

Integration of Atomistic and Continuum-Level Electromigration Models

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Abstract—Interconnect scaling and the introduction of new processes and materials raise an issue of justifiability and applicability of phenomenological continuum-level electromigration models. The parameters of continuum-level models are averages over values which generally vary on microscopic and atomistic scale. Therefore it is necessary to investigate under which conditions these microscopic or atomistic spatial variations influence the validity of continuum-level models. Regarding both important parameters of continuum-level electromigration models, effective valence and vacancy diffusivity, their variations depend on the crystal orientation and the variations between bulk, grain boundaries, and interfaces. We apply the results of quantum mechanical calculations of the effective valence in order to parameterize the continuum-level electromigration model and subsequently investigate the impact of parameter variation on the variability of the electromigration behavior. With the effective valence and vacancy diffusivity, which depend on the crystal orientation inside the grains as follows from atomistic simulations, we obtain a substantially more accurate electromigration behavior compared to that predicted with previous models. This difference implies the necessity of application of atomistic simulations in order to increase the predictive capability of continuum-level models.

I. INTRODUCTION

Extensive electromigration experiments have produced an ample amount of data, indicating that the copper interconnect lifetime has decreased for every new interconnect generation, even when tested at the same current density [1]. The reason is that newer interconnects, due to their reduced size, require a smaller void volume for failure and a larger fraction of atoms is transferred, along the fast interface, to the capping layer and the grain boundary diffusion paths. The bamboo-like copper grain structure, observed in interconnects above the 65nm technology node, does not exist in interconnects below the 65nm node, where line sections of the polycrystalline grain structure dominate.

The improvement of electromigration behavior for the 22nm technology node and beyond will face a new challenge, because the electromigration-induced mass transport will increasingly depend on the copper microstructure and the interface properties related to the fabrication conditions [2].

Improving the overall interconnect reliability can only be achieved with a combination of different techniques, such as

copper alloying, thicker liner, large via size, embedded via, strengthening of copper/dielectric interface, etc.

The electromigration lifetime, depending on the variability of material properties at the microscopic and atomistic level, has always distributed values.

Under microscopic properties we understand grain boundaries and grains with their crystal orientation; under atomistic properties the specific configuration of atoms inside the grain boundaries, inside the interfaces to surrounding layers, and at the cross-section between grain boundaries and interfaces [3].

The dimensions of modern interconnect are in a region, where microscopic and atomistic properties are gaining importance. Therefore, in order to understand the distribution of electromigration life time, the variability of the impact parameters and their influence on electromigration must be well understood and appropriately modeled.

II. THEORETICAL BACKGROUND

In the modeling of electromigration the primary motivation for connecting the atomistic and the continuum-level description is to enable a correct parameterization of the continuum-level models. Experimental methods for the determination of the effective valence are based on two approaches: one is the compositional change induced by the current flow; the other measures the mass transport relative to a fixed reference frame. The principles of these two types of measurements apply to bulk materials as well as thin films [9].

The method based on the compositional change is more complex but also more accurate. One of the reasons for the higher accuracy is that it is not necessary to initially determine a self-diffusion coefficient, which may cause an additional error. The determination of a self-diffusion coefficient is part of the simpler mass transport method. The value of the effective valence Z^* can be reliably determined experimentally only for the bulk of metals [5]. Extending experimental methods for grain boundaries and interfaces demands additional, often questionable assumptions [9].

The significance of ab initio methods lays in the fact that they cannot only provide the values of the effective valence in the grain boundaries but also the insight into the process of

electromigration induced atomistic transport in the grain boundaries.

A. Parameterization of Continuum-Level Models

Electromigration on the atomistic level includes a complex multi-scattering process, where local fields and the local configuration of atoms play a decisive role. The quantum mechanical expression for the electron wind force is given by [4]

$$\vec{F} = - \int \delta n(\vec{r}) \frac{\partial V}{\partial \vec{R}} d^3r, \quad \delta n(\vec{r}) = \sum_k g_k |\psi_k(\vec{r})|^2, \quad (1)$$

where V is the interaction potential between an electron and the migrating atom, $\delta n(\vec{r})$ is the part of the electron density at position \vec{r} which depends on the electric field, $\psi_k(\vec{r})$ are the scattering states for electrons in the absence of an external electric field, and g_k is the shifted electron distribution which has the form

$$g_k = - \frac{e\hbar\tau(\vec{k})}{m} v(\vec{k}) \cdot \vec{E} \delta(\mathcal{E}_F - \mathcal{E}_k), \quad (2)$$

$\tau(\vec{k})$ is the relaxation time due to scattering by phonons, $v(\vec{k})$ is the electron group velocity, and \vec{E} is the external electric field. For practical evaluation (1) is transformed into

$$\vec{F}(\vec{r}) = \frac{e\Omega}{4\pi^3} \iint_{\text{FS}} \frac{dS_k}{|\nabla_k \mathcal{E}_k|} \tau(\vec{k}) \vec{v}(\vec{k}) \cdot \vec{E} \iint d\vec{r}' \psi_k(\vec{r}')^* \nabla_R V(\vec{r}' - \vec{R}) \psi_k(\vec{r}'), \quad (3)$$

where Ω is the atomic volume. The first integration is over the Fermi surface and the second over the volume of the crystal.

There are several different approaches for the calculation of the electron states and the Fermi surfaces needed in (3), but the most promising and the most sophisticated one is the Korringa-Kohn-Rostoker (KKR) method [5]. A difficult issue in electronic structure calculation is to take into account the polyhedral shape of the unit cell. To avoid this difficult boundary value problem Green's function techniques are used in the KKR method, where the Schrödinger equation is transformed into an integral equation. The results of the KKR method [5] are utilized in the present work to evaluate effective valence variations on the surface of copper.

In general, the microscopic force-field can depend on the position of the atom along the diffusion jump path.

The appropriate driving force, to be used in continuum electromigration models [7], is the average of the microscopic force over the i -th diffusion jump path between locations $\vec{r}_{i,1}$ and $\vec{r}_{i,2}$ [4]

$$\vec{F}_m = \left\langle \frac{1}{|\vec{r}_{i,2} - \vec{r}_{i,1}|} \int_{\vec{r}_{i,1}}^{\vec{r}_{i,2}} \vec{F}(\vec{r}) \cdot d\vec{r} \right\rangle, \quad (4)$$

where the outer brackets signify that an average is performed over the set of all equivalent diffusion jump paths, i.e., paths that have the same activation energy or diffusion coefficient, in the absence of an electric field and electron current.

B. Electromigration Force in Grain Boundaries

Quantum mechanical theory of electromigration has been successfully applied for ab initio calculation of electromigration in metallic bulk in many different ways. However, there are only few publications regarding electromigration in grain boundaries, interfaces, and surfaces. Among them, the jellium model and atomic cluster model are applicable on grain boundaries.

In the jellium model the grain boundary is regarded to be a disordered region confined to a slab like domain [4]. Since on average there are fewer atoms in this region than in the regular lattice, the grain boundary region presents a repulsive potential to the electrons. The potential has been taken to be a positive constant inside the grain boundary and to vanish elsewhere. The electromigration force is calculated for an impurity atom which is modeled by a delta-function potential.

Calculations have shown [4,8] that the electromigration force is strongly diminished, when the impurity is inside the grain boundary. The interpretation is that the outer surface of the grain boundary scatters electrons and thereby acts as a shield which keeps electrons from entering the inner region of the grain boundary. Thus, when the atom is well inside the grain boundary it is subjected to a smaller flux of electrons and to less electron scattering and smaller electromigration forces.

The KKR method has proven to be powerful for the calculation of the electromigration force in crystal bulk and on crystal surfaces. It was a natural step to extend this method to other crystal heterogeneities, like dislocations and grain boundaries. An important simplification of the original KKR approach [5] was carried out in [11], where a muffin-tin representation of the crystal bulk was replaced by a jellium model and heterogeneities were represented by a cluster of isolated atoms embedded in jellium.

As an illustration of this method we give a draft of a scheme for the calculation of the electromigration force on an atom in the vicinity of a grain boundary.

The momentum transfer between the atom and the current carrying electrons is influenced by multiple scattering of electrons on the atom and the cluster. The grain boundary itself can be constructed by the method of molecular statics.

The grain boundary is modeled as an atomic cluster embedded into the crystal bulk modeled as jellium, cf. Fig. 1. From (3) it is apparent that a calculation of the wind force requires a self-consistent determination of the single particle states of the system at the Fermi energy, and the effective one-electron potential in the vicinity of the test atom. In order to calculate these quantities it is necessary to self-consistently solve the Schrödinger equation for the atomic cluster in jellium.

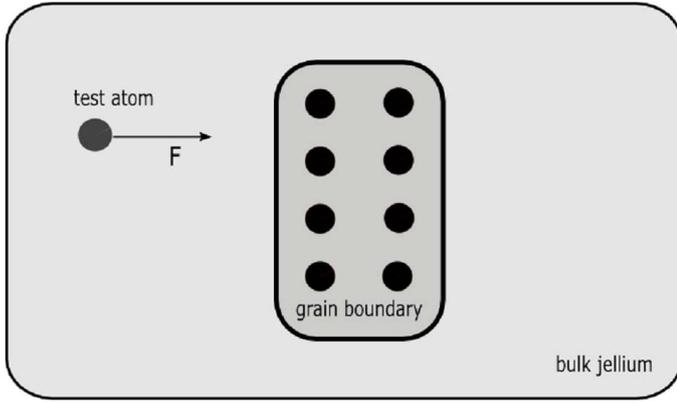


Fig. 1. Schematic illustration of a test atom interacting with an atomic cluster embedded in jellium.

The effective potential in the vicinity of the test atom is replaced with a spherical potential of muffin-tin form. Inside the muffin-tin, the Schrödinger equation is solved and the obtained wave function surrounding the test atom has to fulfill a continuity condition at the muffin-tin surface.

The wave function continuity can be enforced by expanding the solution of the Schrödinger equation into spherical harmonics and a suitable choice of the free parameters of the expansion.

In such a way the wave function $\psi_k(\vec{r})$ is defined in the whole simulation domain and can then be used for the calculation of the electromigration force by (3).

The above described procedure turned out to be accurate through comparison with a calculation performed by the layer-KKR method for the case of surface electromigration [11] of Na.

III. STATISTICAL SIMULATION

For a given interconnect layout and monocrystalline material, simulation provides a unique time-to-failure. All impact factors, e.g. geometry of the layout, bulk diffusivity, interface diffusivity, and mechanical properties, are deterministic and so this time-to-failure is deterministic. However, the situation changes, when the interconnect possesses a microstructure. The microstructure has a significant impact on electromigration, since it introduces a diversity of possible electromigration paths and local mechanical properties, e.g. the Young modulus and Poisson factor depend on the crystal orientation in each grain. However, the microstructure itself cannot be completely controlled by a process technology. In other words, the position of grain boundaries, angles in which they meet the interfaces, etc. cannot be designed, the process itself determines only statistics of grain sizes and textures.

In order to include the grain distribution in the numerical simulations, a microstructure generator tool has been developed. Given a specific interconnect structure and providing the tool with a median grain size and corresponding standard deviation, it generates a lognormal distribution of grain sizes (Fig. 2). Then, following this distribution, the interconnect line is cut along its length by the planes which form the grain boundaries.

Furthermore, the angles between the grain boundaries' planes and the line surface follow a normal distribution with a median value of 90° . The corresponding standard deviation can also be specified.

IV. SIMULATION RESULTS

By extrapolating effective valence value variations from quantum-mechanical calculations, we parameterize our continuum-level electromigration model. The applied effective valence profile along the (100) oriented crystal surface (Fig. 3) is presented in Fig. 4. Analogously, effective valence profiles for (111) and (110) are calculated. Currently, none of the available electromigration models accounts for the varying self-diffusion coefficient and the effective valence caused by different crystal orientations. However, when these variations were implemented, assuming a lognormal distribution of grain sizes, a significant variation in failure times (time to reach certain failure-triggering stress threshold) was observed.

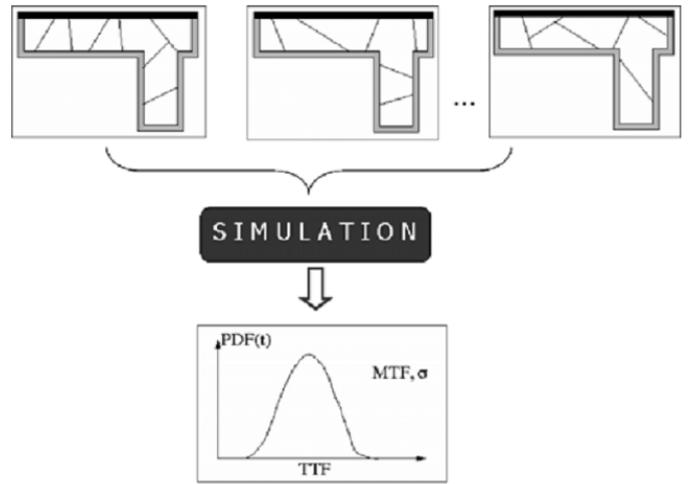


Fig. 2. Schematic simulation procedure.

When compared with the results from our previous work [7], the growth of the failure time variance is much more pronounced (Fig. 5). An additional effect is that the effective valence in grain boundaries is not constant, but rather varies depending on the angle between the grain boundary and the electric field [8]. If we consider only grain boundaries as the fast diffusivity path, our simulations show that a significant variability in stress levels, attained for a pre-defined electromigration time, is reached (Fig. 6). In this case results of the grain boundary jellium model are utilized. The weakness of this model is that one cannot include details of the grain boundary structure, such as tilt angle and reciprocal density of coincident sites. These features characterize different atomic spacings and thus different electron densities which cause additional variations in the effective valence. For more accurate simulation the usage of the atomic cluster model is advised.

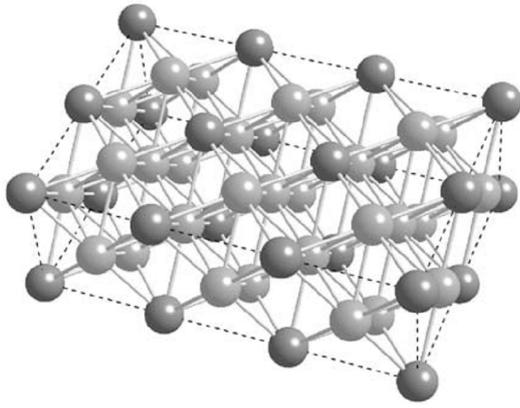


Fig. 3. Surface portion of the copper fcc-type lattice used for evaluation of the effective valence Z^* .

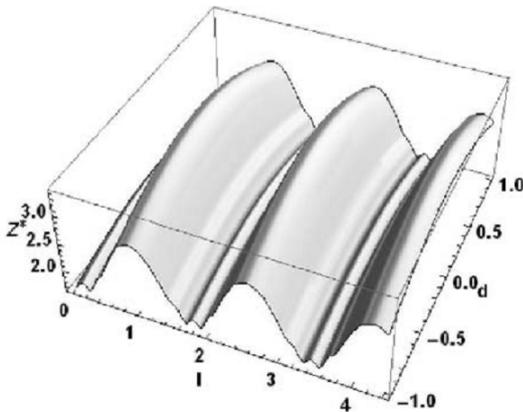


Fig. 4. Variation of the effective valence Z^* along the crystal surface. Valleys correspond to the face atomic positions and hills to the transition regions. The length l and width d are given in angstroms.

V. CONCLUSION

The application of ab initio models is a necessity for modeling of electromigration at the current and the future levels of miniaturization. The crucial parameters, such as the effective valence in grain boundaries, material surfaces, and interfaces, are not obtainable from experimental results, or their determination is very unreliable. The quantum mechanical theory of electromigration offers a spectrum of methods for the calculation of the effective valence and some of them are presented in this work. The effective valence calculated by ab initio methods is used for the parameterization of the continuum-level models which are, in turn, used for the statistical simulation of electromigration. Simulation results have clearly shown that the variability of the effective valence at the copper interfaces and inside the grain boundaries has a significant impact on the electromigration failure time distribution.

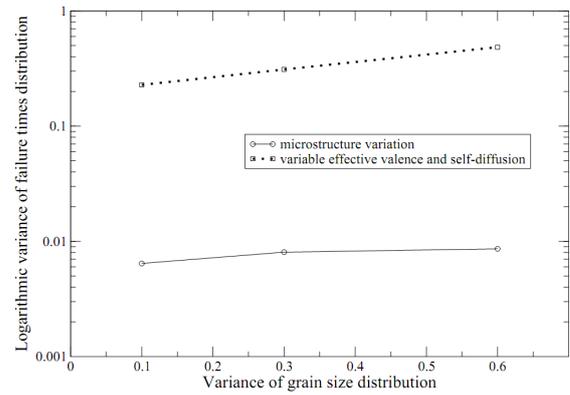


Fig. 5. Failure time variance due to microstructure variability.

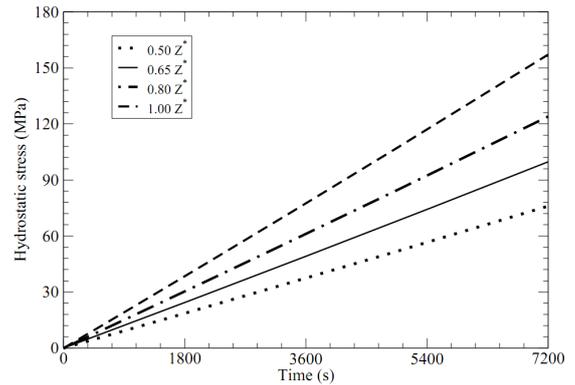


Fig. 6. Variation of stress levels due to variation of the effective valence Z^* .

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