Application of Molecular Dynamics to the Simulation of Deposition

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Introduction

Ultra thin films are needed as contact layers, seed layers, and barriers for the fabrication of present and future Deep Submicron Interconnection Systems (DSM). As long as possible the deposition of such thin metal films is performed by Physical Vapor Deposition (PVD) or Ionized Physical Vapor Deposition (IPVD). See Fig. 1 for a simplified illustration of the PVD / IPVD process. Conformal (homogeneous) deposition in vias and trenches of increasing aspect ratio as well as uniform bottom and sidewall coverage in the features across a large wafer diameter require a near normal incidence of the film-forming particles. This can be achieved by a combination of a long target-to- wafer distance, a high degree of (post-) ionization, and wafer bias voltages in the order of –100 V. Because of their increased energy the ions undergo various interactions with the surfaces they hit: adsorption, reflection, and resputtering of one or more film particles. An optimization of the process conditions has to be supported by a multi-scale simulation of particle generation, transport, and deposition.

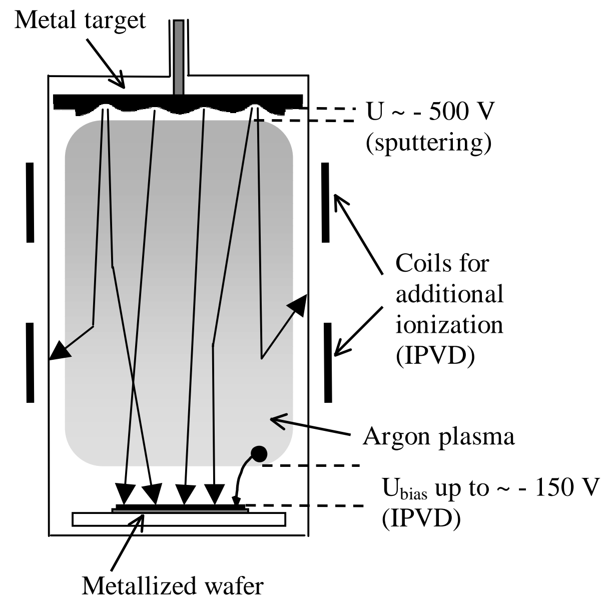

Fig. 1: A simplified illustration of the PVD / IPVD process

Objectives of PVD / IPVD simulation

The reactor scale simulation comprises firstly calculation of target emission spectra using the Molecular Dynamic (MD) approach and secondly simulation of transport at the reactor scale by the Monte Carlo (MC) approach. The goal of the reactor scale simulation is to obtain the profile of the film across the whole wafer disregarding the features, and the energy and angular distributions of particles arriving on the wafer. The results of the reactor scale simulation serve as input for the feature scale simulation.

The feature scale simulation comprises firstly simulation of transport at the feature scale using the MC approach, and secondly simulation of interactions of the arriving film-forming particles with the film surface using the MD approach. The main goal of the feature scale simulation is to obtain the topography of the film in the features (trenches and vias) for various positions on the the wafer (from wafer centre to wafer edge), and thus to be able to predict for given process conditions whether the bottom and sidewall coverage of the features will be sufficient or not.

Particle-surface interactions

A lot of research has been done in the field of particle-surface interactions. In the next paragraph let us summarize some basic facts relevant for this work. For a detailed analysis of this problematics we refer to [1,2].

As an incident ion in collisions with atoms and electrons of a metal slows down, energy in excess of the lattice binding energy (in the order of 10 eV) may be transferred to an atom of the metal. Atoms removed from their original sites are subsequently slowed down in the solid as well. They can also transfer energy to other atoms in the lattice. Thus, a so called collision cascade develops. Collision cascade evolution is influenced by the crystal lattice structure through channeling, blocking, and focusing. Some atoms involved in the collision cascade can be ejected out of the lattice. The ejected atoms are called as sputtered and the phenomenon of the ejection of lattice atoms out of the crystal by particle bombardment as sputtering. The projectile itself need not be absorbed in the crystal, it can be reflected and escape from the lattice as well. Sputtering yield is the average number of atoms ejected from the lattice by one incident projectile. The sputtering yield and the probability of projectile absorption / reflection and also the energy and angular spectra of emitted atoms (sputtered metal and reflected projectile atoms) depend on the projectile species, the composition of the metal target, the texture of the target, the projectile energy and the angle of projectile incidence.

The collision cascade spans over relatively large areas. If we want to properly model a projectile-surface interaction by atomistic simulations, for a projectile energy in the order of 100 eV the target size should be in the order of thousands of atoms.

Molecular (Classical) Dynamics approach

It is technically impossible to simulate a system consisting of thousands of atoms from first principles, i.e. by quantum mechanics. The approach of modelling the interactions on atomic scale is based on the approximation of quantum interactions by classical ones. Instead of solving the Schrödinger equation, a semiempirical model of classical interaction between atoms is constructed and then the Newton equations are solved [3].

For MD simulations we use an effective code Kalypso written by Marcus Karolewski [4] designed for simulating interactions of an atomic projectile with a metal crystal. The interaction potential used consists of three parts. The first acts at a short interatomic distance and it is a pairwise repulsive potential, so called screened Coulombic potential of Ziegler-Biersack-Littmark type [2].

$$E_{rep} = \frac{1}{2} \sum_i \sum_{j \neq i} \frac{Z_\alpha Z_\beta e^2}{4\pi\varepsilon_o r_{ij}} \sum_{k=1}^{4} c_k^{\alpha\beta} e^{-b_k^{\alpha\beta} r_{ij}/a^{\alpha\beta}} \tag{1}$$

E_{rep} is the total energy contribution resulting from the pairwise repulsive interactions. α and β denote the atomic types of the interacting atoms. Z is the atomic number, r_{ij} is the distance between atoms i and j; a, c_k and b_k are parameters. The repulsive part is important for high energy collisions that take place at the beginning of the collision cascade. At larger interatomic distances the interaction is modeled by an attractive potential consisting of a pairwise part and a many-body part based on so called tight-binding approximation [5].

$$E_{attr} = \sum_i \left[\sum_{j>i} A\, e^{-p\, x_{ij}} - \sqrt{\sum_{j \neq i} \xi^2 e^{-q\, x_{ij}}} \right] \quad \text{where } x_{ij} = \frac{r_{ij}}{r_o} - 1 \tag{2}$$

E_{attr} is the total energy contribution resulting from the attractive interactions. A, p, ξ, q and r_0 are parameters depending on the types of the interacting atoms α and β. The square root is the many-body part. The expression under the radical sign represents the local electron density at the site of atom i. To simplify the matter, the square root accounts for the fact that the total bond energy does not increase linearly with the number of bonds. This is important for a proper description of interactions at the surface. Thus, the surface binding energy should be automatically correct and it is not necessary to introduce an additional correction. An appropriate attractive potential is important for a proper description of the collective interaction in the collision cascade [2,6].

Note that the potential form defined by relations (1) and (2) does not show any explicit directional dependence that is in accord with the behaviour of transition metals. Because of a diffusive character of their valence f-orbitals the transition metals do not form bonds with a pronounced directionality.

The parameters in the interaction functions are usually obtained by fitting on experimental data of the material like cohesive energy, elastic constants, phonon spectra, heat of sublimation, and others or by fitting on data calculated ab initio by quantum mechanics.

The time step for integration of the Newton equations is in the order of 0.1-1 fs. The duration of the collision cascade is in the order of 100 – 1000 fs. After this time there is not enough energy for further atoms be sputtered.

MD simulation of the target emission spectra

Fig. 2 shows kinetic energy distributions of sputtered atoms for different faces of the hcp Ti crystal. It is obvious that the difference between the spectra for the particular faces is small. Note that despite the high energy of the projectile the energy of the most sputtered particles does not exceed 25 eV. It is a general phenomenon. The dependence of energy spectra of sputtered particles both on the projectile species and energy and even on the target metal is not strong. The maximum always lies in the order of several eV (depending on the cohesive energy of the metal crystal) and kinetic energy of the most sputtered atoms does not exceed several tens eV. Though, sputtering yield strongly depends on the materials used and the projectile energy.

On the other hand, the polar angle distributions of sputtered atoms can significantly differ depending on crystal structure and texture. For a perfectly polycrystalline target where the crystallites are randomly oriented, the angular distribution of sputtered particles has a cosine form. In this case the probability of emission is proportional to the cosine of the polar angle of the sputtered atom. Though, for particular textures the angular distribution can significantly differ from the cosine distribution. See Fig. 3 for comparison of the cosine distribution of a polycrystalline target with angular distributions calculated by MD simulations for different faces of the hcp-Ti target. For a proper simulation of the deposition process at the reactor scale it is necessary to know

the target texture (the percentage of crystallite orientations present on the target surface) and the corresponding spectrum of sputtered atoms resulting from this texture.

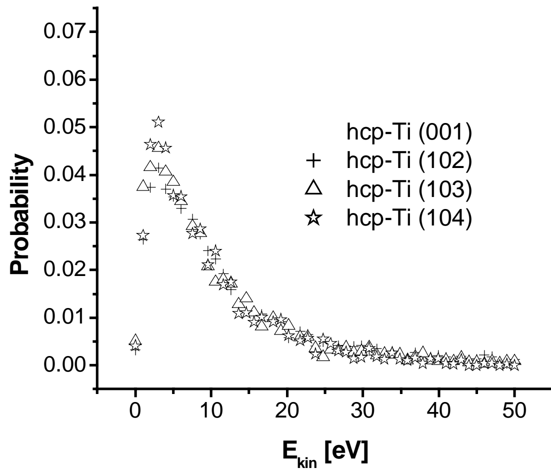

Fig. 2: Kinetic energy spectrum of sputtered atoms, MD calculation
(Projectile: Ar+, 441 eV, normal incidence)

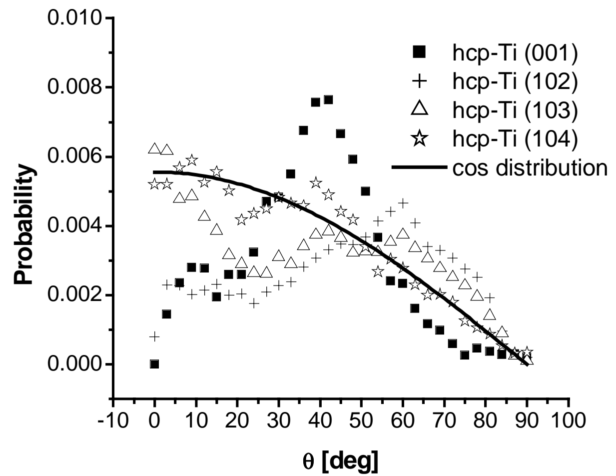

Fig.3: Polar angle spectrum of sputtered atoms, MD calculation
(Projectile: Ar+, 441 eV, normal incidence)

MD simulation of surface interactions for the Feature scale simulation

Fig. 4 and 5 show the dependence of the (re-)sputtering yield on the incident kinetic energy E_{kin} and the incident polar (off-normal) angle θ for an argon atom (Fig. 4) or a metal atom (Fig. 5) arriving on the surface of the growing thin film for three different metal surfaces: bcc Ti (100), fcc Cu (111), and bcc Ta (110), as obtained by MD simulations.

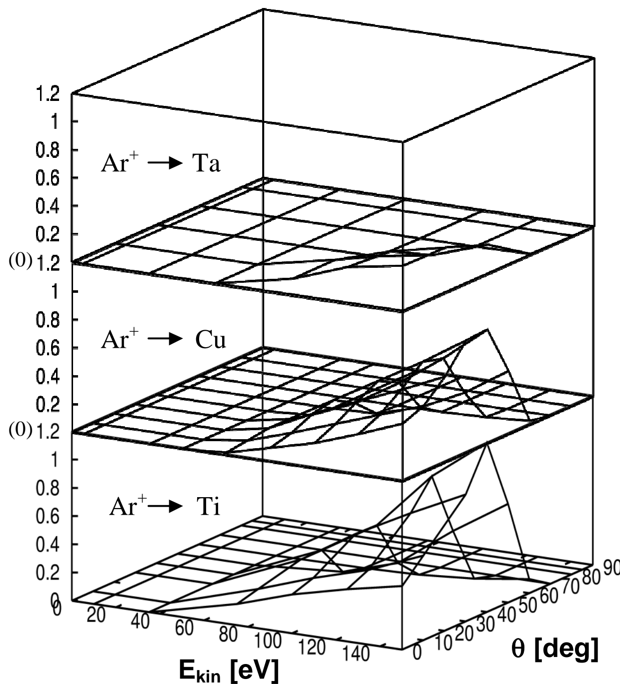

Fig. 4: Dependence of the (re-)sputtering yield on E_{kin} and θ for Ar^+ as projectile
(down – Ti, middle – Cu, up – Ta)

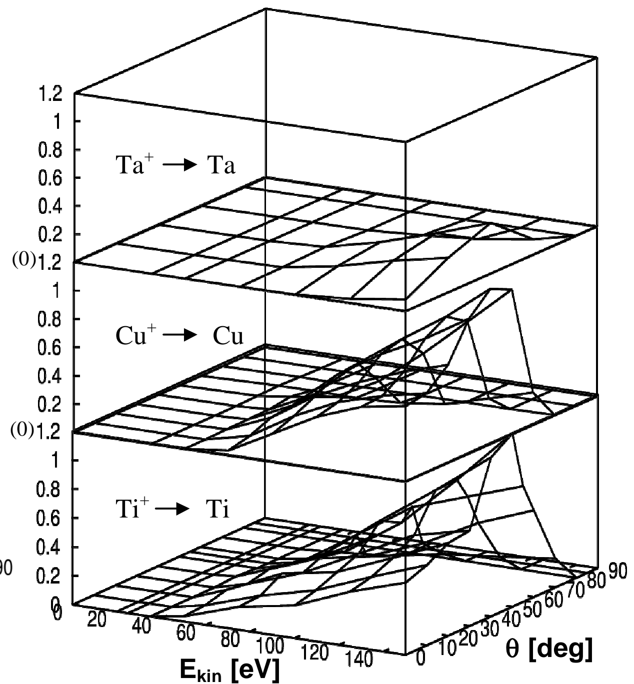

Fig. 5: Dependence of the self-(re-)sputtering yield on E_{kin} and θ
(down – Ti, middle – Cu, up – Ta)

Except these resputtering spectra, also spectra for reflection are important for a proper simulation of thin film deposition in high-aspect-ratio features. It can be seen that there is a threshold for sputtering in the range of several tens eV. The resputtering yield usually shows a maximum in the range from 40 to 50 degrees. Below 40° there is a high probability of projectile absorption and above 50° the probability of reflection starts to increase.

Further, let us point out the big difference in sputtering yield for titanium and copper on one side and the heavy tantalum on the other side. The masses of Cu and Ti are similar (63.5 and 47.9 a.u.) while Ta is much heavier (180.9 a.u.). The most effective energy transfer in an elastic collision occurs if both collision partners have the same mass. This is reason why in the case of Ta the sputtering yield for Ar^+ projectile (39.9 a.u.) is the lowest one. But, even for the self-sputtering, the yield is lowest for Ta (Ta sputtering Ta). It can be explained by a longer interaction time of the slower Ta projectile with the lattice atoms and with a higher value of lattice binding energy of Ta.

Thus, in a PVD process, where the energy of arriving particles is low, effectively no film resputtering occurs. On the other hand, in an IPVD process, where the energy of arriving ions is increased by a bias voltage applied on the substrate, resputtering can occur. The metallization of the lower part of the sidewalls in very high-aspect-ratio features occurs practically only due to the resputtering of the bottom film because on the sidewall only few atoms arrive, moreover if so, they arrive under low angles with a high probability of their nearly specular reflection.

The following figures show the results of the feature scale simulation using an in-house developed multiscale simulator T2.

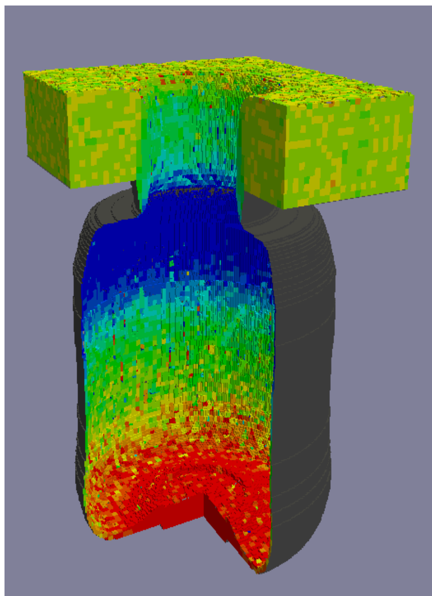

Fig. 6: Energy deposition in eV/atom, 3D representation

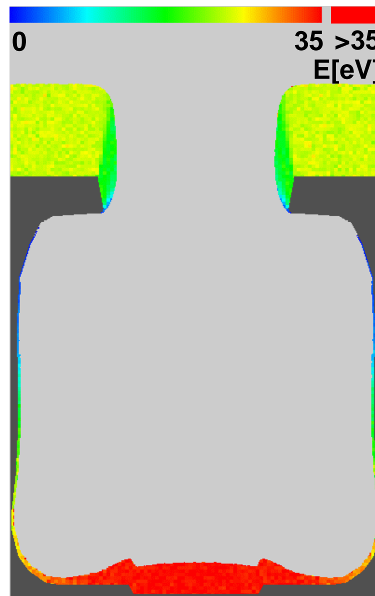

Fig. 7: Energy deposition in eV/atom, 2D profile

Fig. 8: TEM micrograph of the film in the feature

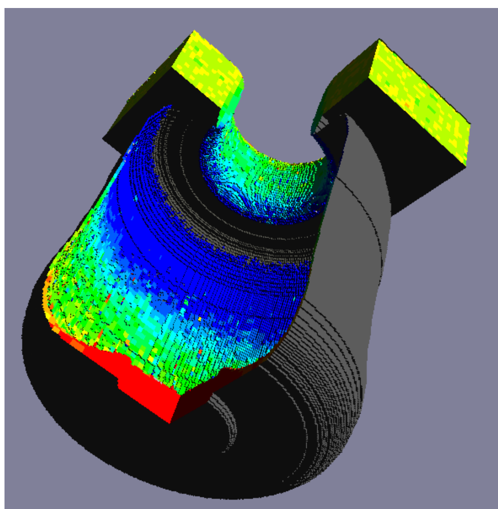

Fig. 9: Energy deposition in eV/atom, 3D representation (without resputtering and reflection)

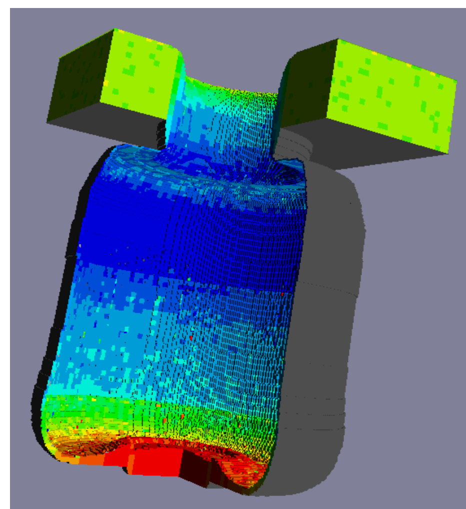

Fig. 10: Energy deposition in eV/atom, 3D representation (with resputtering and reflection)

Figures 6 and 7 show the simulated film profile and the distribution of the energy deposition (in eV per deposited metal atom) for a Ti deposition into a bottle-shaped test structure using a Trikon Advanced Hi-Fill process [7]. To have a good picture how the atoms arrive on the surface, resputtering, reflection, and diffusion models in T2 have been switched off deliberately. The absence of diffususion and resputtering effects is the reason for the occurrence of the sharp spikes in the bottom film profile. Fig. 8 is a TEM photo of an experimental film in the bottle-shaped feature for comparison.

Fig. 9 shows the same as Fig. 6, the feature is just rotated so that also the clean upper wall can be seen. Fig. 10 shows again a 3D representation for the same process when resputtering and reflection events were switched on in the simulation. It can be seen that thanks to these effects also the upper wall gets metallized.

Conclusions

The simulation of PVD and IPVD metallization processes for microelectronic applications at the reactor scale requires the knowledge of the energy and angular distributions of sputtered particles. If the metal target has a texture these distributions must be obtained by atomistic simulations.

The simulation of the film profiles at the feature scale for an IPVD process turned out to be impossible if the adsorption probability of all arriving atoms is assumed to be 1. The very different angles and an increased energy at which the atoms arrive on different parts of the feature make it necessary to consider reflection and resputtering events. The probabilities of these events must be obtained by atomistic simulations.

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