Modeling of Microstructural Effects on Electromigration Failure

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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. The reasons are 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. 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. 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.

It is well known today that the microstructure of copper has a significant impact on electromigration failure. Grain boundaries are fast diffusivity paths and vacancy recombination sites. The diffusion of vacancies on the grain boundary is faster compared to diffusion in the grain bulk, because a grain boundary generally exhibits a larger diversity of point defect migration mechanisms. Formation energies and migration barriers of point defects are in average lower than those for lattice.

Current electromigration models used for simulation and analysis of interconnect reliability lack the appropriate description of metal microstructure and consequently have a very limited predictive capability. Therefore, the main objective of our work was obtaining more sophisticated electromigration tools. The problem is addressed through a combination of different levels of atomistic modeling and already available, continuum level macroscopic models. An integral part of the applied methodology is understanding of the relationship between macroscopic models and the models which contain detailed information about the atomistic structure. This kind of analysis leads to the modification and improvement of the initial continuum model. At this point the necessity of the here presented research effort is evident, since today only very rough methods to characterize electromigration in amorphous interfaces and grain boundaries exist.

Quantum-mechanical methods contribute to understand the nature of the electromigration force in the presence of a specific atomic configuration which appears at the copper interfaces to surrounding layers and inside the grain boundaries. A natural next step is the incorporation of the obtained knowledge into a molecular dynamics model, with which one can simulate electromigration induced material transport on the atomistic level. Additionally, for a statistical investigation of the influence of the microstructure on the electromigration failure behavior we apply a compact model. The model takes into account the kinetics of nucleation and growth, so it provides a better description of the early EM lifetimes and also a more precise extrapolation of accelerated test results to use conditions.

This talk gives an overview over our research and consists of the following 4 major parts:

1) **Investigation of the copper microstructure development by simulation:** The interconnect microstructure depends on many parameters such as the core material deposition technique, the barrier material types, the barrier material deposition technique, the copper seed layer deposition technique and thickness, and the line width. As an example, for a given line width, the grain size may differ significantly, when the copper deposition technique changes from CVD to electroplating. Using a model based on the van der Drift algorithm we have developed a software tool which enables the simulation of grain boundary formation and the competitive growth of grains. We present results of investigations of copper microstructures with different statistical properties which depend on specific process conditions during deposition of copper.

2) **Molecular dynamics simulation of grain boundaries and interfaces:** Prior to carrying out the *ab initio* calculation of the electromigration force and the effective valence it is necessary to construct grain boundaries with exact positions of atoms. For this purpose an in-house molecular dynamic simulator with a many-atom interatomic potential based on the effective-medium theory is used. Depending on crystallization conditions, as for example the temperature regime, grain boundaries with different properties such as tilt angle and reciprocal density of coincident sites are produced. These features characterize different atomic spacings and thus different electron densities which cause additional variations in the effective valence for electromigration. For the construction of the grain boundary a three-dimensional cell with 200-500 atoms and periodic boundary conditions have been used. Starting with completely disordered atoms in the cell and subsequently reducing the temperature results in the emergence of a realistic grain boundary structure.

3) **Atomistic method for analysis of electromigration:** The reliability of interconnects in modern integrated circuits is determined by the magnitude and direction of the effective valence for electromigration. The effective valence depends on local atomistic configurations. In order to study electromigration on the atomistic level an application of *ab initio* methods is a necessity. We present a computationally efficient *ab initio* method for calculation of the effective valence for electromigration and the atomistic electromigration force. The consideration of the accurate effective valence in grain boundaries enables a realistic simulation of the electromigration behavior. We demonstrate that for the same interconnect layout and operating conditions, different copper microstructures exhibit a significantely different behavior of electromigration driven vacancy transport due to the variation of the effective valence between bulk and grain boundaries. In addition, the presented combination of atomistic force calculation with a kinetic Monte Carlo simulation enables a sophisticated analysis of vacancy dynamics.

4) **Compact modeling for early electromigration failures:** For copper dual-damascene interconnects two main electromigration failure modes have been identified, namely the late (strong) mode and the early (weak) mode. The late failure mode is commonly characterized by the growth of a void which spans the line cross section. For a line/via structure subjected to downstream electron flow, the early failure mode is typically characterized by the growth of a slit void under the cathode via. A compact model for early electromigration failures in copper dual-damascene interconnects is proposed. The model is based on the combination of a complete void nucleation model together with a simple mechanism of slit void growth under the via. It is demonstrated that the early electromigration lifetime is well described by a simple analytical expression, from where a statistical distribution can be conveniently obtained. Fast diffusivity paths and microstructure are properly considered. It is shown that the simulation results provide a reasonable estimation for the interconnect lifetimes.

Two primary goals of research presented in this talk are the parameterization and the refinement of continuum level models by means of atomistic simulation. 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 knowledge obtained from atomistic simulations, theoretical considerations, and the analysis of experimental results lead to improvement and sophistication of continuum level models. These models are subsequently used for the prediction of long time interconnect failure statistics and will enable a systematic study of the influence of different geometrical and microstructural properties on the failure behavior.