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

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## 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

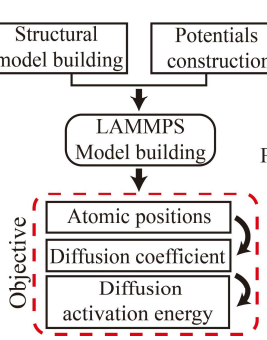
**Metal Passivation:**
Ag, Au, Ti, and poly crystalline Au

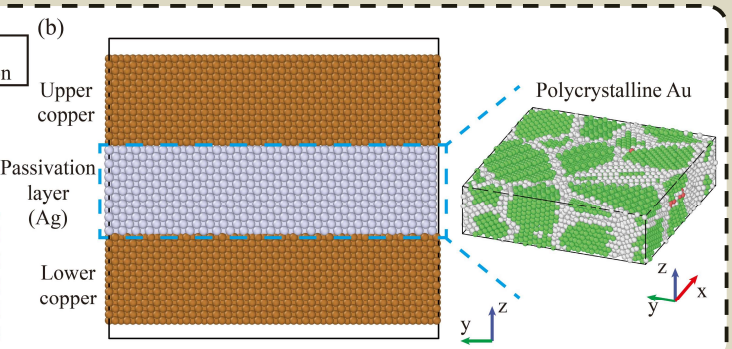
**Atomic Lattice:**
Cu, Ag, and Au are FCC, Ti is HCP

**Target Temperature:**
973K, 1023K, 1073K, 1123K,and 1173K

**Boundary Conditions:**
X-axis and Y-axis (Periodic boundary), Z-axis (non-periodic boundary) with the top and bottom fixed two layers

**Potential and Ensemble:**
MEAM potential, NVT (at target Temp.)




## 3.Diffusion of Cu-Passivation-Cu

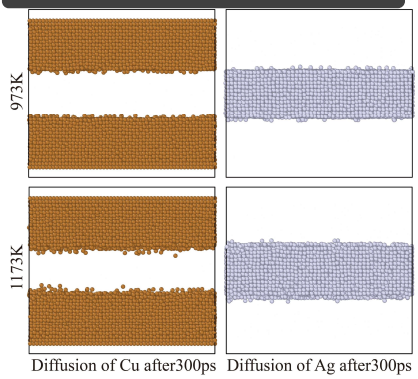



**Fig.1 Diffusion between Cu and Ag obtained at different temperatures after 300 ps**

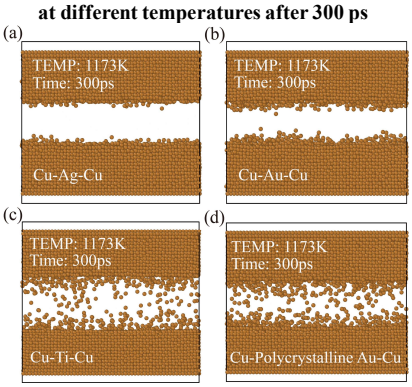
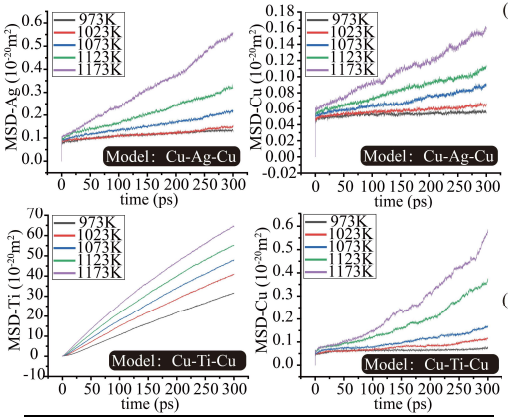
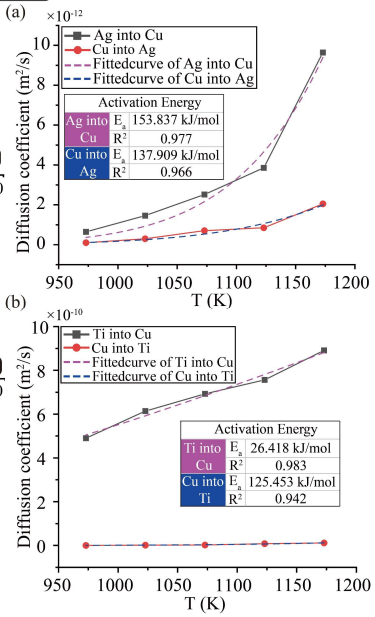



**Fig.2 Diffusion of Cu adding different metal passivation layers under 1173 K after 300 ps**

- With the rise of time and temperature, more atoms diffuse and the diffusion deepens.
- Within limited duration, Ag and Au passivation yield shallow Cu diffusion, while Ti passivation results in deeper diffusion.
- In polycrystalline Au, initial grain boundaries expedite Cu diffusion.

## 4. Diffusion Coefficient and Activation Energy




| Activation energy | My research | Ref (Bulk metal) |
|---|---|---|
| Cu into Ag | 137.909 kJ/mol | 142.1 kJ/mol |
| Ag into Cu | 153.837 kJ/mol | 183.8 kJ/mol |
| Cu into Au | 156.451 kJ/mol | 169~172 kJ/mol |
| Au into Cu | 175.973 kJ/mol | 178~197 kJ/mol |
| Cu into Ti | 125.453 kJ/mol | 195 kJ/mol |
| Ti into Cu | 26.418 kJ/mol | 196 kJ/mol |
| Cu into Poly Au | 139.051 kJ/mol | — |
| Poly Au into Cu | 51.997 kJ/mol | — |

- 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.
- The $E_a$ with the metal layer as passivation is lower than the diffusion between bulk metal and Cu. With Ti as the passivation layer, diffusion is primarily through grain boundaries, resulting in a notable decrease in $E_a$.
- Initial grain boundaries exacerbate diffusion, further lowering $E_a$ compared to single-crystal Au.

## 5. Conclusion

- Initially, diffusion with the metal layer as passivation likes bulk metal. As diffusion continues, more and deeper grain boundaries form within the passivation layer. Low-energy grain boundary diffusion gradually becomes dominant, enabling low temperature Cu-Cu bonding.
- Reducing the thickness of the passivation layer will accelerate the dominance of grain boundary diffusion, providing direction for process optimization.
- Introducing initial grain boundaries can reduce activation energy, offering new optimization theories for bonding processes. Refining grain size aids low-temperature bonding.

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