Molecular Dynamics Simulation on Microstructure and Deformation Properties Related to Porosity in Al Thin Film Sputtered on Si Substrate*

Takashi IIZUKA**, Akira ONODA**
and Toshihiko HOSHIDE***

A material system of Al sputtered on crystalline Si was dealt with as one of the simple material models for semiconductor material systems. To investigate qualitative properties of sputtered films on an atomic scale, simulations were conducted by a molecular dynamics (MD) method using two film models; i.e. a deposition model based on MD simulations of sputtering process and a crystal model using a crystalline Al film instead of a deposited one. The surface roughness and porosity, which are defined in this work, were found to decrease with an increase in the incident energy of atoms. Relationships between tensile deformation properties and porosities in simulated thin films were also investigated. Although the porosity was found to affect the tensile strength in the direction parallel to the substrate surface, it was revealed that the tensile strength in the direction perpendicular to the substrate surface was hardly influenced by the difference in the porosity.

Key Words: Molecular Dynamics, Thin Film, Sputtering, Microstructure, Porosity, Tensile Strength, Silicon, Aluminum

1. Introduction

Mechanical properties of thin films should be clarified to improve the performance and reliability of micro-devices having film structures. Although experimental works on the subject have been carried out, computer simulations of molecular dynamics (MD) and Monte Carlo types are also applied to obtain atomic scale information. These simulations inform us of characteristics such as film structures, residual stresses⁽¹⁾, and collision behavior of atom moving toward the substrate⁽²⁾, among others. However, only few works are available regarding the fracture behavior of thin films including their formation processes. This may be associated with the difficulty in evaluating interfaces with a long-term periodicity due to misfit in experiments and due to the large cell required in MD simulations. However,

qualitative properties of sputtered films on an atomic scale can be elucidated by appropriate applications of MD simulations for metallic and covalent bonding systems. Such simulations are performed on the basis of the effective medium theory⁽³⁾, the embedded atom methods (EAM)⁽⁴⁾ for metals and the Tersoff potential for silicon⁽⁵⁾.

The preset work deals with Al sputtered on a Si system as one of the simple material models for semiconductor material systems. The process of deposition and the resultant film structures with pores are investigated by MD simulations. Potential functions to be used are first stated, and two models of the Al film deposited on the Si substrate are proposed to clarify the difference in film characteristics due to the variation of film structure. Using the proposed models, surface roughness, porosity and tensile properties are evaluated, and the relationships among them are also discussed.

2. Interatomic Potential

The embedded atom method (EAM) potential is widely used for metallic materials, though the modified embedded atom method (MEAM) potential

* Received 10th May, 2000

** Graduate Student, Graduate School of Energy Science, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan. E-mail: tiizuka@ipc.kit.ac.jp

*** Department of Energy Conversion Science, Kyoto University, Sakyo-ku, Kyoto 606-8501, Japan

is developed as an extension to the EAM one⁽⁴⁾ in particular to describe the structure of covalent bonding⁽⁶⁾. In this simulation, the MEAM potential is used to specify interactions between atoms in the system under consideration, because it is desirable that both covalent and metallic bonding structures can be dealt with on the same theoretical basis. In this system, the total energy E_{tot} is expressed by

$$E_{\text{tot}} = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j \neq i} \phi_{ij}(r_{ij}) \right\}. \quad (1)$$

In Eq. (1), F_i and $\bar{\rho}_i$ are the embedding function and the background electron density of atom i , respectively. The pair potential ϕ_{ij} is the function of the distance r_{ij} between atoms i and j . The potential functions used in this simulation are given elsewhere⁽⁷⁾. To restrict the range of atomic interaction, a cutoff function f_c , which includes only interactions between the first neighbor atoms, is introduced instead of the screen function. Si-Si and Al-Al interactions are described using the potential parameters given by Baskes⁽⁶⁾. On the other hand, the parameters for Si-Al interaction are determined by the procedure recommended by Baskes et al.⁽⁸⁾ In addition, the equilibrated structure of Al_{12}Si cluster^{(9),(10)} is adopted as the reference system for lack of detailed information available about metastable bulk structures for the Si-Al binary system. Although such a cluster structure as a reference system is insufficient for the description of properties of a bulk system, it is convenient to use a small system for considering the symmetry of the system and formulating the binary pair potential.

The pair potential functions are given as follows. For the same atom,

$$\phi_{\text{elm}}(r_{ij}) = \frac{2}{Z_{\text{elm}}^{\text{ref}}} \{ f_c(r_{ij}) E_{\text{elm}}^{\text{u}}(r_{ij}) - F_{\text{elm}}[\bar{\rho}_{\text{elm}}^{\text{ref}}(r_{ij})] \} \quad (\text{elm} = \text{Si or Al}) \quad (2)$$

and for the Si-Al system,

$$\begin{aligned} \phi_{\text{Si-Al}}(r_{ij}) = & \frac{13}{12} f_c(r_{ij}) E_{\text{cls}}^{\text{u}}(r_{ij}) - \frac{1}{12} F_{\text{Si}}(\bar{\rho}_{\text{Si}}^{\text{cls}}) \\ & - F_{\text{Al}}(\bar{\rho}_{\text{Al}}^{\text{cls}}) - \frac{5}{2} \phi_{\text{Al}}(n_2^{\text{cls}} r_{ij}). \end{aligned} \quad (3)$$

The superscripts and subscripts 'ref' and 'cls' present parameters for the reference and cluster systems, respectively. Functions and parameters in Eqs. (2) and (3) are specified in the following.

E^{u} is the universal equation of state proposed by Rose et al.⁽¹¹⁾, and is expressed as

$$E_{\text{elm}}^{\text{u}}(r) = -E_{\text{elm}}^{\text{c}}(1 + a_{ij}^*) \exp(-a_{ij}^*), \quad (4)$$

$$a_{ij}^* = \alpha_{\text{elm}} \left(\frac{r_{ij}}{r_{\text{elm}}^{\text{eq}}} - 1 \right), \quad (5)$$

$$\alpha_{\text{elm}}^2 = \frac{9\Omega_{\text{elm}}^{\text{eq}} B_{\text{elm}}^{\text{eq}}}{E_{\text{elm}}^{\text{c}}}. \quad (6)$$

In the above equations, the subscript 'elm' denotes parameters in each reference system (i.e. Al, Si and

Al_{12}Si cluster), and the superscript 'eq' indicates those for the equilibrium state. The parameter α is determined by the atomic volume Ω , the bulk modulus B and the cohesive energy (the energy for binding cluster) E^{c} . For cluster systems, the universal function is not always appropriate, though it is used in this simulation for convenience. Z is the number of first neighbors, and n_2 is the ratio of the second nearest neighbor distance to the first nearest one in the cluster Al_{12}Si . In the cluster structure, the distances of the first and second nearest neighbors for Al is so short that both interactions should not be ignored. Therefore, the terms associated with the second nearest neighbor interaction for Al are also included in this formulation.

For the embedding function, the following equations are applied.

$$F_{\text{elm}}(\bar{\rho}_i) = A E_{\text{elm}}^{\text{c}} \frac{\bar{\rho}_i}{Z_{\text{elm}}^{\text{ref}} \rho_{\text{elm}}^0} \ln \frac{\bar{\rho}_i}{Z_{\text{elm}}^{\text{ref}} \rho_{\text{elm}}^0} \quad (\text{elm} = \text{Si or Al}). \quad (7)$$

The background electron density $\bar{\rho}_i$ for atom i is assumed to be a spherically symmetric partial density $\bar{\rho}_i^{(0)}$ modified by including angular contributions; i.e.

$$\bar{\rho}_i = \rho_i^{(0)} G(\Gamma_i), \quad (8)$$

$$G(\Gamma_i) = \frac{2}{1 + \exp(-\Gamma_i)}, \quad (9)$$

$$\Gamma_i = \sum_{h=1}^3 t_i^{(h)} \left(\frac{\rho_i^{(h)}}{\rho_i^{(0)}} \right), \quad (10)$$

where $t_i^{(h)}$ ($h=0 \sim 3$) are weight constants for atom i . Partial electron densities $\rho_i^{(h)}$ ($h=0 \sim 3$) are given by the summation of the atomic density contribution $\rho_j^{a(h)}(j \neq i)$ from neighboring atoms as follows.

$$\rho_i^{(0)} = \sum_{j \neq i} \rho_j^{a(0)}(r_{ij}), \quad (11)$$

$$(\rho_i^{(1)})^2 = \sum_k \left[\sum_{j \neq i} \rho_j^{a(1)}(r_{ij}) \frac{r_{ij}^k}{r_{ij}} \right]^2, \quad (12)$$

$$(\rho_i^{(2)})^2 = \sum_{k,l} \left[\sum_{j \neq i} \rho_j^{a(2)}(r_{ij}) \frac{r_{ij}^k r_{ij}^l}{r_{ij}^2} \right]^2 - \frac{1}{3} \left[\sum_{j \neq i} \rho_j^{a(2)}(r_{ij}) \right]^2, \quad (13)$$

$$(\rho_i^{(3)})^2 = \sum_{k,l,m} \left[\sum_{j \neq i} \rho_j^{a(3)}(r_{ij}) \frac{r_{ij}^k r_{ij}^l r_{ij}^m}{r_{ij}^3} \right]^2, \quad (14)$$

where k , l and m imply three orthogonal directions in a given coordinate system. The partial electron densities describe structural contributions from different symmetries of the system. Each atomic density is presented by the following exponential form.

$$\rho_{\text{elm}}^{a(h)}(r) = f_c(r) \rho_{\text{elm}}^0 \exp \left[-\beta_{\text{elm}}^{(h)} \left(\frac{r}{r_{\text{elm}}^{\text{eq}}} - 1 \right) \right] \quad (\text{elm} = \text{Si or Al}), \quad (15)$$

where the cutoff function $f_c(r)$ is defined as

$$f_c(r) = \begin{cases} 1 & \text{for } x \geq 1 \\ [1 - (1 - x(r))^4]^2 & \text{for } 0 < x < 1, \\ 0 & \text{for } x \leq 0 \end{cases} \quad (16)$$

$$x(r) = \frac{r_c - r}{\Delta r}. \quad (17)$$

Table 1 Potential parameters for Si-Al interaction

$E_{\text{cls}}^{\text{c}}(\text{eV})$	$r_{\text{cls}}^{\text{eq}}(\text{\AA})$	α_{cls}	ρ_{Al}^0
2.96	2.59	4.635	1.975

The cutoff distance r_{c} and the cutoff region Δr are set to be 3.6 and 1.0 ($\text{\AA}$), respectively.

New parameters to be given for simulations are density scaling parameters ρ_{Si}^0 , ρ_{Al}^0 and Si-Al pair potential parameters $E_{\text{cls}}^{\text{c}}$, $r_{\text{cls}}^{\text{eq}}$ and α_{cls} . Although the Si-Al pair potential parameters may be directly available elsewhere⁽⁹⁾, ρ_{Si}^0 is set to be 1 for convenience. Another parameter ρ_{Al}^0 can be determined if Al adsorption properties on the Si(001)2 $\times$ 1 reconstruction surface^{(12),(13)} are used. Finally, ρ_{Al}^0 , $E_{\text{cls}}^{\text{c}}$ and α_{cls} are adequately modified so that the properties of adsorption, e.g. the energy and position of Al atoms, can be roughly described using the parameters. Potential parameters to be used in this work are listed in Table 1. However, these parameters can only reproduce the Al₁₂Si cluster structure and energetic tendency of a single Al atom on the Si(100)2 $\times$ 1 reconstructed surface. Using these parameters, it is impossible to discuss Si-Al interaction and interfacial properties in detail.

For this potential function, the stress of the system σ_{kl} is calculated using the general equation as below.

$$\sigma_{kl} = \frac{1}{2V} \sum_i \sum_{j(\neq i)} \frac{\partial E_{\text{tot}}}{\partial r_{ij}^k} r_{ij}^l, \quad (18)$$

where V is the volume of the system considered about.

3. Thin Film Models

In the present simulation, two kinds of models are considered. One is a deposition model and the other is a crystal model. In the deposition model, thin films are formed by MD simulations of sputtering processes. Since the deposited thin films obtained by MD simulations may have some porosity, crystal models are also prepared to investigate the effect of porosity. Details of these models are presented in the following.

3.1 Deposition model

Al thin films are deposited on Si(001)2 $\times$ 1 reconstructed surfaces by MD simulations. The model of the system is illustrated in Fig. 1. The substrate is constructed by arranging eight primitive lattices of Si diamond structure under a periodic boundary condition imposed in the x_1 and x_2 directions. This results in 128 atoms existing in a plane of the unit cell. The aforementioned periodicity is selected because it is known that the Si(001) reconstructed surface usually

Fig. 1 Schematic illustration of deposition process modeling

shows 4 $\times$ 2 periodicity. After ten layers of the (001) plane are stacked in the x_3 direction, atoms in the lowest two layers are fixed and velocities of atoms in the two layers above them are rescaled to keep the system temperature at 300 K. Atoms in the top layer are initially arranged to be similar to the Si(001)2 $\times$ 1 reconstructed surface, but not the crystalline Si(001) surface. After the relaxation calculation of 10 000 steps is carried out, the resultant configuration is used as the initial state of the substrate. The time-step is fundamentally 2 fsec.

Incident Al atoms are placed in the plane 6 $\text{\AA}$ above the highest atom in the substrate or the film, and their positions in the plane are randomly given. The velocity of every incident atom is determined so that a given incident energy can be obtained from the velocity distribution. Incident directions of atoms are randomly assigned within the angle range of 0 to $\pi/3$ against the perpendicular direction to the x_1 - x_2 plane (see Fig. 1). For atoms moving over the length of $r_{\text{c}}/100$ per step, the time-step is changed to be the time interval during which the fastest atom in the system moves by this distance.

An atom incidence is given for every 1 000 steps. If an atom in the system moves up to 6 $\text{\AA}$ over any other atoms in the system, the atom is removed from the system. The simulation is continued until a total of 1 452 atoms is finally deposited on the substrate. In this simulation, two incident conditions are set so that the incident energy of the atom should be 1 eV and 5 eV. Final configurations for both cases are shown in Fig. 2(a). Large and small circles in the figure represent Si and Al atoms, respectively.

For 1 eV incidence, the temperature of the system is held at almost 300 K during the deposition process. For 5 eV incidence, however, the energy incident density is too high to hold it at 300 K and the temperature increases above 1 000 K. Consequently, for 5 eV incidence, a mixed state of atoms of the substrate and

Fig. 2 Configurations of thin films in each model

Fig. 3 Spatial distribution of atoms in x_3 direction

the deposited film appear around the interface. The number distribution of atoms in the x_3 direction is shown in Fig. 3. The distance in the x_3 direction in Fig. 3 is measured from the initial substrate surface. As shown in Fig. 3, it is found that no mixing appears for 1 eV incidence while there is a large amount of mixing in the case of 5 eV incidence. Figure 4 shows the radial distribution function for each element, which indicates amorphous structures of films for both incident energies. For 5 eV incidence, in particular, an amorphous phase is partially seen in the substrate because of the atom mixing as noted above.

3.2 Crystal model

An Al crystal film on a Si substrate is also prepared to compare with the Al deposited film including pores. The Al film is constructed to have a (001) fcc plane on the Si(001) crystalline surface of diamond structure. Eleven primitive lattices in the Al fcc

Fig. 4 Radial distribution functions for deposited films and substrate

structure are arranged in the x_1 and x_2 directions so that 242 atoms exist in a plane of a unit cell. Six layers of the (001) plane are piled up in the x_3 direction, and the crystallographic direction $\langle 100 \rangle$ of Al film is set in the same direction as that of $\langle 100 \rangle$ of the Si substrate.

The aforementioned configuration is chosen, because it is easy to fit the film to the substrate and the configuration is that of the metastable structures. For the crystal model, of course, no pore is introduced in the film. The same relaxation calculation as in the case of only the substrate is executed after the film is placed on the substrate to have no stress in the x_3 direction. The final configuration is shown in Fig. 2 (b).

4. Evaluation of Porosity and Surface Roughness

To evaluate porosity and surface roughness of the deposited film, the surface morphology should be determined. In the atomic view, the surface has a discrete character if the atoms are regarded as rigid spheres. However, it is convenient to consider that the surface is continuous as the surface appears in the macroscopic view. Because atomic radius is approximately defined using the background electron density in addition to continuousness, the background electron density is used for determining the surface morphology in this work. A preliminary calculation is carried out for Al (001) surface as follows. Assuming the Al (001) surface to be a plane in the Al crystal, positions of atoms in the Al film are determined so that the equilibrium volume might be obtained. In this case, the average value of the background electron density in the plane is considered as the background electron density on the surface. It should be noted that only spherical symmetric density is taken into account for calculating the background density. Once the surface

Fig. 5 Division of x_1 - x_2 plane for modulation in characterization of surface morphology

morphology is specified, the surface roughness and the film porosity can be investigated.

It is reasonable to assume that the surface roughness and porosity of the perfect crystal should be nil. Therefore, the following modulations are proposed in this work to eliminate surface roughness and porosity for achieving the perfect crystal surface. The modeling is shown in Fig. 5. A planar modulation introduced first implies that a plane is divided into 11×11 blocks and the average value of all the heights calculated at 20×20 points in each block is evaluated as the height of the block. Although such a modulation can almost exclude the roughness on the scale of the order of one atom, slight differences in height, depending on the procedure of cell division, are still present. To reduce these differences, another modulation is required in the depth direction of the film. After the modulation in the depth direction, the roughness within $0.5 \text{ \AA}$ may be ignored in this simulation.

Using the height evaluated as above, the surface roughness, the volume and surface porosities are evaluated as follows. As illustrated in Fig. 6(a), the surface roughness is calculated as the deviation from the center line of the roughness curve at each block. The height difference from the maximum height of the film is considered to be the depth of a macroscopic surface pore (see Fig. 6(b)). The volume ratio of surface pores to the film volume is defined as the volume porosity. Another porosity, designated as the surface porosity, is also defined as the ratio of the porous area below the average height of the film to the whole surface area of the film (see Fig. 6(c)). The whole surface area corresponds to the area of the x_1 - x_2 plane. The latter porosity is considered to be in the atomic scale.

Generally speaking, the surface roughness is a continuous property and the surface porosity is a discrete property present on the surface. In addition to that, another difference is that the former is the

Table 2 Surface properties in each model

Incident energy (eV)	1	5
Surface roughness ($\text{\AA}$)	1.51	0.593
Volume porosity	0.210	0.126
Surface porosity	0.331	0.339

Fig. 6 Schematic illustrations for definition of surface characteristics

property of only the surface itself and the latter is considered to be related to the inner porosity which differs from surface roughness. However, on an atomic scale of this simulation, surface roughness and surface porosity have almost the same values. In this work, it is required to evaluate the surface porosity because of the reason mentioned above, and the surface roughness is dealt with as the reference value to the surface porosity because that value has clear definition.

Results evaluated as above are listed in Table 2. The surface roughness and the volume porosity are found to decrease with increasing incident energy of atoms. The result may be associated with the substrate temperature during the deposition process. Since the increase in the substrate temperature is observed in the case of 5 eV as mentioned previously, the smoothing behavior of film surface for 5 eV may be explained by the following two phenomena. The collision between an incident atom and an island formed on the film surface may get filled in the

concave regions between islands with atoms. Another possibility is that incident atoms have sufficient energy to move the surface atoms toward the porous regions by collisions.

Regarding the surface porosity, there is no significant difference due to the incidence condition. The result may be attributed to the porosity definition on an atomic scale and may also be related to the unit cell size.

5. Deformation Properties

To investigate the relationship between transformation property and porosity of thin films, two tensile tests in directions parallel and perpendicular to the substrate surface are simulated using the three models prepared as above. In this work, the strength is evaluated for the film-substrate composite system to avoid confusion with film-substrate interface. The results are discussed qualitatively.

5.1 Tensile properties in the direction parallel to the substrate surface

In this simulation, the lowest two layers of the substrate are fixed and the system is located in the direction parallel to the substrate surface, i.e. the x_1 direction. To remove the effect of thermal fluctuation, rescaling is imposed on atoms in the rest of the system so that the system temperature can be maintained of 5 K. After the total stress in the system is relaxed to become 0 MPa, the uniform deformation is carried out for the system.

In general, only the local deformation is essential for an amorphous structure and uniform deformation is not valid. However, a fixed region exists in this model and it is difficult to express the local deformation. On the other hand, the effect of porosity can be considered to appear to some extent using the uniform deformation. Hence, although the uniform deformation is considered in this work, it is insufficient.

The uniform strain of 0.005 is imposed on all the atoms in the system every 1 000 steps and the relaxation calculation is performed in the interval. In the deformation process, the strain in the x_2 direction is forced to be 0.

Figure 7 indicates the final configurations of atoms. A larger deformation in the film part is observed in the deposition models compared with the crystal model. It is assumed that the difference in the film deformation is associated with the film porosity. Stress(σ_{x1})-strain(ϵ_{x1}) curves in the x_1 direction are shown for each model in Fig. 8. The plastic deformation for the deposition model is found to be larger compared with that for the crystal model. A quasi-brittle behavior rather than a ductile behavior appears in particular in the case of the crystal model. In this

Fig. 7 Final configurations of thin films under tension in x_1 direction

Fig. 8 Stress-strain curves in tensile loading in x_1 direction

simulation, the tensile strength of a sputtered material is defined as the peak stress in its stress-strain curve. It is revealed that a larger porosity results in a smaller tensile strength. Consequently, it may be concluded that the film porosity affects the stress relaxation and plastic behavior in the direction parallel to the substrate surface.

5.2 Tensile properties in the direction perpendicular to the substrate surface

For the deposition model, the lowest two layers of the substrate and the upper part of the deposited film are fixed, and the system is loaded in the direction perpendicular to the substrate surface, i.e. the x_3 direction. To reduce the effect of thermal fluctuation, the motion of atoms in the rest of the system is rescaled so that the system temperature can be maintained at 5 K. After the total stress in the system is relaxed to become 0 MPa, a constant strain of 1.0×10^{-5} /step is imposed on the fixed atoms only, and the rest of the atoms are relaxed all the time. The strains

Fig. 9 Final configurations of thin films under tension in x_3 direction

in the x_1 and x_2 directions are forced to become 0.

The final configurations of atoms are depicted in Fig. 9. For the deposition model, a ductile fracture seems to be initiated from defects in the simulated film. For the crystal model, however, a quasi-brittle fracture is seen near the interface region. Figure 10 presents stress(σ_{x3})-strain(ϵ_{x3}) curves in the x_3 direction for each model. Contrary to the load in the x_1 direction, there is no significant difference in the tensile strength for the three models. After reaching the peak stress, the stress in the deposition model gradually decreases, while a faster decrease in the stress is found in the crystal model.

It is considered that fixed regions have an effect on the result, but fractures occur sufficiently far from these regions in all cases. These results show that the effects of the fixed region are small in this work.

5.3 Relationship between porosity and strength

The relationship between the porosity and the tensile strength in the x_1 and x_3 directions are plotted in Fig. 11.

The strength in the direction parallel to the substrate surface is decreased with an increase in the porosity. The fracture in this direction is initiated from a larger pore as illustrated in Fig. 7 because the region with a smaller cross section is subjected to a larger stress. In this simulation, it may be concluded that the size of a dominant pore directly influences the strength. It is known that film hardness is decreased by the increase of the porosity of the film, experimentally and by simulation⁽¹⁴⁾. It is likely that the result of film strength in this work is similar to that of film hardness.

In loading perpendicular to the substrate surface, no significant difference is observed in the relationship

Fig. 10 Stress-strain curve in tensile loading in x_3 direction

Fig. 11 Relationship between surface porosity and tensile strength

even if the porosity varies. In this case, it is suggested that the interfacial property is a more important factor to be considered in addition to the porosity. Atoms of deposited films are more relaxed on the interface, around which atoms of the substrate and the film are scrambled. On the other hand, the crystal film is assumed to have a lower lattice fitness with the substrate, which yields a weaker bonding at the interface of the crystal model. This results in the quasi-brittle fracture seen in the crystal model. This result related to interfacial property is discussed only as a general tendency of sputtered films. For detailed discussions of the Si-Al interface, precise potential values of Si-Al interactions are required.

6. Conclusions

In this work, a porosity-related microstructure and its correlation with strength properties in an Al film sputtered on a Si substrate were investigated by

an MD simulation. Simulations were conducted using the MEAM potential, on which the interaction potential for Si-Al was discussed and then determined for the simulations. Two film models were proposed to clarify microstructure-dependent properties. One was a deposition model and the other was a crystal model. In the deposition model, Al atoms were deposited on the Si substrate using the MD simulation, while a crystalline Al film was adaptively allocated to the Si substrate in the crystal model.

Films simulated by the deposition model were found to be amorphous. In the case of the substrate maintained at high temperature during the deposition process, atoms of the film and the substrate were observed to be scrambled around the interface.

Procedures to evaluate the surface roughness and the porosity of film were also proposed to characterize the film structure. The surface roughness and the volume porosity were observed to decrease with increasing the incident energy of atoms, although the surface porosity was hardly influenced by the incidence condition.

The relationship between tensile deformation property and porosity in a simulated film, was investigated by simulations for loading in the directions parallel and perpendicular to the substrate surface. The film porosity was found to affect the tensile strength in the direction parallel to the substrate surface. On the other hand, it was revealed that the tensile strength in the direction perpendicular to the substrate surface was hardly influenced by the variation in the film porosity. It was suggested that the latter behavior was attributed to a greater sensitivity to the interface characteristics rather than the film porosity.

In this work, Si-Al interaction is not reproduced completely and these results are considered to be valid in this context.

References

- (1) Fang, C.C., Prasad, V. and Jones, F., Molecular Dynamics Modeling of Microstructure and Stresses of Sputter-Deposited Thin Films, *J. Vac. Sci. Technol. A*, Vol. 11, No. 5 (1993), p. 2778.
- (2) Sanders, D.E. and DePristo, A.E., Metal/Metal Homo-Epitaxy on fcc (001) surfaces: Is there Transient Mobility of Adsorbed Atoms?, *Surf. Sci.*, Vol. 254 (1991), p. 341.
- (3) Jacobsen, K.W., Norskov, J.K. and Puska, M.J., Interatomic Interactions in the Effective-Medium Theory, *Phys. Rev. B*, Vol. 35, No. 14 (1987), p. 7423.
- (4) Foils, S.M., Baskes, M.I. and Daw, M.S., Embedded-Atom-Method Functions for the Fcc Metals Cu, Ag, Au, Ni, Pd, Pt, and Their Alloys, *Phys. Rev. B*, Vol. 33, No. 12 (1986), p. 7983.
- (5) Tersoff, J., Empirical Interatomic Potential for Silicon with Improved Elastic Properties, *Phys. Rev. B*, Vol. 38, No. 14 (1988), p. 9902.
- (6) Baskes, M.I., Modified Embedded-Atom Potentials for Cubic Materials and Impurities, *Phys. Rev. B*, Vol. 46, No. 5 (1992), p. 2727.
- (7) Baskes, M.I., Determination of Modified Embedded Atom Method Parameters for Nickel, *Mater. Chem. Phys.*, Vol. 50 (1997), p. 152.
- (8) Baskes, M.I., Angelo, J.I. and Bisson, C.L., Atomistic Calculations of Composite Interfaces, *Modelling Simul. Mater. Sci. Eng.*, Vol. 2 (1994), p. 505.
- (9) Gong, X.G., Structure and Stability of Cluster-Assembled Solid $\text{Al}_{12}\text{C}(\text{Si})$: A First-Principles Study, *Phys. Rev. B*, Vol. 56, No. 3 (1997), p. 1091.
- (10) Gong, X.G. and Kumar, V., Enhanced Stability of Magic Clusters: A Case Study of Icosahedral Al_{12}X , $\text{X}=\text{B}, \text{Al}, \text{Ga}, \text{C}, \text{Si}, \text{Ge}, \text{Ti}, \text{As}$, *Phys. Rev. Lett.*, Vol. 70, No. 14 (1993), p. 2078.
- (11) Rose, J.H., Smith, J.R., Guinea, F. and Ferrante, J., Universal Features of The Equation of State of Metals, *Phys. Rev. B*, Vol. 29, No. 6 (1984), p. 2963.
- (12) Brooks, G. and Kelly, P.J., The Energetics of Adatoms on the Si(100) Surface, *Surf. Sci.*, Vol. 269/270 (1992), p. 860.
- (13) Khoo, G.S. and Ong, C.K., The Interactions of Metallic and Semiconducting Adsorbates with Si(100), *J. Phys. Condens. Matter.*, Vol. 6 (1994), p. 8141.
- (14) Iizuka, T., Onoda, A. and Hoshida, T., to be submitted to *JSME Int. J.*, Ser. A.
- (1) Fang, C.C., Prasad, V. and Jones, F., Molecular Dynamics Modeling of Microstructure and Stres-