

Molecular dynamics simulation of sputter trench-filling morphology in damascene process

Shin-Pon Ju, Cheng-I Weng,^{a)} and Jee-Gong Chang^{b)}

Department of Mechanical Engineering, National Cheng Kung University, Tainan, Taiwan, Republic of China

Chi-Chuan Hwang^{c)}

Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan, Republic of China

(Received 7 May 2001; accepted 18 March 2002)

This article presents the use of molecular dynamics (MD) simulation to investigate the influence of process parameters on sputter trench-filling morphologies in the damascene process. We focus not only upon the mechanisms of trench-filling formation, but also upon the coverage percentage at various transient states during the deposition process. The MD simulation includes a three-dimensional trench model and a deposition model, and uses the many-body, tight-binding potential method to represent the interatomic force acting between atoms. The results of the study indicate that an ideal trench-filling morphology, i.e., one in which the trench is completely filled, with no trapped voids, is most likely to occur as the incident energy of the deposited atom increases, and for higher substrate temperatures. It is found that the principal influence of an increased incident energy is to improve the migration ability of deposited atoms, particularly along the two sidewalls of the trench. This is beneficial since it alleviates the self-shadowing effect, thereby improving coverage of the trench bottom by deposited atoms, particularly in the corners. An increased substrate temperature is influential in improving the fluidity of the atoms deposited within the trench. This promotes the filling of the voids which tend to form at the intermediate stage of the deposition process. Finally, it is found that of the two process parameters investigated in this study, the filling pattern of the trench is most strongly influenced by the incident energy of the deposited atoms.

© 2002 American Vacuum Society. [DOI: 10.1116/1.1477423]

I. INTRODUCTION

As device density increases,¹ the challenges faced in the manufacturing of multiple-layer interconnects, such as vias, contacts, and trenches also greatly increase. These challenges include developing alternative metallization materials which can provide lower resistivity² and higher electromigration resistance.³ A further challenge is to then modify the existing deposition processes as necessary in order to incorporate these new materials.⁴ The most recently developed copper metallization process is known as the damascene process,^{2,3} and is a way of improving the performance of devices whose dimensions are measured on a submicrometer scale. Several methods have been developed to fill high aspect ratio trenches or holes, including collimated magnetron sputter deposition,⁵⁻⁸ and chemical vapor deposition.⁹ However, it is found that as the trench depth increases, the self-shadowing effect caused by the growth of clusters at the trench opening leads to poor coverage by the deposited atoms, and tends to trap voids within the trench.¹ Since these defects significantly affect the reliability of the device, it is important to develop a thorough understanding of the void formation mechanism, and its relationship with the process parameters,

in order that it is possible to improve the manufacturing process in such a way as to produce void free trenches.

Due to the very small scale of the devices involved, it is not easy to observe the trench-filling morphology at a transient state, and therefore physical experimentation is not really very beneficial in developing a deep insight into the trench-filling mechanisms. Accordingly, several numerical methods have been developed as aids to understanding the growth mechanisms of deposited films, including continuum-based methods such as the shock tracking algorithm,^{5,10} finite element methods,¹¹ and particle-based methods, e.g., the Monte Carlo method^{12,13} and molecular dynamics (MD) simulation. The latter method describes the atomic motion of constituent particles, which satisfy the laws of classic mechanics at the atomic scale.¹⁴ The superiority of the MD approach becomes apparent as the characteristic size of the system decreases. An analysis of existing literature reveals that most studies to date have used the first three methods referenced herein, and that MD simulations of the trench-filling process are comparatively scarce. However, as features continue to decrease in size, there is undoubtedly a requirement for atomic simulation of the trench-filling process if a deeper insight into film growth mechanisms is to be acquired. Furthermore, the requirement to speed up the deposition process development¹⁵ demands simulation models which are able to reflect the physical process accurately. One example of MD simulation used as part of a trench-filling process investigation was the work carried out by Saito

^{a)}Author to whom all correspondence should be addressed; electronic mail: weng@mail.ncku.edu.tw

^{b)}Electronic mail: changjg@mail.ncku.edu.tw

^{c)}Electronic mail: chchwang@mail.ncku.edu.tw

et al.,¹⁶ in which the reflow process for sputtered aluminum films was analyzed. The pairwise, Morse and Lennard–Jones potentials method was employed to simulate the atomic forces between the aluminum film and the silicon substrate. In their work, it was found that droplet formation is strongly dependent upon the initial film-thickness distribution, the film temperature, and the bond energy between the film and the substrate. In their analysis, distribution of the sputtered aluminum was assumed to have been completed before the reflow process was initiated, even though this is not truly the case in the physical process.

Fairly recently, the many-body, tight-binding potential method has been developed, which addresses the long-range force existing among atoms.^{17,18} In this method, the interaction between any pair of atoms is assumed to depend upon the local environment surrounding the atoms, as well as just upon the two atoms themselves, as in the pair-wise potential method. This method offers the advantages that the Cauchy discrepancy of the elastic constant is well satisfied, and that the surface relaxation, adatom diffusion can be appropriately modeled.^{19,20–22} The validity of the method as compared to other many body potential models such as the embedded atom method (EAM) has been well proven, and in some cases it has been shown that its prediction of material properties is actually better than other non-pair-wise potential methods.¹⁷ An additional advantage of this method is that its calculation methodology is straightforward.

The main objective of this study is to employ MD simulation to investigate the influence of process parameters on the sputter trench-filling morphology. A three-dimensional model of the trench is established, which comprises a Ti film and a thermal control layer. A model which governs the deposition of the Cu atoms is also created. The tight-binding potential method is used to simulate the interatomic forces which exist between the atoms. The trench-filling formation mechanisms and coverage percentage at various transient states during the deposition process are studied, and an assessment is made of the influence of incident energy and substrate temperature upon the coverage of the trench by the deposited atoms.

II. SIMULATION MODEL

A schematic diagram of the trench which is to be filled via the Damascene process is presented in Fig. 1(a), while Fig. 1(b) shows the simplified trench-filling model which is incorporated into the MD simulation. As can be seen in Fig. 1(b), the surface of the trench is uniformly covered by a Ti film. In this study, an assumption is made that deposition of the copper atoms does not commence until this barrier film is in place. In this way, the behavior of low-*k* dielectric material within the trench material may be neglected without affecting the validity of the simulation results. This is because the thickness of the Ti film is greater than the truncation distance of the interaction between the low-*k* material and the deposited atoms, i.e., the Ti film acts as a barrier which prevents the low-*k* material from influencing the motion of the deposited Cu atoms.

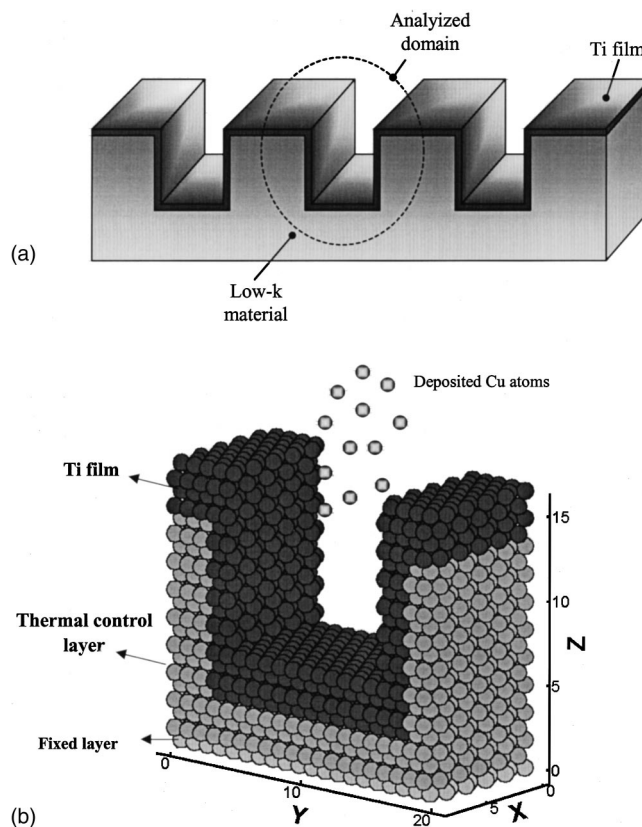


FIG. 1. (a) Schematic diagram of damascene process and (b) simplified model used in MD simulation.

The layers below the Ti film, which are indicated as gray dots in Fig. 1(b), are used to control the thermal state of the Ti film, and will henceforth be referred to as the thermal layer. The scaling method is used to maintain the thermal layer at a constant temperature. Therefore, the lowest layer of the Ti film is also close to a constant temperature. The function of the thermal layer is to model the introduction of thermal energy into the trench. The velocities of the atoms in thermal layers over the fixed layer are in the Maxwell–Boltzmann’s distribution, which is rescaled at each time step according to the prescribed substrate temperature in the simulation. The rescaling method is used to model the energy transformation (adsorption) from the top layers to bottom layers of the trench in the deposition process. In later sections of this article, the words “substrate temperature” are used to refer to the state of the thermal layer when modeling the thermal layers maintain at a steady state.

Both the Ti film and the thermal layer are arranged according to their hexagonal-close-packed structure. The trench model, composed of the Ti film and the thermal layer, comprises 2770 atoms, and represents an equal aspect ratio trench with both its depth and its width equal to 2.5 nm. The lowest layer is fixed to prevent the trench atoms from shifting, and periodic boundary conditions are applied in the *x* and *y* directions.

In the sputter deposition process, the copper atoms, which are to be used to fill the trench, are generated by bombarding a copper target with ions. The ion bombardment increases

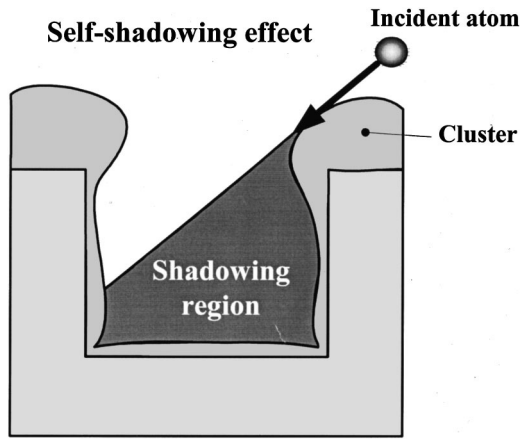


FIG. 2. Schematic diagram of self-shadowing effect in damascene process.

the kinetic energy of the copper atoms causing them to be sputtered from the target. They are then deposited on the substrate. The current simulation does not attempt to provide a detailed representation of the atom sputtering process, but instead uses a spatial distribution of the incident atoms to represent the actual distribution of sputtered atoms. The initial velocity of each incident atom is assumed to be the same, and is calculated according to the specified incident energy, as follows:

$$V_{\text{atom}} = \sqrt{\frac{2 \cdot E_{\text{atom}}}{M}}, \quad (1)$$

where E_{atom} represents the incident energy and M is the atomic mass.

During the conventional sputter deposition process, bombardment of the target with Ar atoms results in incident atoms which have a wide angle of distribution. Although this situation is suitable for deposition processes on flat surfaces, it is less practical for the damascene process since it will tend to cause a significant shadowing effect, resulting in the trench-filling pattern shown in Fig. 2. Therefore, it is assumed that the incident angle is well controlled within the deposition process. In the current simulation, the incident atom angles are generated by a random function and are constrained such that they fall within a range -5° to $+5^\circ$. This range takes the vertical z axis as its zero-angle reference, and is also known as the cutoff angle.⁵ In practice, the angular distribution is controllable in several deposition processes, including collimated magnetron sputter deposition, and ionized magnetron sputter deposition. The current simulation uses two sets of random distribution functions to generate the incident angle, and the incident position of the deposited atoms, respectively. It is known that atoms rarely

interact with each other before reaching the substrate due to the distribution of atoms in a vacuum, and therefore in the simulation, the distance between two subsequently deposited atoms is set to be larger than their truncated distance. Interaction between the incident atoms and the trench atoms commences when their proximity is less than their truncation distance. These atomic interactions include Cu–Ti, Cu–Cu, and also Ti–Ti. The motion trajectories of the deposited atoms, and of the trench atoms, are governed by their equations of motion. Usually, the interatomic force which acts between atoms is represented by a potential function, e.g., Eq. (2), below. The interaction force on a particular atom, i , is obtained by taking the first negative derivation of the potential function, as shown in Eq. (3).

In this simulation, the many-body potential of the tight-binding second-moment approximation (TB-SMA) model is employed to simulate the interatomic force among atoms. The main difference between the TB potential model and pair-wise potential models is that it considers the interaction between two atoms to depend on their local environment, as well as upon the two atoms themselves. It has been found that the prediction of some material properties when using the TB-SMA method is more accurate than when the EAM method is employed. Moreover, the computing algorithm of the TB-SMA method is more straightforward than that of the EAM method. This model commences by summing the band energy, which is characterized by the second moment of the d -band density of state, and a pair-wise potential energy of the Born–Mayer type.¹⁸

$$E_i = - \left\{ \sum_j \xi^2 \exp \left[-2q \left(\frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{1/2} + \sum_j A \exp \left[-p \left(\frac{r_{ij}}{r_0} - 1 \right) \right], \quad (2)$$

where ξ is an effective hopping integral, r_{ij} is the distance between atom i and j , and r_0 is the first-neighbor distance. The parameters A , p , q , and ξ are determined by experimental measurement of the following material properties; cohesive energy, lattice parameter, bulk modulus, and shear elastic constants. The parameters of tight-binding potential corresponding to Cu–Cu and Ti–Ti which are used in the current simulation, are listed in Table I.¹⁷ However, to the best of the authors' current knowledge, the parameters describing the interatomic potential of Cu–Ti have never been published. Rather than resorting to a rigorous mathematical method, or to theory, to determine the value of these parameters, a simpler method may be adopted in which an average is taken of the corresponding parameters for the pure atomic potential of Cu–Cu and Ti–Ti.

The interaction force on atom i can be expressed as

$$\vec{F}_i = \sum_{j \neq i} \left(\frac{\partial E_i}{\partial r_{ij}} + \frac{\partial E_j}{\partial r_{ij}} \right) \frac{\vec{r}_{ij}}{r_{ij}}. \quad (3)$$

Finally, a complete derivation of the equations of motion of

TABLE I. Parameters used in tight-binding potential.

Parameters	A (eV)	ξ (eV)	P	Q	r_0 (Å)
Cu–Cu	0.0855	1.224	10.960	2.278	2.556
Ti–Ti	0.0741	1.4163	11.418	1.643	2.492

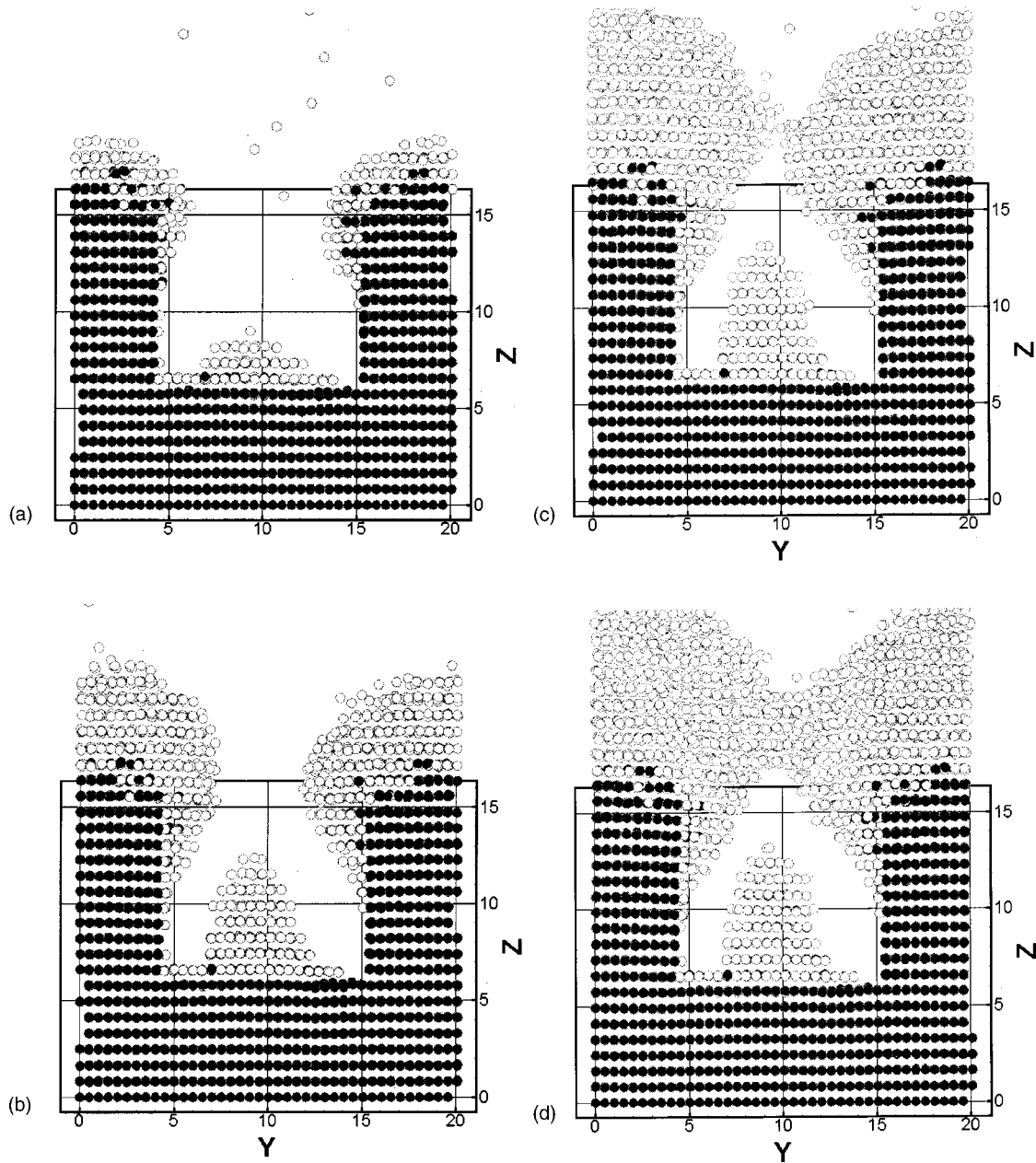


FIG. 3. Snapshots of trench-filling morphology at incident energy of 1 eV, substrate temperature of 300 K: (a) 100 ps, (b) 250 ps, (c) 400 ps, and (d) 450 ps.

the atoms, i.e., their trajectories of motion, can be obtained by substituting this force term into the right-hand side of the motion equation given as

$$m_i \dot{v}_i = \bar{F}_i. \quad (4)$$

The initial velocity of the incident atoms is determined from Eq. (1). Before the deposition process begins, the trench atom velocities must attain a state of thermal equilibrium (i.e., a constant temperature), at which point their velocities conform to a Maxwell-Boltzmann distribution. The Gear's predictor-corrector algorithm²³ is used to calculate the trajectories of both the Cu and the Ti atoms in the simulation.

III. RESULTS AND DISCUSSION

In this study the trench-filling morphology is investigated for different incident energies and for different substrate temperatures.

A. Effect of the incident energy

In order to investigate the influence of incident energy, the filling morphology is observed for three different values of incident energy, namely 1, 5, and 10 eV, while maintaining a constant substrate temperature of 300 K in each case. Figures 3(a) to 3(d) show four snapshots of the trench filling process for a low incident energy of 1 eV. Observation of the morphology within the trench showed that there was little varia-

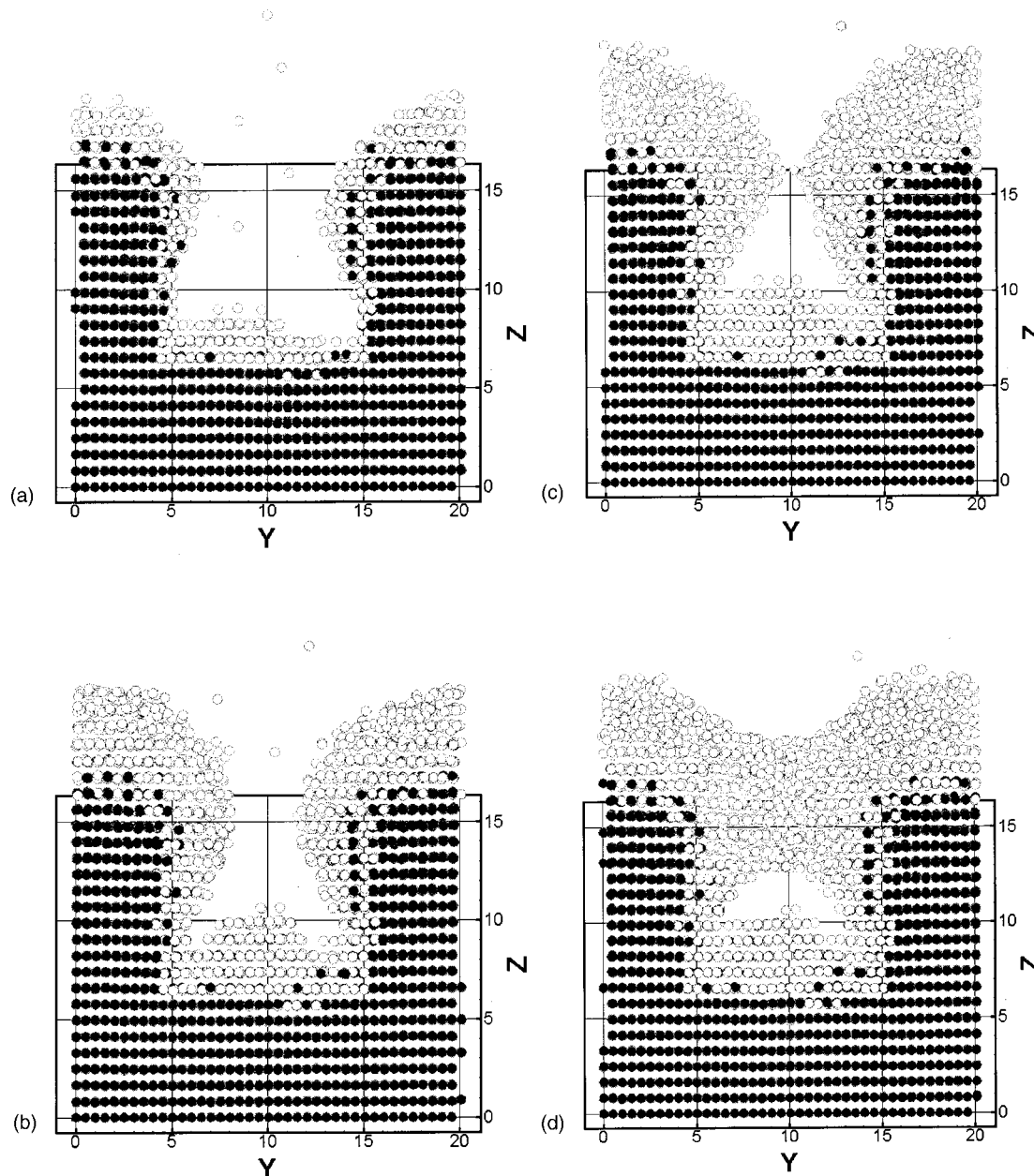


FIG. 4. Snapshots of trench-filling morphology at incident energy of 5 eV, substrate temperature of 300 K: (a) 150 ps, (b) 300 ps, (c) 350 ps, and (d) 400 ps.

tion in the morphology in the x direction, and therefore in the discussions which follow, the morphological result is represented by a typical two-dimensional cross section in the x - y plane rather than by a three-dimensional cross section. Figures 3(a) to 3(c) indicate that the deposited atoms form overhanging clusters at the trench opening. These clusters grow as the deposition process continues, and eventually join, as shown in Fig. 3(d), thus preventing subsequently deposited atoms from entering the trench. As a result of the self-shadowing effect,²⁴ caused by the cluster formations, it will be observed that the bottom corners of the trench are scarcely covered at all by the incident atoms.

Figures 4(a) to 4(c) show the trench-filling sequence for an incident energy of 5 eV. Although the results are broadly similar to the previous case, e.g., an overhanging structure is

again formed at the trench opening, there is one difference which will be noted when comparing Figs. 4(a) and 4(b) with the results shown in Figs. 3(a)–3(c), namely that the coverage of the two bottom corners of the trench is much better when the incident energy is higher. This may be explained by the fact that a higher incident energy promotes the ability of deposited atoms to migrate along the two sidewalls of the trench towards its bottom corners. The detailed mechanism may be explained as follows: During the migration process, the initial kinetic energy of an incident atom gradually diminishes as a result of a series of collisions with the substrate atoms. An individual incident atom will continue to migrate until its kinetic energy is insufficient to overcome the potential energy barrier imposed by the substrate. Since the initial kinetic energy of an incident atom is dependent upon its

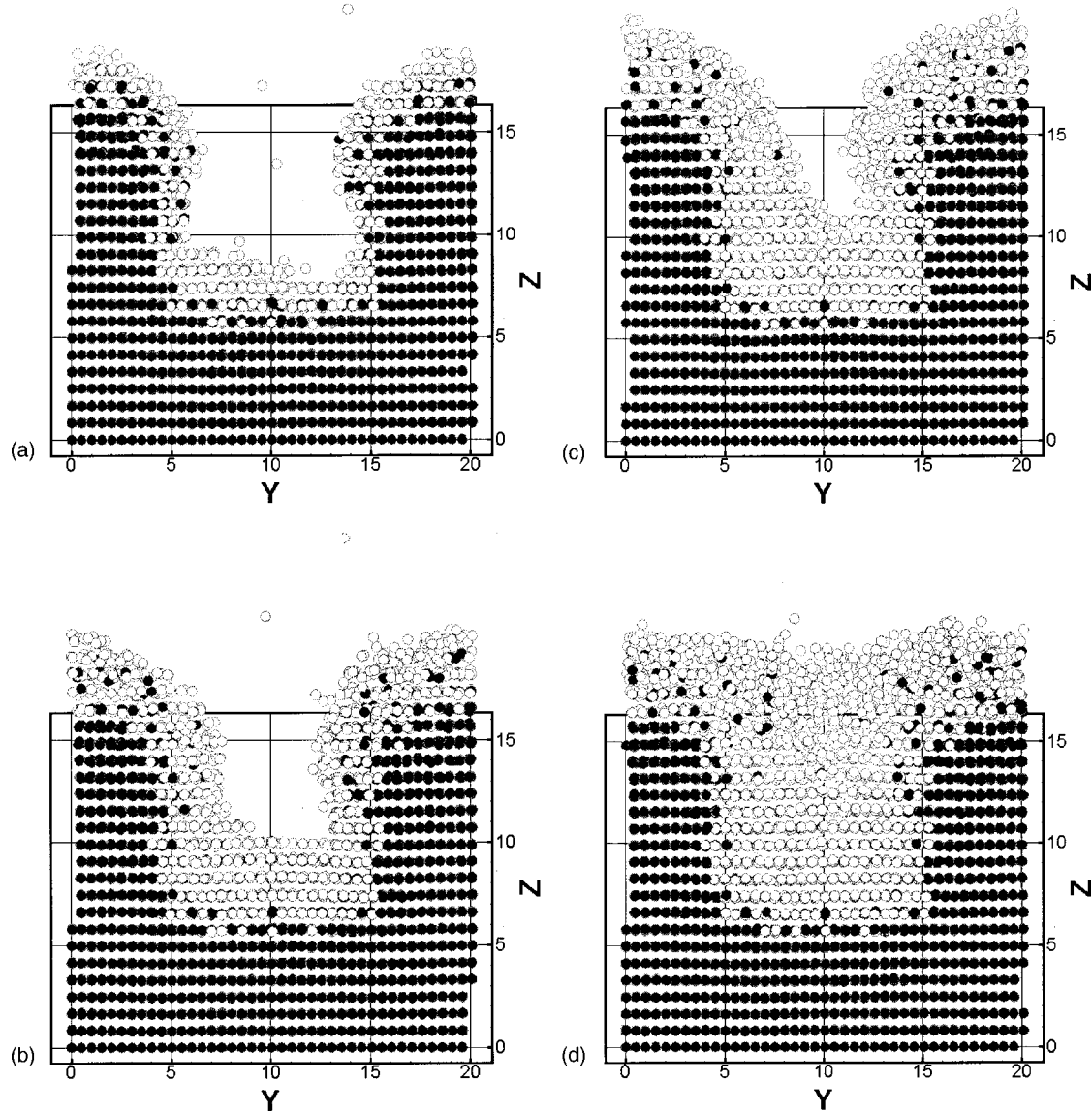


FIG. 5. Snapshots of trench-filling morphology at incident energy of 10 eV, substrate temperature of 300 K: (a) 150 ps, (b) 250 ps, (c) 300 ps, and (d) 380 ps.

incident energy, it will be clear that atoms which impact with a higher incident energy possess a greater migration ability than low incident energy atoms, and will therefore be able to migrate a longer distance along the two sidewalls towards the bottom corners of the trench. As may be seen in Fig. 4(d) a trapped void is finally formed in the center of the trench, although it will be noted that its size is smaller than the void shown in Fig. 3(d), for which the incident energy is 1 eV. It is interesting to note that in the case of a higher incident energy, there is a significant movement of the deposited atoms after the two overhanging clusters join at the trench opening, as witnessed in Figs. 4(c) and 4(d). Although Figs. 3(c) and 3(d) also demonstrate some movement of the deposited atoms after the overhanging clusters join, this movement is only limited compared to the higher incident energy results, and therefore subsequently deposited atoms are not

particularly beneficial in decreasing the size of the void within the trench.

Figures 5(a) to 5(d) present four snapshots of the trench filling process for an incident energy of 10 eV. As may be seen in Fig. 5(d), this level of incident energy results in an ideal morphology, i.e., a complete filling of the trench with no trapped voids. The absence of a void within the trench may be explained by the fact that the elevated incident energy results in a significant increase in the migration ability of deposited atoms along the sidewalls of the trench. Compared to the results presented in Figs. 3(a) and 3(b), and in Figs. 4(a) and 4(b), the size of the overhanging clusters at the trench opening is much smaller when the incident energy is 10 eV. This reduces the self-shadowing effect, and is therefore beneficial to an ideal filling of the trench. Furthermore, it will be noted that the trench-filling characteristic with an

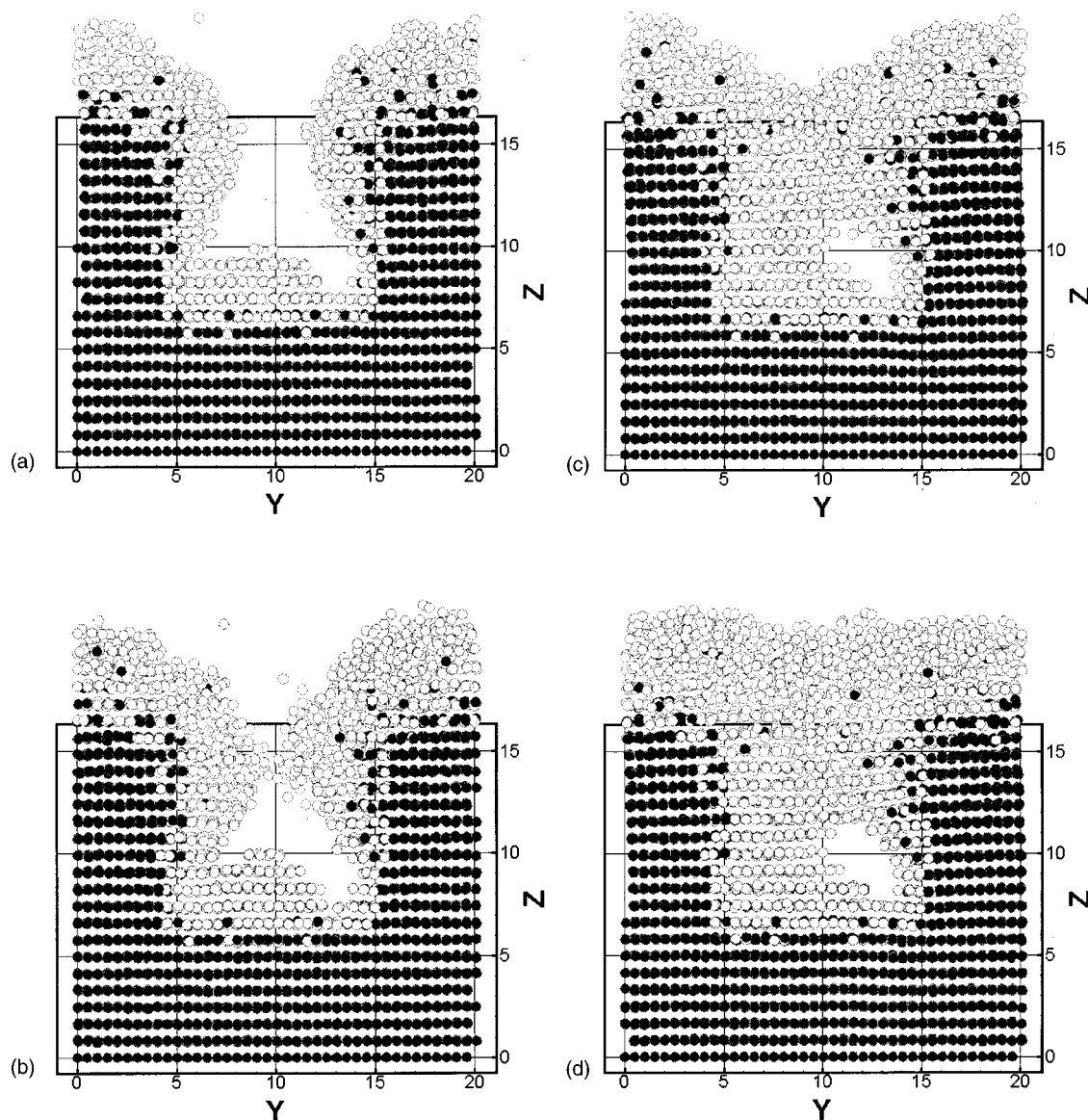


FIG. 6. Snapshots of trench-filling morphology at incident energy of 5 eV, substrate temperature of 500 K: (a) 250 ps, (b) 300 ps, (c) 350 ps, and (d) 400 ps.

incident energy of 10 eV is different than when lower incident energies of 1 or 5 eV are used, namely that in the case of a higher incident energy the deposited atoms tend to accumulate at the bottom of the trench, rather than along the sidewalls, i.e., the trench fills progressively from the bottom towards the top.

B. Effect of substrate temperature

In order to investigate the influence of substrate temperature upon the deposition process, the incident energy was maintained at 5 eV, and the filling morphology was simulated for two different substrate temperatures, i.e., 500 and 1000 K. The results are presented in Figs. 6 and 7, respectively, and may be compared to the nominal case of a substrate temperature of 300 K with an incident energy of 5 eV presented in Fig. 4. A comparison of Figs. 6(d) and 4(d) indi-

cates that a higher substrate temperature tends to reduce the size of the trapped void within the trench. Furthermore, it will be noted that there is a change in the shape of the trapped void, i.e., the left-hand side of the void which is trapped at a lower substrate temperature becomes filled as the temperature of the substrate is increased, so that only the right-hand side of the original void remains. A careful observation of Figs. 6(a)–6(c) shows that an increase in substrate temperature causes a “flow” of the atoms accumulated along the left-hand sidewall toward the bottom of the trench, thereby filling the left-hand side of the original void. In other words, it would appear that an increase in substrate temperature enhances the fluidity of the deposited atoms within the trench. This assertion is borne out by a comparison of the morphology presented in Figs. 6(b) and 4(b). These two results show the morphology at the same time instant and

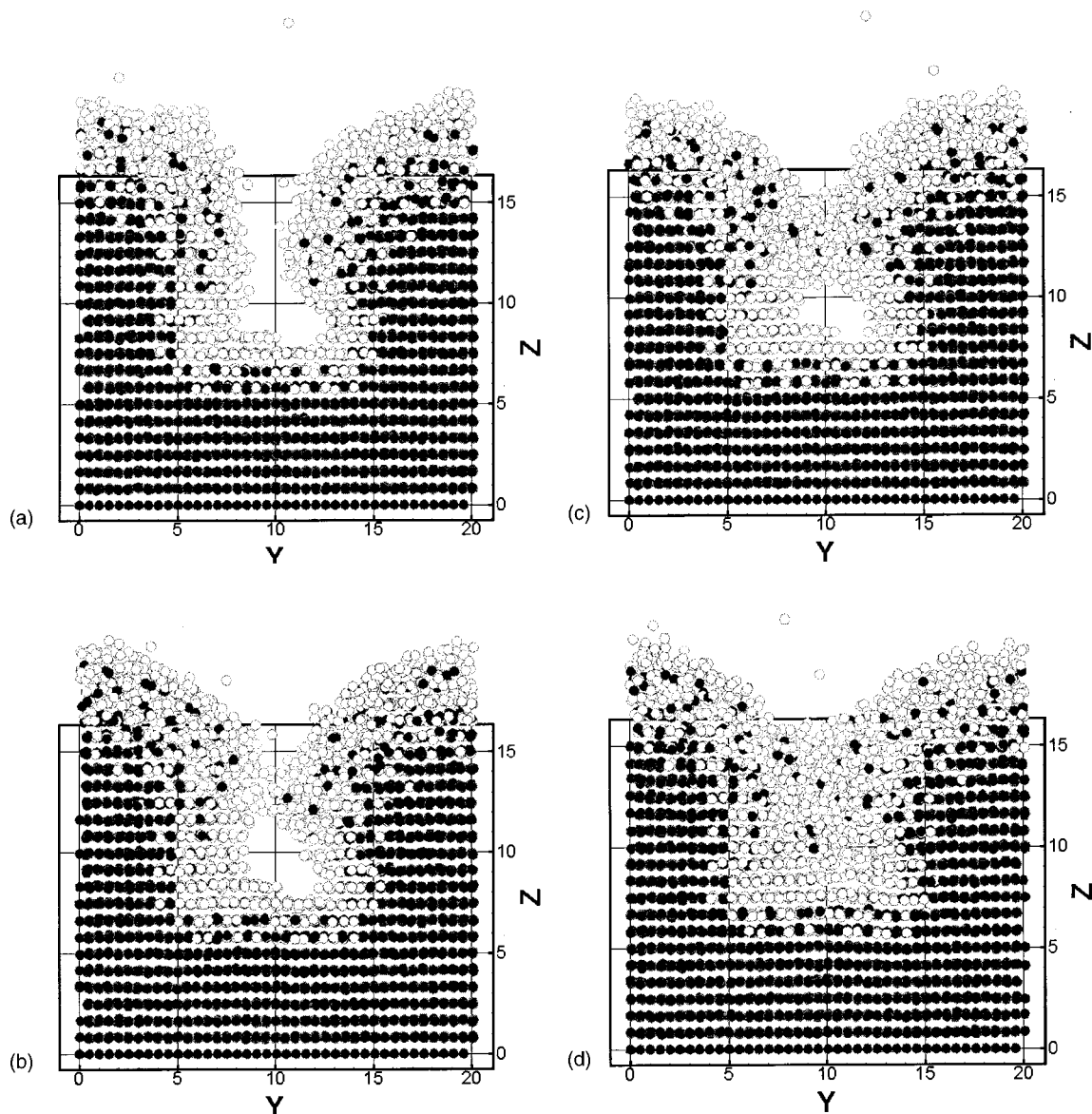


FIG. 7. Snapshots of trench-filling morphology at incident energy of 5 eV, substrate temperature of 1000 K: (a) 260 ps, (b) 270 ps, (c) 280 ps, and (d) 290 ps.

therefore any difference in morphology is due mainly to the effect of substrate temperature difference. In Fig. 6(b), it will be seen that the two clusters almost touch, whereas in Fig. 4(b) there is a significant gap between the two atom clusters.

It will be seen in Fig. 7(b) that a void is initially formed within the trench during the deposition process, but that this void is completely filled as deposition continues, as shown in Fig. 7(d). As has been mentioned previously, the elevation of substrate temperature enhances the fluidity of the deposited atoms, which tends to result in an ideal trench morphology.

C. Filling pattern comparison for elevation of incident energy and substrate temperature

In order to better understand the relative influence of increasing incident energy and increasing substrate tempera-

ture on the trench-filling mechanism, a comparison is made between the improvement in morphology observed as each of these parameters is increased. It is noted that increasing the incident energy significantly affects the filling patterns within the trench. For a lower incident energy, it is found that a void is trapped within the trench, while a higher incident energy results in an ideal filling of the trench, i.e., with no void formation. However, an increase in substrate temperature does not change the filling pattern; it merely enhances the fluidity of the deposited atoms during the trench-filling process. As can be seen in Figs. 6 and 7, which show the trench-filling process for substrate temperatures of 500 and 1000 K, respectively, voids are formed in both deposition processes. The different influence on filling patterns is the chief difference noted between increasing incident energy and increasing substrate temperature.

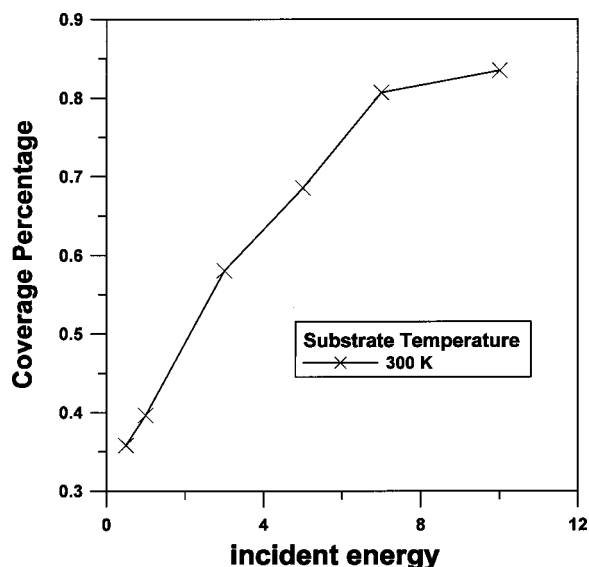


FIG. 8. Coverage percentage at different incident energies.

D. Evaluation the influence of incident energy and substrate temperature on the filling morphology

Figures 8 and 9 show the relationship between the coverage percentage and the process parameters of incident energy and substrate temperature. A comparison between Figs. 8 and 9 demonstrates the different influence of each parameter on the trench coverage. For the chosen substrate temperature of 300 K, it can be seen that the coverage percentage initially increases rapidly as the incident energy is increased. However, when the incident energy is greater than 7 eV, the rate of increase in coverage percentage reduces. Therefore, during the tuning process it should be noted that a linear increase in incident energy does not necessarily result in a linear improvement of the trench-filling morphology.

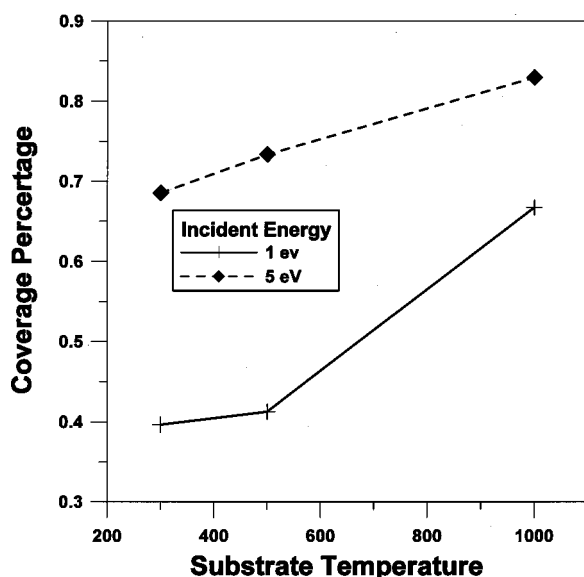


FIG. 9. Coverage percentage at different substrate temperatures.

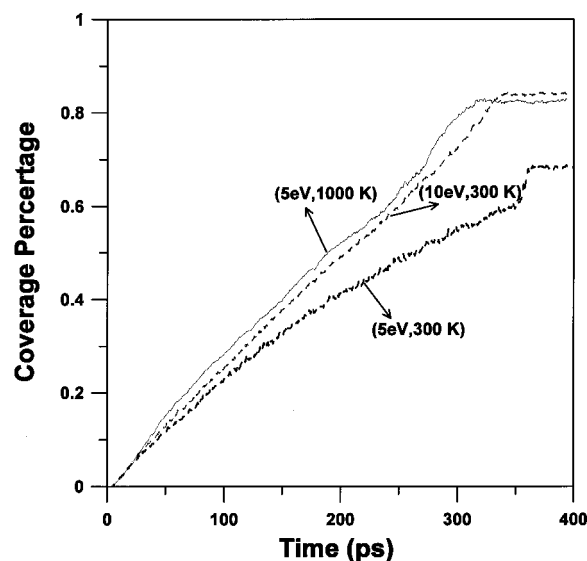


FIG. 10. Transient coverage percentage for the cases of (5 eV, 300 K), (10 eV, 300 K), and (5 eV, 1000 K).

The influence of substrate temperature on the coverage percentage is presented in Fig. 9. In order to investigate the improvement in coverage which is obtained as the substrate temperature is increased, two nominal cases are chosen for reference purposes. As may be seen in Fig. 9, the incident energy is 1 eV for one of these nominal cases, and is 5 eV for the other. As has been noted previously, the poor trench coverage which is obtained with an incident energy of 5 eV and a substrate temperature of 300 K can be improved to an ideal filling state by increasing the temperature to 1000 K. However, for an incident energy of 1 eV, it can be seen that even though there is a significant improvement in coverage as the substrate temperature is increased to 1000 K, the final result is still not one of ideal filling. It is interesting to note that the magnitude of the improvement in coverage percentage obtained as the substrate temperature is increased depends upon its initial state, i.e., applying a substrate temperature elevation of 700 K (i.e., 300 to 1000 K) has a much more dramatic impact upon the coverage percentage for an incident energy of 1 eV than in the case where the incident energy is 5 eV.

Although higher values of incident energy and higher substrate temperatures are both beneficial in generating ideal trench filling, it is noted that of these two parameters, the effects of incident energy are more significant than increasing substrate temperature in promoting an improvement in the trench coverage.

Figure 10 shows the coverage percentage at various transient states of the deposition process for three incident energy/substrate temperature combinations, i.e., incident energy 5 eV and substrate temperature 300 K, incident energy 5 eV and substrate temperature 1000 K, and incident energy 10 eV and substrate temperature 300 K. In the discussion which follows, these various cases are abbreviated to (5 eV, 300 K), (5 eV, 1000 K), and (10 eV, 300 K) for the sake of convenience. The results indicate that in all cases the coverage percentage increases as the process proceeds, and that the

coverage percentage finally attains a steady value. Comparing the transient coverage percentage obtained with (5 eV, 300 K) and (5 eV, 1000 K), it will be observed that increasing the substrate temperature not only improves the coverage percentage, but also increases the rate at which the coverage percentage improves, thereby reducing the time required for the coverage percentage to obtain a steady value. An implication of this is that less time is required to complete the trench filling process. The time required for the coverage percentage to obtain a steady value is even less in the case of (10 eV, 300 K). An abrupt increase in the coverage percentage is noted at approximately 350 ps in the case of (5 eV, 300 K). This is due to the sudden collapse of the two clusters joining caused by the subsequently deposited atoms.

Inspection of Fig. 10 shows that the percentage coverage obtained with (5 eV, 1000 K) is higher than that of (10 eV, 300 K) at any point prior to the steady state values being attained, and that the time to reach this steady value is shorter for the higher substrate temperature. However, it can also be seen that the final trench coverage percentage is slightly worse in the case of a substrate temperature of 1000 K compared to the substrate temperature of 300 K. Therefore, it would appear to be necessary to find a compromise between trench-filling time and coverage percentage. A detailed investigation into the optimal process parameters should be the subject of further investigation, but in the meanwhile it is suggested that the values of these parameters fall somewhere between 5 eV and 10 eV for the incident energy, and between 300 and 1000 K for the substrate temperature.

IV. CONCLUSION

In this study, MD simulation has been employed to investigate the influence of process parameters on the trench-filling morphology in the damascene process. This study of the trench-filling process is beneficial in developing an understanding of the dominant mechanisms which occur at the atomic scale. It is possible to summarize the conclusions which may be drawn from this study as follows:

- (1) Increasing the incident energy of the deposited atoms, or increasing the substrate temperature, both tend to promote an ideal trench-filling morphology, i.e., one in which there are no voids trapped within the trench.
- (2) The main influence of the increase in incident energy is to increase the migration ability of deposited atoms, especially those along the two sidewalls of the trench. Furthermore, increasing the incident energy tends to reduce the size of the atom clusters overhanging the trench opening, thereby reducing the effects of self-shadowing on coverage of the trench bottom.
- (3) The increase of substrate temperature primarily improves the fluidity of the deposited atoms within the trench. This

improvement in fluidity enables the deposited atoms to fill the void which forms at the intermediate stage of the process.

- (4) The trench filling patterns are influenced mainly by the incident energy rather than by the substrate temperature. The filling pattern changes from one of void formation at a lower incident energy to an ideal filling pattern at a higher incident energy.
- (5) Of the two parameters investigated in this study, it was found that the influence of incident energy is much more significant than substrate temperature in improving the coverage percentage.
- (6) The time required to complete the filling process is greatly reduced if the substrate temperature is increased.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the support given to this research by the National Science Council, Republic of China, under Grant Nos. NSC89-2215-E-006-002 and NSC89-2212-E-006-024.

¹C. S. Pai, Mater. Chem. Phys. **44**, 1 (1996).

²D. Bollmann, R. Merkel, and A. Klumpp, Microelectron. Eng. **37/38**, 105 (1997).

³K. Abe, S. Tokitoh, S. C. Chen, J. Kanamori, and H. Onoda, Proceedings of the IEEE 38th Annual International Reliability Physics Symposium, San Jose, California (2000), p. 333.

⁴P. Siemroth and T. Schulke, Surf. Coat. Technol. **133/134**, 106 (2000).

⁵S. Hamaguchi and S. M. Rossnagel, J. Vac. Sci. Technol. B **14**, 2603 (1996).

⁶P. F. Cheng, S. M. Rossnagel, and D. N. Ruzic, J. Vac. Sci. Technol. B **13**, 203 (1995).

⁷P. Siemroth, C. Wenzel, W. Klimes, B. Schultrich, and T. Schulke, Thin Solid Films **308**, 455 (1997).

⁸S. M. Rossnagel, Semicond. Int. **19**, 99 (1996).

⁹P. Doppelt, Coord. Chem. Rev. **178**, 1785 (1998).

¹⁰S. Hamaguchi and S. M. Rossnagel, J. Vac. Sci. Technol. B **13**, 183 (1995).

¹¹C. A. Ross, J. Vac. Sci. Technol. A **14**, 2511 (1996).

¹²T. Smy, R. V. Joshi, N. Tait, S. K. Dew, and M. J. Brett, IEEE IEDM 1998, p. 311.

¹³T. Smy, L. Tan, K. Chan, R. N. Tait, J. N. Broughton, S. K. Dew, and M. J. Brett, IEEE Trans. Electron Devices **45**, 1414 (1998).

¹⁴D. Frenkel and B. Smit, *Understanding Molecular Simulation from Algorithms to Applications* (Academic, New York, 1996).

¹⁵T. Smy, S. K. Dew, and M. J. Brett, Can. Metall. Q. **34**, 195 (1995).

¹⁶Y. Saito, S. Hirasawa, T. Saito, H. Nezu, H. Yamaguchi, and N. Owada, IEEE Trans. Semicond. Manuf. **10**, 131 (1997).

¹⁷F. Cleri and V. Rosato, Phys. Rev. B **48**, 22 (1993).

¹⁸V. Rosato, M. Guillope, and B. Legrand, Philos. Mag. A **59**, 321 (1989).

¹⁹I. Meunier, G. Treglia, B. Legrand, R. Tetot, B. Aufray, and J.-M. Gay, Appl. Surf. Sci. **162**, 219 (2000).

²⁰F. Hontinfinde, R. Ferrando, and A. C. Levi, Surf. Sci. **366**, 306 (1996).

²¹M. Ladeveze, G. Treglia, P. Muller, and F. Arnaud d'Avitay, Surf. Sci. **395**, 317 (1998).

²²T. Iwasaki, Comput. Mech. **25**, 78 (2000).

²³J. M. Haile, *Molecular Dynamic Simulation* (Wiley, New York, 1992).

²⁴S. P. Ju, C. I. Weng, J. G. Chang, and C. C. Hwang, J. Appl. Phys. **89**, 7825 (2001).