

Dual Damascene Simulation for Ionized Physical Vapor Deposition Process: Investigation on Incident Energy and Via Geometry Effects

Chi-Chuan HWANG^{1*}, Jee-Gong CHANG^{2†}, Jian-Ming LU¹ and Hong-Chang LIN¹

¹*Department of Engineering Science, National Cheng Kung University, Tainan, Taiwan, Republic of China*

²*National Center for High-Performance Computing, No. 21, Nan-Ke 3rd Rd., Hsin-Shi, Tainan, Taiwan, Republic of China*

(Received June 3, 2003)

This paper employs a dual damascene simulation to study the filling mechanisms of a dual via for the ionized physical vapor deposition (IPVD) process. The study focuses principally upon the influence of incident atom energy and via geometry upon the final dual via coverage. Additionally, the improvement in coverage which results from the use of beveled edges within the via is also considered. The molecular dynamics (MD) method is employed to simulate the filling process. The simulation is based upon three MD models, namely the dual via model, the deposition model and the potential model. Furthermore, the simulation incorporates the thermal control layer marching algorithm in order to increase the accuracy of the solution and to reduce the computational time. The results of the study show that in general, the coverage of both vias improves as the incident energy of the deposited atom increases, i.e. the filling pattern changes from anti-conformal to conformal, and then finally to super-filling as the incident energy increases. Typically, the optimum coverage of the upper via is obtained for a large via-radius ratio. However, it is found that coverage of the lower via is not only dependent upon the via-ratio, but that it is also strongly influenced by the incident energy of the deposited atoms. At lower incident energy levels, the via geometry effect governs the coverage results. However, as the incident energy increases, the incident energy effect becomes the dominant factor in determining the final coverage. It is determined that the interaction of these two effects influences the nature of the relationship between the coverage percentage and incident energy for different ranges of the via-radius ratio.

KEYWORDS: molecular dynamics, dual damascene, ionized physical vapor deposition
DOI: 10.1143/JPSJ.72.3151

1. Introduction

The dual damascene process is a batch operation which consolidates the original two-step metallization procedure into a single-step process. This technique involves filling multiple-layer interconnects etched into a dielectric inter-layer to form a dual via configuration, as shown in the schematic diagram presented in Fig. 1. The dual damascene process provides two major improvements to the traditional two-step technique, namely a reduction in the process time and a lower connector resistance, i.e. because the additional resistance arising from the adjacent surfaces in the two-step process^{1–4)} is eliminated. However, the filling characteristics become more complicated for the dual via configuration due to the additional interactions which occur between the various process parameters, *e.g.* incident energy, geometry parameter and via-radius ratio. Therefore, producing defect-free interconnects¹⁾ becomes more problematic. Clearly, a detailed understanding of the influence of process and geometry parameters upon the filling characteristics is essential if defect-free dual via interconnects are to be produced.

Several deposition processes have been developed in order to meet the special filling requirements for particular geometries such as corrugated structures or high aspect ratio vias. These processes include long throw deposition, collimated deposition and ionized physical vapor deposition (IPVD).^{5–7)} The key characteristic of each of these processes is the ability to focus the incident atoms within a narrow

angular bandwidth by means of various control strategies. In the IPVD process, the atoms which are to be deposited are first emitted from a magnetron cathode and then enter an inductively coupled plasma (ICP) region^{8,9)} where some of them subsequently become ionized. The fraction of emitted atoms which are ionized as they pass through this region can be controlled by adjusting the power of the ICP and the magnetron.⁸⁾ Further, the direction of the ionized atoms can be manipulated by applying a bias potential to the substrate. This ability to control the direction of the deposited atoms is the intrinsic advantage of the IPVD method over the collimated sputtering process⁹⁾ or the long throw deposition process. An experimental study using the IPVD process to produce dual via interconnects showed that the technique was effective in producing improved interconnects with lower defects.⁹⁾

A review of the available literature determines that the dual damascene process has seldom been investigated using numerical analysis techniques. Most of the previous studies were based upon an experimental approach and discussed either the analytic or technical aspects of the process.¹⁾ However, due to the very small characteristic size of the devices considered within these studies, it is very difficult to explore the filling mechanisms experimentally. Therefore, numerical simulation techniques have been developed to provide a detailed understanding of the filling morphology evolution during the deposition process. Many closely related studies^{10–13)} have employed a numerical technique to investigate the filling of a single trench or via using the conventional damascene process. Hamaguchi and Rossnagel¹⁰⁾ used the shock-tracking method to obtain the filling morphology evolution during the IPVD process. Later, Vyvoda¹¹⁾ employed a hybrid technique combining the

*To whom all the correspondence should be addressed.

E-mail: chchwang@mail.ncku.edu.tw

†E-mail: n00cjg00@nchc.org.tw

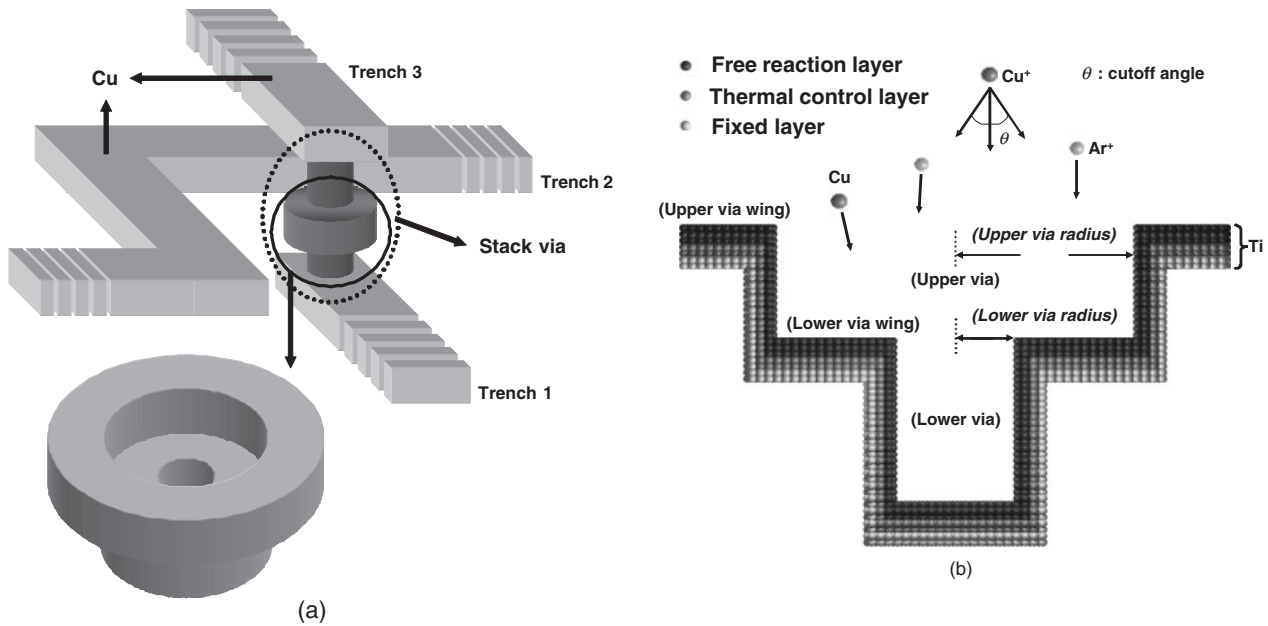


Fig. 1. Schematic diagram of stack via used in dual damascene process; (b) MD simulation model.

shock-tracking method and a molecular dynamics (MD) approach to study the IPVD filling profile evolution. In their study, the effects of sputtering and sticking were first determined by a separate MD simulation and were then incorporated into the shock-tracking method. In a very recent investigation, Hwang *et al.*^{12,13)} adopted MD simulation to study the role of incident Ar⁺ and Cu⁺ ions in the IPVD process. Their study pointed out that the use of the MD technique to simulate the IPVD process enables the direct treatment of sputtering and sticking effects without the need for any additional treatment. They concluded that Ar⁺ and Cu⁺ ions play a similar role in determining the filling characteristics, i.e. they both promote the migration ability of the deposited atoms.

The objective of the present study is to use MD simulation to conduct a detailed investigation of the filling mechanisms of dual vias in a dual damascene process. The MD simulation is based upon three discrete models, namely the dual via model, the deposition model and the potential model. Additionally, the thermal control layer marching (TLM) algorithm is adopted in order to increase the computational accuracy and to reduce the computational time.¹⁴⁾ The filling morphologies and filling characteristics are investigated for different incident energies and different via-radius ratios. The relationship between the dual via geometry parameter and the filling percentage is explored.

2. Simulation Model

The schematic diagram of the dual via arrangement and the molecular dynamics simulation model are depicted in Figs. 1(a) and 1(b), respectively. The stack via configuration is usually found within complementary metal–oxide–semiconductors (CMOS).^{15,16)} As shown in Fig. 1(b), the analyzed domain in the molecular dynamics simulation consists of two rectangle regions, which together form the cross-section of the two-via structure.

The MD simulation of the dual damascene process

comprises three models: a model of the dual via structure, a deposition model and a potential model. The simulation also incorporates the thermal control layer marching (TLM) algorithm. For the sake of brevity, detailed descriptions of the simulation model and the TLM algorithm are deliberately omitted from the current paper. Interested readers are invited to refer to the present authors' previous publications^{12–14)} for further information.

2.1 Dual via model

An assumption is made that the deposition process is symmetrical about the vertical axis of the three-dimensional stack via shown in Fig. 1(a). This simplification allows a two-dimensional MD model of the dual via to be developed, as shown in Fig. 1(b). The influence of the low- k material lying beneath the Ti barrier layer on the incident atoms is not included in this model since the Ti film thickness is larger than the truncation distance of the interaction between the low- k material and Cu. The atoms lying on the upper surface of the free reaction layer are subjected to direct impact by the deposited atoms and undergo migration as a result. The purpose of the thermal control layer is to model the energy transfer which takes place as the impact energy of the deposited atoms is gradually absorbed within the substrate. In a traditional damascene simulation, the location of the thermal control layer is fixed. However, as described in §2.4, the current dual damascene simulation adopts a moveable thermal control layer. Finally, the outmost layer of the model is fixed to prevent the whole model from shifting.

2.2 Deposition model

The incident ions and the atoms emitted from the magnetron cathode are accelerated into impact on the dual via structure under the influence of an applied substrate bias. Within the simulation, the incident atoms are characterized by their incident velocity and by their spatial and angular distributions. The velocities of the incident atoms are

determined by their incident energy in accordance with the following expression:

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

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

A random distribution function is used to generate the incident positions of the deposited atoms and ions within the dual via structure. It is also necessary to specify the incident angle of each atom and ion. This is again achieved by means of a random function which ensures that the incident angle of each atom falls randomly within a cutoff angle, θ specified relative to the vertical axis, as shown in Fig. 1(b). Finally, the elapsed time between two successive deposited atoms is determined by the specified deposition rate.

2.3 Potential model

The interaction between the atoms and the ions in the IPVD process is complex. It is necessary to simultaneously consider both the neutral atom interactions, i.e. Ti–Ti, Cu–Cu and Ti–Cu, and the interactions between the Ar^+ and Cu^+ ions and the neutral Ti and Cu atoms. A detailed description of these interactions has been published previously by the current authors.^{12,13)} A recent investigation¹⁷⁾ reports that the incident ions are neutralized via a fast Auger process or by resonance well before they impact on the substrate. Consequently, the interaction between the ions and the neutral atoms may be simplified to the case of interaction between two neutral atoms. This approach has been adopted in several previous MD simulations of ion-related processing^{18–20)} and the results have been in good agreement with experimental results.

This paper adopts the many-body, tight-binding potential method to model the atomic interaction among the Cu atoms, among the Ti atoms and between the Cu and Ti atoms. The remaining inter-atomic forces, i.e. Ar–Cu and Ar–Ti, are modeled using the Molière potential method.

The interactions for Ti–Ti, Cu–Cu and Cu–Ti are characterized by the many-body, tight-binding potential, which is given by the following:

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

where ξ is an effective hopping integral, r_{ij} is the distance between atoms i and j and r_0 is the first-neighbor distance. The parameters A , p , q and ξ used in the simulation to describe the Cu–Cu and Ti–Ti interactions are listed in Table I.²¹⁾

The pairwise Molière potential method is used to simulate the interatomic force acting between the Ar ions and the

neutral atoms. The repulsion force is represented by an exponential decayed function and depends only on the neutral charges and the inter-nuclear distance. The Molière potential is introduced in ref. 22 and is expressed by:

$$V_{ij}(r) = \frac{Z_1 Z_2 e^2}{r_{ij}} (0.35 e^{-0.3 r_{ij}/a} + 0.55 e^{-1.2 r_{ij}/a} + 0.1 e^{-6.0 r_{ij}/a}) \quad (3)$$

where a is the Firsov screening length, given by:

$$a = 0.4683 (Z_1^{1/2} + Z_2^{1/2})^{-2/3} \quad (4)$$

where Z_1 and Z_2 are the atomic numbers of the relevant ion and the neutral atom, respectively.

The trajectories of the atoms and ions are calculated by the Newton equation of motion by manipulating the potential forms given in eqs. (2) and (3).

2.4 Thermal control layer marching algorithm

In the traditional simulation deposition model, the position of the thermal control layer is fixed. However, this straightforward approach increases the computational time required to simulate the complete outward transfer of the impact energy through the thermal control layer. The thermal control layer marching (TLM) algorithm has been developed to address this problem. The TLM algorithm employs a moveable thermal control layer whose location shifts upwards during the deposition process such that it always remains at a constant distance from the surface. The adoption of a moveable thermal control layer is shown to be a convenient and effective means of removing the impact energy of incident atoms, thus preventing an accumulation of energy within the deposited atoms.

The main procedures of the TLM algorithm involve first determining the locations of the surface atoms, i.e. the upper surface of the free reaction layer. Then, given a specified thickness of the free reaction layer, it is possible to locate the upper surface of the thermal control layer. Similarly, the lower surface of the thermal control layer can be located once the thermal control layer thickness is specified. Since the lower surface of the thermal control layer forms a boundary with the upper surface of the fixed layer, the location of the fixed layer is also determined. A detailed description of the TLM algorithm is provided in ref. 14. Figure 2 presents a schematic diagram of the TLM algorithm during the simulation process. Figure 2 clearly indicates the atoms which lie beneath the fixed layer. These atoms lie within the so-called non-reaction layer and are excluded from the simulation activity.

3. Result and Discussion

In this section, the effects of the incident energy and the via-radius ratio on the filling characteristics of the dual via in the dual damascene process are extensively investigated. The simulation considers incident Ar ions and Cu atom/ions with incident energy levels of 2-eV, 5-eV, 10-eV, 20-eV and 30-eV, and dual via structures with via-radius ratios of 1.5, 1.75, 2, 2.5 and 3. Note that this ratio is defined by dividing the upper via radius by the lower via radius. The cutoff angle is specified to be 5° for both Ar ions and Cu atoms. An assumption is made that almost all of the Cu atoms become

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

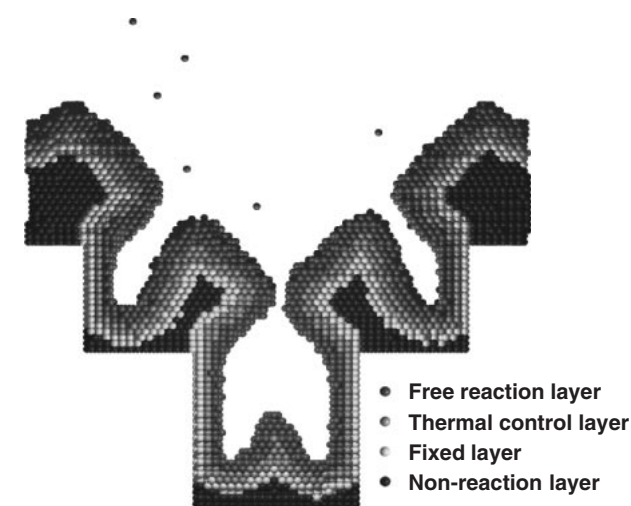


Fig. 2. Schematic diagram of thermal control marching algorithm [a snapshot of filling morphology of Fig. 3(u) at an instant of 3250 ps].

ionized,^{5,6,9,12)} and therefore no distinction is made between Cu atoms and copper ions when specifying their incident energy and incident angle. An equal number of Cu atoms and Ar ions are introduced into the simulation system. The simulation case studies considered in this investigation adopt a lower via aspect ratio of 1.5 (defined as the ratio of the via depth to the diameter of the lower via).

3.1 Filling morphology comparison

Figure 3 shows the filling morphology for different combinations of incident energy and via-radius ratio. The 25 individual filling morphologies may be classified as belonging to one of 5 possible filling patterns, namely anti-conformal/anti-conformal, anti-conformal/super-filling, an-

ti-conformal/conformal, super-filling/anti-conformal, and conformal/conformal, where the first filling pattern mentioned within each pair refers to the upper-via, and the second pattern refers to the lower via. A more detailed view of each possible filling pattern combination is presented in Figs. 4(a) to 4(e). It is noted that a number is assigned to each filling pattern, i.e. (i)–(v). This number appears in the upper-right hand corner of each of the 25 snapshots in Fig. 3 for reference purposes. From Fig. 4, it can be seen that the anti-conformal filling pattern results in an unsatisfactory filling of the trench. With this pattern, deposited atoms accumulate on both wings of the via and form an overhanging structure which prevents subsequently deposited atoms from reaching the bottom corners of the via. The effects of this so-called shadowing effect are clearly visible in Fig. 4(a), in which it is noted that the corners of the via are scarcely covered with deposited atoms. As may be seen in the lower via of Fig. 4(c), the conformal filling pattern is a more satisfactory filling pattern, which results in the thickness of the layer of deposited atoms increasing uniformly in all directions. However, it is also noted that this filling pattern may result in small voids becoming trapped within the filled via. As may be seen in Fig. 4(b), the super-filling pattern, in which the lower via is filled progressively from its base to its upper edge, is found to be the most successful.

Table II summarizes the filling pattern results presented in Fig. 3. As before, the initial filling pattern within each pair refers to the upper via coverage pattern, while the second filling pattern refers to the lower via coverage. It is possible to draw several fundamental conclusions from Table II. At smaller values of incident energy, anti-conformal filling patterns are noted within both the upper and the lower vias. When the incident energy is increased to 10-eV, it is noted that an increase in the via-radius from 1.75 to 2.0 has no

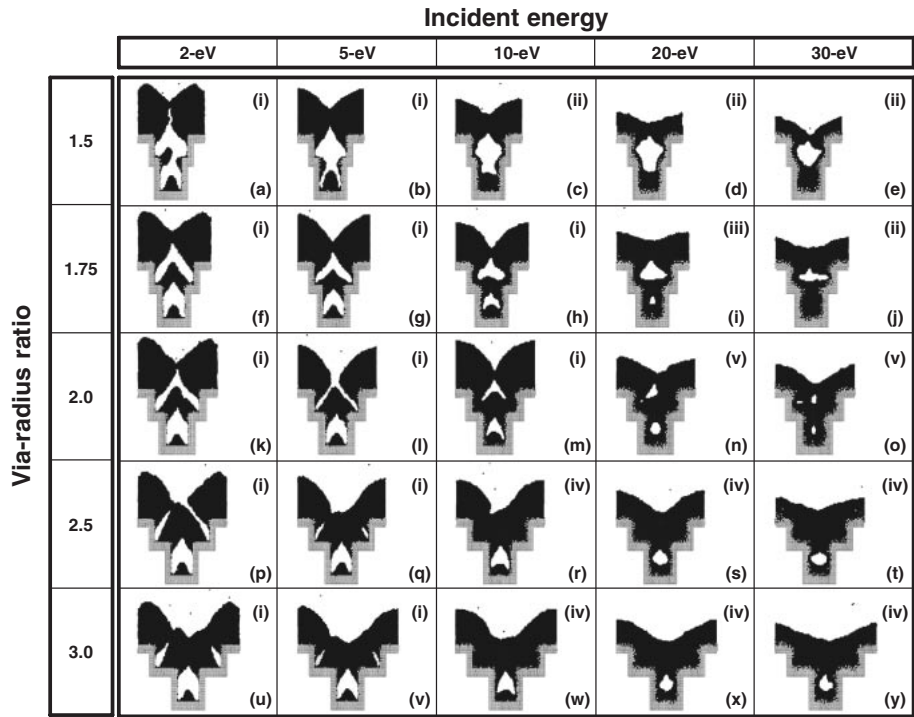


Fig. 3. Final filling morphology at different incident energy and via-radius ratios [Note that the filling pattern of each snapshot is given by a number (i–v) in the upper right corner, where these numbers refer to the filling patterns detailed in Fig. 4].

Table II. Summary of filling patterns of Fig. 2 for different incident energies and via-radius ratios.

Via-radius ratio	Incident energy				
	2-eV	5-eV	10-eV	20-eV	30-eV
1.5	Anti/Anti ^{a)}	Anti/Anti	Anti/Supe	Anti/Supe	Anti/Supe
1.75	Anti/Anti	Anti/Anti	Anti/Anti	Anti/Conf	Anti/Supe
2.0	Anti/Anti	Anti/Anti	Anti/Anti	Conf/Conf	Conf/Conf
2.5	Anti/Anti	Anti/Anti	Supe/Anti	Supe/Anti	Supe/Anti
3.0	Anti/Anti	Anti/Anti	Supe/Anti	Supe/Anti	Supe/Anti

a) which is in “upper via/lower via” order, and the “Conf”, “Anti” and “Supe” are the abbreviations for Conformal, Anti-conformal, Super-filling, respectively.

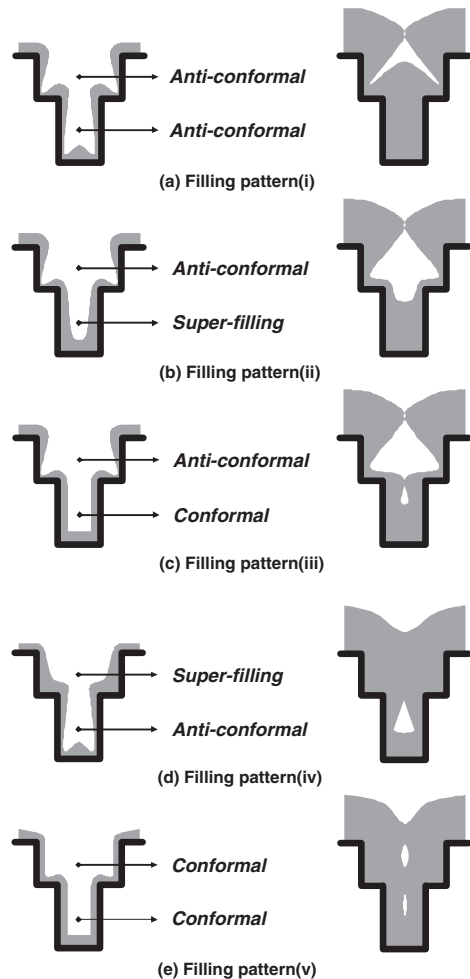


Fig. 4. Schematic of the five possible filling patterns: (a) anti-conformal/anti-conformal, filling pattern (i); (b) anti-conformal/super-filling, filling pattern (ii); (c) anti-conformal/conformal, filling pattern (iii); (d) super-filling/anti-conformal, filling pattern (iv); (e) conformal/conformal, filling pattern (v).

effect upon the filling pattern of the upper via; it retains a anti-conformal filling pattern. However, when the via radius is further increased to 2.5, the filling pattern in the upper via changes to one of super-filling. For the case of incident energies of 20-eV and 30-eV, the filling pattern in the upper via changes from anti-conformal to conformal, and from conformal to super-filling, as the via-radius ratio is increased from 1.75 to 2.0, and from 2.0 to 2.5, respectively. [Snapshots (i), (n) and (s) and snapshots (j), (o) and (t) in Fig. 3 apply.] Regarding the lower via, for an incident energy of 20-eV, the filling pattern changes from super-

filling at a via radius ratio of 1.5 [i.e. Fig. 3(d)] to conformal at radius ratios of 1.75 and 2.00 [i.e. Figs. 3(i) and 3(n)], and finally to an anti-conformal filling pattern for radius ratios of 2.5 and 3.0 [i.e. Figs. 3(s) and 3(x)]. The change in filling pattern of the lower via follows the same trend for the highest incident energy of 30-eV, i.e. the lower via filling pattern changes from super-filling for a via radius of 1.5 and 1.75, to conformal for a via radius of 2.0, and finally to anti-conformal for via radius ratios of 2.5 and 3.0. [Snapshots (e), (j), (o), (t) and (y) apply, respectively.] At incident energies of 10-eV and 20-eV, it is noted that as the filling condition of the upper via improves due to an increasing via-radius ratio, the filling coverage in the lower via deteriorates. In addition, it is observed that the filling pattern transition does not cycle strictly from anti-conformal to conformal, and then to super-filling (or vice versa). As may be seen from Figs. 3(c) and 3(h) for the case of an incident energy of 10-eV, the filling pattern may change directly from super-filling to anti-conformal.

From the discussion above, it is clear that the transition between the filling patterns is strongly dependent upon the interaction between the incident energy and the dual via geometry effects. This interaction is now discussed in detail.

3.2 Incident energy effect

Figure 5 presents the relationship between coverage percentage and incident energy for different values of the via-radius ratio. Note that the solid lines represent the coverage percentage of the upper via, while the dashed lines refer to coverage of the lower via.

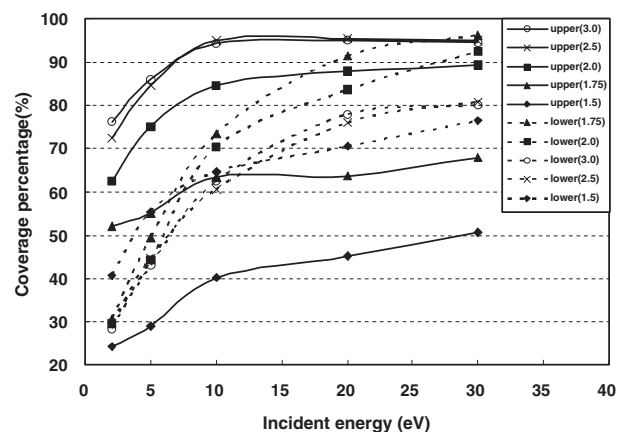


Fig. 5. Relationship between upper and lower via coverage and incident energy for different values of via-radius ratios.

In general, it is observed that the coverage percentage of both the upper and the lower via tends to increase as the incident energy increases. However, it is noted that the degree of improvement depends upon the via-radius ratio. In the case of the upper via, increasing the via-radius ratio improves the coverage percentage. This phenomenon is clearly visible in Fig. 3 by comparing the coverage of the upper via in snapshots (a)–(e) for a via-radius ratio of 1.5 with snapshots (u)–(y), which present the coverage for a via-radius ratio of 3.0.

An inspection of the coverage percentage of the lower via shows that the relationship between coverage percentage and via-radius for different levels of incident energy is less straightforward than in the case of the upper via. At higher values of incident energy, i.e. between 15-eV and 30-eV, the optimal coverage of the lower via is achieved for a via-radius ratio of 1.75. The coverage percentage then reduces progressively as the via-radius ratio is changed to 2.0, then to 3.0 and then finally to 2.5, i.e. the results indicate that the poorest coverage percentage is obtained for the smallest via-radius of 1.5. At the lower incident energy of 10-eV, the best coverage results are again obtained with a via-radius ratio of 1.75, followed by a ratio of 2.0. However, thereafter the sequence of via-radius ratios which results in a progressive reduction of coverage is different than in the previous case, i.e. 1.5, 3.0 and 2.5 for 10-eV, compared to 3.0, 2.5 and 1.5 for the incident energy range of 15-eV to 30-eV. Finally, at the smaller incident energies of 2-eV and 5-eV, the best coverage percentage is obtained for the smallest via-radius, i.e. 1.5.

From the discussions above, it is clear that the relationship between the percentage coverage and the via-radius ratio is straightforward in the case of the upper via. The results show that the coverage improves as the via-radius increases for a constant incident energy, i.e. the coverage is improved when a larger upper via opening is adopted. However, the relationship between these parameters is more complex for the lower via and requires a rigorous investigation.

3.3 Via-radius ratio effect

For a constant value of incident energy, the relationship between the coverage percentage and the via-radius ratio may be investigated by rearranging the data of Fig. 5 into the format shown in Fig. 6. As before, the solid lines represent coverage of the upper via, while the dashed lines refer to the lower via. For incident energies of 2-eV and 5-eV, it is noted that there appears to be an inverse relationship between the coverage percentage of the upper via and the lower via, i.e. an improvement in the coverage of the upper via is accompanied by a deterioration in the coverage of the lower via as the via-radius ratio increases. However, an exception to this trend is the improvement in coverage identified in both the lower and the upper via as the via-radius ratio is increased from 1.5 to approximately 1.75 for incident energies of 10-eV, 20-eV and 30-eV. This phenomenon is investigated further in the paragraphs which follow.

Incident energy and via geometry both have a significant influence upon the filling pattern of the dual via. Regarding the via geometry, the length of the lower wing [see Fig. 1(b)] is a particularly significant factor and is reflected by the via-radius ratio parameter. The significance of the lower wing

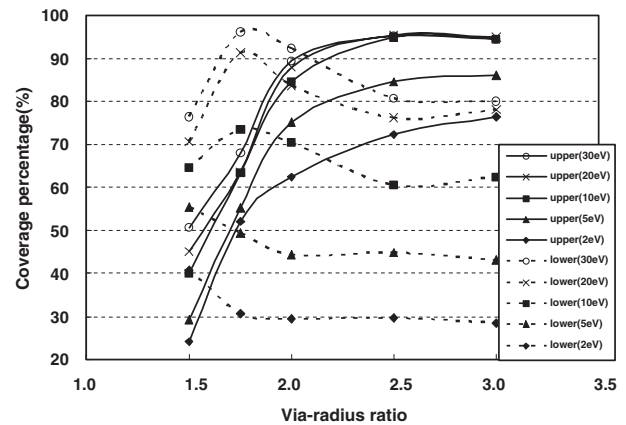


Fig. 6. Relationship between upper and lower via coverage and via-radius ratio for different values of incident energy.

length becomes clear if the filling morphology at the smallest incident energy of 2-eV is observed in Fig. 3 as the via-radius ratio increases from 1.5 to 3.0 [i.e. Figs. 3(a), 3(f), 3(k), 3(p) and 3(u)]. As the length of the lower via wing increases, i.e. as the via-radius ratio increases, it is observed that the deposited atoms accumulate at the lower via opening and form inclined columnar clusters. At a via-radius of 1.75, it can be seen that these columns meet and subsequently grow in size as further atoms are deposited. As the incident energy increases to 5-eV, the influence of the lower via wing length is still dominant. However, as shown by a comparison of Figs. 3(a) and 3(b), 3(f) and 3(g), 3(p) and 3(q) and 3(u) and 3(v), the height of the inverse triangle columnar structure forming a bridge over the lower via opening is smaller than in the previous case of 2-eV.

As the incident energy increases to 10-eV, the incident energy effect becomes more significant and begins to interact with the via geometry effect in determining the coverage of the two vias. A comparison of Figs. 3(f), 3(g) and 3(h) or Figs. 3(k), 3(l) and 3(m) shows that the most obvious effect of the increased incident energy is to reduce the bulgy part of the inverse triangle columnar structure. Furthermore, observation of Figs. 3(a)–3(c) shows that the accumulation of deposited atoms at the lower via wing gradually disappears as the incident energy increases to 10-eV. This phenomenon may be attributed to the higher migration ability of the deposited atoms along the trench walls at elevated incident energies, which allows the deposited atoms to move towards the base of the lower via rather than to accumulate on the lower via trench wing.

A careful comparison of the filling morphologies of Figs. 3(c) and 3(h), 3(d) and 3(i) and 3(e) and 3(j) confirms that the coverage in both the upper and the lower via improves as the via-radius ratio increases from 1.5 to 1.75 for incident energies of 10-eV, 20-eV and 30-eV. As stated previously, this phenomenon is different from the trend noted at higher values of via-radius ratio. From these figures, it would appear that the elapsed time prior to the touching of the clusters overhanging the upper via opening and the increase in incident energy are the two principal factors causing this phenomenon. It is noted that the accumulation of deposited atoms on the lower via trench wings is smaller in the case of the low via-radius configurations. Therefore, the shadowing

effect is reduced and the coverage of the lower via is improved. Therefore, it might be expected that the coverage of the lower via would deteriorate as the via-radius ratio increases, as stated previously for the smaller incident energy levels of 2-eV and 5-eV. However, the effect of the increased incident energy is to improve the migration ability of the deposited atoms. This effect enables the accumulated atoms on the lower trench wing to overcome the geometry effect imposed by the longer lower trench wing. The increased migration ability allows the atoms which would otherwise accumulate on the lower trench wing to flow into the lower via, thus improving its coverage. Meanwhile, the elapsed time before the clusters which overhang the upper via opening touch is shorter in the case of a lower via-radius ratio. The formation of this bridge structure prevents incident atoms from entering the dual-via, thus preventing any further improvement in the lower via coverage. This explains why the lower via coverage is worse at the lower via-radius configuration of 1.5 than it is at a via-radius configuration of 1.75 for higher incident energy levels of 10-eV, 20-eV and 30-eV.

4. Conclusion

This investigation has employed MD simulation to investigate the influence of incident energy and dual via geometry upon the filling mechanisms for the IPVD process. MD simulation has proven to be an appropriate technique for studying the filling mechanisms from a microscopic viewpoint. A detailed discussion of the various filling mechanisms has been provided and the effectiveness of introducing a beveled edge on both the upper and the lower via corners has been verified.

The results of this study show that in general, the coverage of the upper and lower via improves as the incident energy of the deposited atoms increases. Coverage of the upper and lower vias includes anti-conformal, conformal or super-filling patterns. Generally, the upper via coverage is improved for larger via-radius ratios. However, the coverage of the lower via is dependent not only upon the via-radius ratio, but also upon the incident energy. At incident energy levels of 2-eV and 5-eV, the via geometry effect is the dominant factor in determining the lower via coverage and the coverage deteriorates as the via-radius ratio increases from 1.5 to 1.75. However, as the incident energy level increases, the interaction between the incident energy effect and the geometry effect becomes more significant. At the higher incident energies of 10-eV, 20-eV and 30-eV, the lower via coverage percentage improves as the via-radius ratio increases from 1.5 to approximately 1.75. This phenomenon is attributed to the enhanced migration ability of the deposited atoms at elevated incident energies, which allows the atoms to overcome the "geometry barrier" (i.e. the lower via wing).

In the physical deposition process, control of the substrate temperature is also an important factor in determining the filling mechanisms and the final via coverage.^{13,23–28)} An

intended area of future investigation is to determine the relationship between the substrate temperature and the via filling mechanisms, and specifically, to explore the influence of temperature effects upon the interaction of the upper and lower via filling mechanisms.

Acknowledgment

The authors gratefully acknowledge the support provided to this research by the National Science Council, Republic of China, under Grant Nos. NSC91-2212-E006-161. Grateful thanks are also extended to Dr. Chung-Yi Lin for his technical English writing assistance and to Dr. Shin-Pon Ju for his valuable input to discussions and for his suggestions made during the course of this study.

- 1) R. H. Havemann and J. A. Hutchby: *Proc. IEEE* **89** (2001) 586.
- 2) A. Furuya, M. Tagami, K. Shiba, K. Kikuta and Y. Hayashi: *IEEE Trans. Electron Devices* **49** (2002) 733.
- 3) E. Bar, J. Lorenz and H. Rysse: *Microelectron. Eng.* **50** (2000) 481.
- 4) C. L. Gan, C. V. Thompson, K. L. Pey, W. K. Choi, H. L. Tay, B. Yu and M. K. Radhakrishnan: *Appl. Phys. Lett.* **79** (2001) 4592.
- 5) S. M. Rossnagel and J. Hopwood: *Appl. Phys. Lett.* **63** (1993) 3285.
- 6) S. M. Rossnagel and J. Hopwood: *J. Vac. Sci. Technol. B* **12** (1994) 449.
- 7) E. C. Cooney III, D. C. Strippe, J. W. Korejwa, A. H. Simon and C. Uzoh: *J. Vac. Sci. Technol. A* **17** (1999) 1898.
- 8) C. A. Nichols, S. M. Rossnagel and S. Hamaguchi: *J. Vac. Sci. Technol. B* **14** (1996) 3270.
- 9) S. M. Rossnagel: *J. Vac. Sci. Technol. B* **13** (1995) 125.
- 10) S. Hamaguchi and S. M. Rossnagel: *J. Vac. Sci. Technol. B* **13** (1995) 183.
- 11) M. A. Vyvoda, C. F. Abrams and D. B. Grave: *IEEE Trans. Plasma Sci.* **5** (1999) 1433.
- 12) C. C. Hwang, G. J. Hwang, J. G. Chang and S. P. Ju: *J. Appl. Phys.* **91** (2002) 3569.
- 13) C. C. Hwang, G. J. Hwang, S. P. Ju and J. G. Chang: *Surf. Sci.* **512** (2002) 135.
- 14) C. C. Hwang, J. G. Chang, S. P. Ju and H. C. Lin: submitted to *Phys. Rev. E* (2002).
- 15) F. Caignet, S. Bendhia and E. Sicard: *Proc. IEEE* **89** (2001) 556.
- 16) E. Sicard and S. Bendhia: *EWME 2002*, Vigo, Spain, 23–24 May, 2002.
- 17) G. A. Kimmel and B. H. Cooper: *Phys. Rev. B* **48** (1993) 12164.
- 18) D. G. Coronell, D. E. Hansen, A. F. Voter, C. L. Liu, X. Y. Liu and J. D. Kress: *Appl. Phys. Lett.* **73** (1998) 3860.
- 19) J. D. Kress, D. E. Hansen, A. F. Voter, C. L. Liu, X.-Y. Liu and D. G. Coronell: *J. Vac. Sci. Technol. A* **17** (1999) 2819.
- 20) D. E. Hansen, A. F. Voter and J. D. Kress: *J. Appl. Phys.* **82** (1997) 3552.
- 21) F. Cleri and V. Rosato: *Phys. Rev. B* **48** (1993) 22.
- 22) K. H. Müller: *Phys. Rev. B* **35** (1987) 7690.
- 23) S. P. Ju, C. I. Weng, J. G. Chang and C. C. Hwang: *J. Vac. Sci. Technol. B* **20** (2002) 946.
- 24) M. H. Su, C. C. Hwang, J. G. Chang and S. P. Ju: *J. Vac. Sci. Technol. B* **20** (2002) 1853.
- 25) M. H. Su, C. C. Hwang, J. G. Chang and S. H. Wang: *J. Appl. Phys.* **93** (2003) 4566.
- 26) S. P. Ju, C. I. Weng and C. C. Hwang: *J. Appl. Phys.* **92** (2002) 7062.
- 27) M. Proust, F. Judong and J. M. Gilet: *Microelectron. Eng.* **55** (2001) 269.
- 28) S. Shingubara, H. Kotani and H. Sakaue: *J. Vac. Sci. Technol. B* **17** (1999) 2553.