating above the crack in the -y direction, (v) pile-up region on the Cu surface, (vi) dislocation nucleation from the Cu surface, and (vii) subcrack nucleation ahead of the main crack.

relieve or alter the stress state of the main crack tip and lead to the retardation of crack advance or crack tip closing. It seems that the driving force for crack propagation in the Cu/SiO₂ case is considerably reduced due to the plastic energy dissipation, compared to the Ru/Cu/SiO₂ case.

More importantly, it should be noted that, in previous experiments, the elastic buckling model is employed to determine the interfacial toughness. This model implicitly assumes that the crack tip is apart from the plastic zone and its stress field remains almost elastic during delamination. The previous FEM simulation for the ductile film on elastic substrate demonstrated that the crack tip is located inside the plastic zone, and the above assumptions are not valid [8]. Our atomistic result shown in Fig. 8 supports these earlier findings.

In contrast, our simulation for the $Ru/Cu/SiO_2$ system clearly shows that the dislocation production and evolution in Cu is restricted only near the indenter since the Ru needs high energy to create a new dislocation and can store a lot of elastic energy in the overlayer. As a result, the crack tip completely leaves the plastic zone during crack extension. This would satisfy the above assumptions. Thus, it can be said that nanoindentation test utilizing a Ru overlayer is capable of providing a reasonable measure of interfacial toughness within an elastic framework.

5. Conclusions

To address an atomistic aspect of crack nucleation and propagation at the Cu/SiO_2 interface, we carried out nanoindentation simulations for the $Ru/Cu/SiO_2$ system using the finite-temperature MD–FEM coupling approach. The simulation shows that heterogeneous dislocation nucleation triggers interfacial crack nucleation. The analysis also focuses on the effect of the Ru overlayer on the onset of interfacial cracking through the simulations with and without a high-modulus Ru overlayer. In the system with a Ru overlayer, the crack propagates along the interface in a

Table A.1

Caluculated physical properties of Ru using the present GEAM potential. Values of the cohesive energy E_{hcp} , the lattice constants a_0, c_0 , the bulk modulus K, the elastic constants C_{ij} , the structural energy differences ΔE , the unstable stacking fault energy for basal plane γ_{us} , the intrinsic stacking fault energy for basal plane γ_s , and the heats of solution ΔH for several Cu–Ru binary systems are listed. The experimental values are also shown for comparison.

| | GEAM (this work) | Exp. |
|---|------------------|------------|
| $E_{\rm hcp}~({\rm eV/atom}^{-1})$ | -6.74 | -6.74 [31] |
| a_0 (Å) | 2.69 | 2.70 [32] |
| c_0 (Å) | 4.35 | 4.28 [32] |
| K (GPa) | 310 | 310 [33] |
| <i>C</i> ₁₁ (GPa) | 439 | 563 [33] |
| C_{12} (GPa) | 209 | 188 [33] |
| C_{13} (GPa) | 183 | 168 [33] |
| C ₃₃ (GPa) | 755 | 624 [33] |
| C ₅₅ (GPa) | 117 | 181 [33] |
| $\Delta E_{\rm bcc-hcp}$ (eV atom ⁻¹) | 0.058 | _ |
| $\Delta E_{\rm fcc-hcp}$ (eV atom ⁻¹) | 0.046 | _ |
| $\gamma_{us} (mJ m^- 2)$ | 606 | _ |
| $\gamma_{s} (mJ m^{-}2)$ | 238 | _ |
| $\Delta H_1 \ (\text{eV} \text{ atom}^{-1})^{\text{a}}$ | 0.111 | 0.104 [34] |
| $\Delta H_2 \ (\text{eV} \text{ atom}^{-1})^{\text{b}}$ | 0.088 | 0.062 [34] |
| $\Delta H_3 \ (\text{eV atom}^{-1})^{\text{c}}$ | 0.102 | 0.104 [34] |
| $\Delta H_4 \ (\text{eV} \text{ atom}^{-1})^{\text{d}}$ | 0.082 | 0.073 [34] |

^a ZnS-type RuCu.

^b fcc-type Ru₃Cu₁.

^c fcc-type Ru₂Cu₂.

^d fcc-type Ru₁Cu₃.

brittle manner once the crack nucleates. On the other hand, without a Ru overlayer, the crack propagation is significantly retarded and less driven due to a large number of plastic events during loading. The simulation results provide a clear physical picture of recent experimental results, and demonstrate that nanoindentation utilizing a highmodulus Ru overlayer is an effective test for evaluating Cu film delamination.

Acknowledgement

This research was partially supported by the Ministry of Education, Science, Sports and Culture, Grant-in-Aid for Young Scientists(B), 19760058, 2008.

Appendix A. GEAM potential for hcp Ru

A way of determining the interatomic potential of hcp Ru using an generalized embedded atom method is shown in Ref. [14,15]. Here, Table A.1 provides a list of physical properties of Ru associated with the present potential.

References

- [1] Gerberich WW, Cordill MJ. Rep Prog Phys 2006;69:2157.
- [2] Lane M. Annu Rev Mater Res 2003;33:29.
- [3] Turner MR, Evans AG. Acta Mater 1996;44:863.
- [4] Volinsky AA, Moody NR, Gerberich WW. Acta Mater 2002;50:441.
- [5] Lee A, Clemens BM, Nix WD. Acta Mater 2004;52:2081.
- [6] Kriese MD, Gerberich WW, Moody NR. J Mater Res 1999;14:3007.
- [7] Marshall DB, Evans AG. J Appl Phys 1984;56:2632.
- [8] Li W, Siegmund T. Acta Mater 2004;52:2989.
- [9] Zhang YW, Zeng KY, Thampurun R. Acta Mater 2001;319:893.
- [10] Vliet KJV, Li J, Zhu T, Yip S, Suresh S. Phys Rev B 2003;67:104105.
- [11] Li J, Vliet KJV, Zhu T, Yip S, Suresh S. Nature 2002;418:307.
- [12] Damayanti M, Sritharan T, Gan ZH, Mhaisalkar SG, Jiang N, Chan L. J Elctro Soc 2006;153:41.
- [13] Zhou XW, Wadley HNG, Johnson RA, Larson DJ, Tabat N, Cerezo A, et al. Acta Mater 2001;49:4005.
- [14] Kumagai T, Hara S, Izumi S, Sakai S. Mater Sci Forum 2006;539:2123.
- [15] Kumagai T, Nikkuni D, Hara S, Izumi S, Sakai S. Mater Trans 2007;48:1313.
- [16] Streitz FH, Cammarata RC, Sieradzki K. Phys Rev B 1994;49:10707.
- [17] Kramer DE, Volinsky AA, Moody NR, Gerberich WW. J Mater Res 2001;16:3150.
- [18] Saha R, Xue Zhenyu, Huang Y, Nix WD. J Mech Phys Solids 2001;49:1997.
- [19] Nagao K, Neaton JB, Ashcroft NW. Rhys Rev B 2003;68:125403.
- [20] Kriese MD, Gerberich WW, Moody NR. J Mater Res 1999;14:3019.
- [21] Hara S, Izumi S, Sakai S, Eguchi Y, Iwasaki T. Mater Res Soc Symp Proc 2008;1086:U08–29.
- [22] Curtin WA, Miller RE. Model Simul Mater Sci Eng 2003;11:33.
- [23] Kohlhoff S. Philos Mag A 1991;64:851.
- [24] Qu S, Shastry V, Curtin WA, Miller RE. Model Simul Mater Sci Eng 2005;13:1101.
- [25] <http://www.alphaworks.ibm.com/tech/wsmp>.
- [26] Kelchner CL, Plimpton SJ, Hamilton JC. Phys Rev B 1998;58:11085.
- [27] Ackland GJ, Jones AP. Phys Rev B 2006;73:054104.
- [28] Abdul-Baqi A, Van der Giessen E. J Mater Res 2001;16:1396.
- [29] O'Day MP, Nath P, Curtin WA. J Mech Phys Solids 2006;54:2214.
- [30] Zhu T, Li J, Samanta A, Leach A, Gall K. Phys Rev Lett 2008;100:025502.

4216

- [31] Kittel C. Introduction to solid state physics. New York: Wiley-Interscience; 1996.
- [32] Barrett CS, Massalski TB. Structure of metals. 3rd ed. Oxford: Pergamon Press; 1980.
- [33] Brandes EA, Brook GB. Smithells metal reference book. 7th ed. Oxford: Butterworths; 1992.
- [34] de Boer FR, Boom R, Mattens WC, Miedema AR, Nisessen AK. Cohesion in metals. North-Holland: Amsterdam; 1988.