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A comparative molecular dynamics study of copper trench fill properties between Ta and Ti barrier layers

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Abstract

The copper atoms deposition on tantalum diffusion barrier layer in a damascene process was studied using molecular dynamics simulation with the embedded atom method (EAM) as interaction potential for the present alloy metal system which is based on invariance-preserving alloy model. The present results are discussed in terms of void formation, coverage percentage and alloy fraction. The effects of different process parameters on the trench-filling morphologies and microstructures including incident energies of depositing atoms and substrate temperatures were investigated. Comparing with Ti diffusion barrier under the same process parameters, it is found that due to better thermal stability that significant improvement in coverage percentage can be obtained using the tantalum barrier layer, especially at high incident energies and high substrate temperatures.

Keywords: Tantalum barrier layer; Embedded atom method; Damascene process; Molecular dynamics simulation

1. Introduction

Interconnects are used to connect devices electrically in integrated circuits. As feature sizes decrease below a quarter micron, the scaling of interconnects poses several serious metallization problems such as high RC and electromigration resistance. To improve the electrical properties problems, copper (Cu) is used instead of aluminum for interconnects. A review on the overall requirements for diffusion barrier layers has been given by Kattelus and Nicolet [1]. There are many refractory materials and compounds that are used as barrier layer in Cu interconnect [2–4]. Ta is thermodynamically stable with respect to Cu and Ta is almost completely immiscible up to their melting point and do not react with Cu to produce any compounds. Ta has good adhesion to both Cu and dielectrics and is known to be more effective than Ti as a diffusion barrier in Cu metallization. We shall investigate the effects of using both Ta and Ti barrier layers in Cu Damascene trench filling with physical vapor deposition (PVD). There are many simulation approaches have been explored in deposition simulation [5–9].

In this work, the molecular dynamics simulation is used to study the *trench filling* and microstructures for depositing Cu into Ta diffusion barrier layer in Damascene process. The processes parameters considered including incident energies of depositing atoms and substrate temperatures and

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their effects on the trench-filling morphologies, coverage percentages, and alloy fraction are studied in detail for Ta barrier layer. We also compare the microstructure differences and trench filling between Ta and Ti barrier layers in Cu Damascene process. This paper is a sequel to [10] and we will constantly refer to [10] for the results using Ti barrier layer without duplicating them here.

2. Computational model

The model for trench filling with MD simulation includes a trench model, a deposition model, and a potential model. The trench model is the same as described in previous work [10]. The computational domain is $169.74 \times 25.25 \times 225.30$ Å and the aspect ratio of trench is 1 with the depth of trench 10 nm. The atoms of barrier layer for Ta are arranged by basic cubic crystal (bcc) structure with surface (1 0 0) for Ta barrier layer initially and the single-crystal arrangement hcp and surface (0 0 0 1) is used for Ti barrier layer. Both barrier layers have no grain boundary and amorphous crystal arrangement before simulation. In deposition model, we prepare the incident atoms to add into system before simulation. The positions of incident Cu atoms are arranged randomly in x, y directions. The positions of incident atoms in z direction are started from the height of simulation domain and the gap (Δz) between sequential incident atoms is determined by the depositing rate and the magnitude of velocity is determined by incident energies. As the simulation is advancing, we add nearly 6 incident Cu atoms into the system per 1 ps. The angular distributions deposition is used for incident atoms and are assumed to be confined within the range of zenith angle, from -5° to $+5^\circ$, and the range of azimuth angle, from 0° to 360°. Since only the short-range forces were considered in this work, we did not consider reflected atoms and the resputter atoms which include Cu adatoms and tantalum (titanium) atoms on barrier layer. They are removed from the system when they are far (larger than cutoff-range 6 Å) from the barrier (deposited) layers. We detect free atoms that no longer interact with the substrate by observing force value of every atom. The atoms that have zero force value are labeled as free atoms in our program and these free atoms are removed from the system. As for the interatomic potential model, the embedded atom method (EAM) [11–13] is used which is an isotropic many-body pair-function potential. The total energy acting on each atom is computed from the sum of the local embedded energy and two-body potential as

$$E_{\text{tot}} = \sum_i F(\rho_i) + \frac{1}{2}\sum_i \sum_{j\neq i} \phi_{ij}(r_{ij}), \tag{1}$$

$$\rho_i = \sum_{j\neq i} f(r_{ij}), \tag{2}$$

where E_{tot} is the total internal energy, F is the embedding energy, ρ_i is the local electron density at atom i, $\phi(r_{ij})$ is the pair potential and r_{ij} is the distance between atom i and atom j. A nearest-neighbor analytic form EAM potential is used in this work that *is suitable for* MD simulations has been proposed by Johnson [14]. The analytical forms of EAM have been developed for many metals and have yielded reasonable fits to physical properties [15]. The two-body potential and electron density function as given by Johnson can be written, respectively, as

$$\phi(r) = \frac{A\mathrm{e}^{-\alpha((r/r_{\text{e}})-1)}}{1+((r/r_{\text{e}})-\kappa)^m} - \frac{B\mathrm{e}^{-\beta((r/r_{\text{e}})-1)}}{1+((r/r_{\text{e}})-\lambda)^n}, \tag{3}$$

$$f(r) = \frac{f_{\text{e}}\mathrm{e}^{-\beta((r/r_{\text{e}})-1)}}{1+((r/r_{\text{e}})-\lambda)^n}. \tag{4}$$

The model parameters for Cu, Ti and Ta atoms are listed in Table 1. The embedding energy of the atom i is determined by the local electron density at the position of the atom and the embedding energy is

Table 1
Electron density function and two-body potential parameters for metals of EAM

	r_{e} (Å)	f_{e} (eV/Å)	ρ_{e} (eV/Å)	α	β	A	B	κ	λ	m	n
Cu	2.556	1.554	22.150	7.670	4.091	0.328	0.469	0.431	0.863	20.0	20.0
Ti	2.930	1.860	25.600	8.780	4.680	0.328	0.469	0.431	0.863	20.0	20.0
Ta	2.560	1.550	22.200	8.489	4.528	0.330	0.470	0.430	0.86	20.0	20.0