The 15th International Conference on Surfaces, Coatings, and Nanostructured Materials Theoretical Investigation of metal passivation Layers' Role in Lowering Cu-Cu Bonding Temperature H.J. Dang^{1, a)}, W.C. Tian^{1, 2}, Y.K Wang¹, H.Y. Xu¹, S. Chen³ **1.Background and Highlight** Cu-Cu bonding in 3D packaging is considered the most promising method for extending Moore's Law. However, the high-temperature requirements of direct bonding give rise to challenges such as warpage, bonding misalignment, and thermal failures. Metal passivation strategies directly inhibit the oxidation of Cu surfaces, making it a favorable option for reducing Cu-Cu bonding temperatures. Existing research focused on employing metal passivation to achieve low-temperature bonding, but lacks the underlying mechanisms. Our study aims to analyze the mechanism of metal passivation layer in lowering the temperature of Cu-Cu bonding at the atomic level. 2.Model and Method (b) (a) Structural Potentials □ Metal Passivation: model building construction Ag, Au, Ti, and poly crystalline Au Upper Polycrystalline Au copper □ Atomic Lattice: LAMMPS Cu, Ag, and Au are FCC, Ti is HCP Model building □ Target Temperature: Passivation 973K, 1023K, 1073K, 1123K, and 1173K ᡟ layer Boundary Conditions: (Ag) Atomic positions X-axis and Y-axis (Periodic boundary), Z-axis (non-periodic boundary) with the ecti Diffusion coefficient Lower top and bottom fixed two lavers Diffusion copper Potential and Ensemble: activation energy MEAM potential, NVT (at target Temp.) **3.Diffusion of Cu-Passivation-Cu** 4. Diffusion Coefficient and Activation Energy (a) ×10[.] _ 0.6 (10⁻²⁰ m²) 10 - Ag into Cu ---Fittedcurve of Ag into Cu ----Fittedcurve of Cu into Ag U. Ξ0. 8 (m²/s) L I $\frac{5}{2}$ 0.12 $\frac{10}{2}$ 0.10 973K ы 90.3 V-0.2 0.1 11 0.08 0.06 0.04 0.02 Activation Ener cient E_a 153.837 kJ/mo 11 6 0.977 11 coeff 137.909 kJ/n Model: Cu-Ag-Cu Model: Cu-Ag-Cu 0.0 0.00 -0.0250 100 150 200 250 300 time (ps) 50 100 150 200 250 300 time (ps) ò sion 11 2 70 (II) 0.6 Diffu MSD-Cu (10⁻²⁰m²) 0.4 0.2 0.2 0.2 0.1 () 60 07 50 0 I MSD-Ti (10^{-:} 40 1050 1100 T (K) 1150 1200 950 1000 30 (b) 11 20-×10⁻¹⁰ 10 Ti into Cu Cu into Ti ---Fittedcurve of Ti into Cu 10 Diffusion of Cu after300ps Diffusion of Ag after300ps 0 (m²/s) Model: Cu-Ti-Cu 0.0 Model: Cu-Ti-Cu 8 -10-- Fittedcurve of Cu into T Fig.1 Diffusion between Cu and Ag obtained 50 100 150 200 250 300 , coefficient (. Ò. 50 100 150 200 250 300 at different temperatures after 300 ps time (ps) time (ps) (b) Activation Energy Activation energy My research Ref (Bulk metal) 26.418 kJ/mol Cu into Ag 137.909 kJ/mol 142.1 kJ/mol FEMP: 11731 Fime: 300ps 0.983 11 Ag into Cu 153 837 kJ/mol 183.8 kJ/mol 125.453 kJ/mo Diffusion Cu into Au 156 451 kJ/mol 169~172 kJ/mol 0.943 2 178~197 kJ/mol Au into Cu 175.973 kJ/mol Cu into Ti 125.453 kJ/mol 195 kJ/mol Ti into Cu 26.418 kJ/mol 196 kJ/mol Г 139.051 kJ/mol 1050 1 T (K) Cu into Poly Au 1000 1150 950 1100 1200 I 51.997 kJ/mol Poly Au into Cu (ď) As time and temperature rise, MSD increases, indicating exacerbated diffusion. Diffusion with Ti passivation is more notable. Diffusion with Ag passivation displays higher temperature sensitivity. S.V. Los \Box The E_a with the metal layer as passivation is lower than the diffusion between bulk metal and Cu. L 1 With Ti as the passivation layer, diffusion is primarily through grain boundaries, resulting in a notable decrease in E_{-} \Box Initial grain boundaries exacerbate diffusion, further lowering E_a compared to single-crystal Au. -----Fig.2 Diffusion of Cu adding different metal _____ 5. Conclusion passivation layers under 1173 K after 300 ps □ With the rise of time and temperature, more Initially, diffusion with the metal layer as passivation likes bulk metal. As diffusion continues, more atoms diffuse and the diffusion deepens. and deeper grain boundaries form within the passivation layer. Low-energy grain boundary diffusion □ Within limited duration, Ag and Au gradually becomes dominant, enabling low temperature Cu-Cu bonding. passivation yield shallow Cu diffusion, while Reducing the thickness of the passivation layer will accelerate the dominance of grain boundary Ti passivation results in deeper diffusion. diffusion, providing direction for process optimization. □ In polycrystalline Au, initial grain boundaries > Introducing initial grain boundaries can reduce activation energy, offering new optimization theories expedite Cu diffusion. for bonding processes. Refining grain size aids low-temperature bonding. Your ID CODE goes here! (centralized/ ARIAL BOLD / font size 60) School of Electro-Mechanical Engineering, Xidian University, **NSM143** Xi'an, Shaanxi, China. NANOSMAT Email: d2100710345@outlook.com