ABSTRACT:

Theoretical Investigation of metal passivation Layers' Role in Lowering Cu-Cu Bonding Temperature

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With the complexity of integrated circuits increases and chip size decreases, the number of I/Os increases exponentially, leading to continuous increase in packaging density. Cu-Cu bonding technology has the advantage of vertical integration, hence provides higher interconnect density. However, the direct bonding of Cu-Cu requires high temperature, which poses a risk of thermal damage and impact on the chip. The metal passivation layer can reduce the temperature of direct bonding between copper and copper. As demonstrated by Park, bonding with copper can be achieved at low temperatures (200°C) using a 12nm Ti layer, yielding a shear strength of up to 13.2 MPa. The reason for this is attributed to the decrease in activation energy, but the fundamental mechanism behind it remains unclear.

The study aims to elucidate the basic mechanism by which the addition of a nano-Passivation layer reduces activation energy. Firstly, the LAMMPS was used to analyze the molecular dynamics model of Cu-metal passivation-Cu, and obtained the dynamic position of atoms. Then, the grain boundary morphology and interface diffusion results were visualized, and the diffusion coefficient and activation energy were calculated, refer to Figure 1. Figure 2 illustrates the characterization of the grain boundaries. The results show that, the initial of diffusion is dominated by lattice diffusion, and with time increase the grain boundary was formatted and evolved. According to Einstein's diffusion law, the mean square displacement (MSD) of atoms was calculated, and the diffusion coefficient was obtained by taking the slope of MSD. Besides, the activation energies of three common passivating metals (Ag, Cu, and Ti) were calculated. The activation energy was determined by fitting the diffusion coefficients at temperatures ranging from 973K to 1173K using the Arrhenius relationship. For more details, refer to Figures 5, 7, and 9.

The study finds that the activation energy for Ag diffusion to Cu is 153.84 kJ/mol, while for Cu diffusion to Ag, it is 137.91 kJ/mol. For Au diffusion to Cu, the activation energy is 175.97 kJ/mol, and for Cu diffusion to Au, it is 156.45 kJ/mol. The activation energy of using Ag and Au as the passivation layer is slightly lower than the activation energy of bulk passivation metals under high-temperature experiments, in which bulk activation energy is defined as described in references [5-8]. Analysis reveals that due to the limited number of simulation steps, the diffusion of Cu into Ag and Au is confined to a finite depth, where the diffusion of atoms occurs mainly through lattice diffusion. If given sufficient time, grain boundary diffusion would become the dominant mechanism. When Ti is used as a passivation layer, the activation energy for Ti diffusing into Cu is 26.42 kJ/mol, while the activation energy for Cu diffusing into Ti is 125.45 kJ/mol. It is attributed to the fact that Cu atoms can quickly penetrate through the Ti passivation layer, which promotes the diffusion of grain boundary, and reduce activation energy. The diffusion activation energy of bulk Ti into copper is 196 kJ/mol, while for copper into Ti, it is 195 kJ/mol (Park, 2024). The study indicates that introducing the passivation layer can lower the bonding temperature by forming grain boundaries within the layer, which provides rapid diffusion pathways with lower activation energy for atom diffusion, thus enabling bonding at lower temperatures. In experiments, thinning the barrier layer can facilitate rapid achievement of low activation energy grain boundary diffusion.

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