Structure and Failure of Metallic Interfaces in Microelectronic Devices (DFG)

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Interfaces between dissimilar metals are of significant fundamental interest. The Cu-Ta system is a good model of systems, since Cu and Ta have practically zero mutual solid solubility, have different crystal structures, as well as highly different melting temperatures and mechanical strengths. Heterophase interfaces between Cu and Ta are present in most modern microelectronic devices. Copper is the most widely used interconnect material, while Tantalum is used as a diffusion barrier preventing the copper from penetrating into the silicon chip.

The investigation of fcc/bcc interfaces is difficult. The first step in this DFG project was to develop a new reliable interatomic potential for the Cu-Ta system (A. Hasibon et. al., Phys. Rev. B 76, 2007). This interatomic potential is based on the embedded-atom method (EAM) with an addition of angularly dependent terms. The Cu-Ta ADP potential has been fitted to a large database of first principles calculations.

Various interface systems have been considered, including thin Cu films on Ta, liquid Cu on Ta, and internal bulk interfaces. Molecular dynamics (MD) simulations at various temperatures of thin Cu films composed of a few Cu (111) planes deposited on a free Ta (110) surface resulted in Cu dewetting from the Ta surface, leaving a stable Cu monolayer. Figure 1 shows this behaviour. We also observe a spreading of a stable monolayer of Cu, while the remaining Cu atoms form a 3D island. Experimental evidence for our results is conflicting.

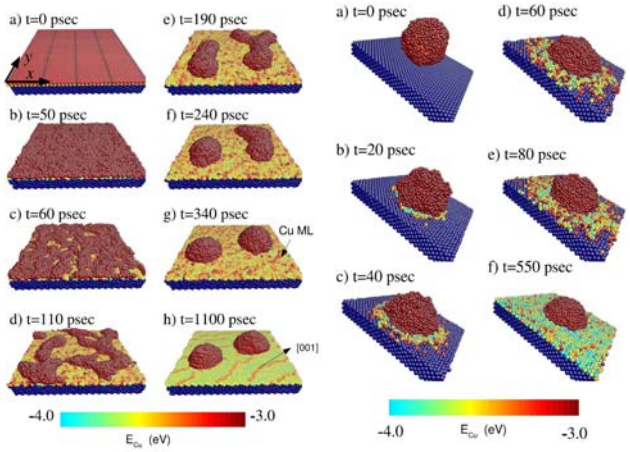

Fig. 1: In the left panel: a sequence of snapshots from a molecular dynamics simulation of two fcc (111) layers on a bcc Ta (110) substrate at T=1400 K, demonstrating dewetting of the top Cu layer and the formation of two Cu drops. The Ta atoms are represented by blue colours, while the Cu atoms are coloured according to their potential energy using the energy scale at the bottom of the figure. The directions indicated by the axes in (a) correspond to the Kurdjumov-Sachs orientation relationship with the lattice directions $[0\text{-}11]_{fcc}$ and $[111]_{bcc}$ pointing along the x axis and the lattice directions $[2\text{-}1\text{-}1]_{fcc}$ and $[\text{-}112]_{bcc}$ pointing along the y axis. In the right panel: a sequence of snapshots from a molecular dynamics simulation of a Cu drop spreading on a Ta (110) substrate at 1400 K. A monolayer of Cu spreads and a stable wetting drop forms on top of it

To resolve this discrepancy in the experimental literature, and as a further test of the validity of the interatomic potential, we conducted additional first principles DFT calculations to investigate the mechanical and thermodynamic stability of thin Cu films on Ta (A. Hashibon et. al., Phys. Rev. B 77, 2008). Two extreme cases were considered: Cu is assumed to be coherent and second, it is assumed to be completely incoherent with respect to the Ta. The coherent Cu monolayer on Ta was found to be unstable, and that this instability is due to excess coherency strains. The incoherent system, and subsequently the semi-coherent monolayer are indeed mechanically and thermodynamically stable, in accordance with our MD simulation results.

Internal bulk interfaces are also considered. In this case, since the interface structure is initially unknown, we start by joining two ideal fcc and bcc lattices, assuming that close packed surfaces are parallel formed in the so called Nishiyama-Wasserman orientation relationship defined by the directions: $[11\text{-}2]_{fcc}$// $[1\text{-}10]_{bcc}$ and $[1\text{-}10]_{fcc}$// $[001]_{bcc}$. The interface structure is optimized by calculation of the vacancy formation energy profile of Cu and Ta atoms. Atoms (or sites) with negative vacancy formation energies indicate a tendency to reduce the density of atoms at that site. We have systematically removed atoms with large negative vacancy formation energies, and subsequently recalculated the vacancy formation energy profile. Figure 2 shows a plot of the excess interface energy as a function of the number of vacancies at the interface. 18 atoms are removed from the Cu plane adjacent to the Ta. This corresponds to removal of two [1-10] rows of atoms from the region of maximal strain in the Cu plane. Only the Cu layer directly adjacent to the interface shows any significant deviations from the ideal fcc structure. This monolayer facilitates the transition from the bcc Ta to the fcc Cu. A simple tensile test simulation on this system further reveals that failure occurs between this layer and the remaining Cu, i.e., not at the interface.

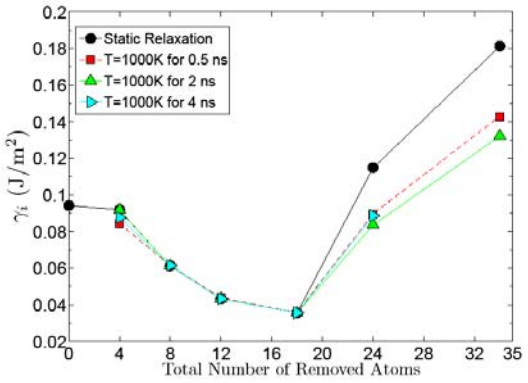

Fig. 2: Interface excess energy as a function of the number of vacancies at the interface