Research on Atomic-scale Tribochemistry Underlying Wafer-Scale Global Planarization of Advanced Integrated Circuits

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Introduction

The development of advanced integrated circuit (IC) manufacturing hinges on constructing multi-layer structures with nanometer-level precision. Chemical mechanical polishing (CMP) serves as an indispensable core process to realize wafer global planarization and ultra-clean surface. The absence of an in-depth atomic-level understanding of the interfacial tribochemical mechanism severely limits the precision of IC manufacturing. Therefore, revealing these atomic-level internal mechanisms to achieve precise control throughout the entire process of CMP and post-CMP cleaning has become a significant challenge.

The metallic copper (Cu) and the non-metallic silicon (Si) constitute the core structural layers of modern IC devices. During the chip manufacturing process, repeated CMP and post-CMP cleaning treatments are inevitable. This research innovatively integrates theoretical simulation, nanomechanical wear experiments, and post-CMP cleaning experiments to systematically reveal the dominant mechanisms underlying the interfacial tribochemical behavior of Cu and Si. Specifically, density functional theory (DFT) calculations quantified the interlayer interactions during CMP, while an atomic-scale CMP model was used in nanomechanical wear experiments to study material removal. A multi-layer model simulated the particle deposition and removal during the post-CMP cleaning process, with particular attention to the evolution of chemical bonds and changes in particle trajectories. Moreover, the simulation results were rigorously verified through the cleaning effect of post-CMP cleaning experiments.

Results

During the CMP process, the theoretical simulation shows that the oxidized interface formed on Cu features the minimum interfacial fracture energy and is prone to interlayer cracking under external mechanical shear load. In contrast, the *OH adsorption on the Si surface weakens the interlayer Si-Si bonding, facilitating atomic-level material removal. Nanomechanical wear experiments combined with microstructure characterization verified the differences in the planarization performance of Cu and Si after material removal, directly demonstrating their different removal mechanisms.

During the post-CMP cleaning process, Cu and Si are dominated by different tribological effects, and the paths of particle detachment on their surfaces are completely different. For Cu, the particle removal controlled by tribochemistry is affected by the change in the solid-liquid interface characteristics due to the cleaning additives, which enhances electrostatic repulsion or steric hindrance effects, thereby removing surface contaminants. For Si, particle desorption depends on frictional mechanics. The formed surface lubricating film enables abrasive particles to be lifted and slide off through fluid dynamics.

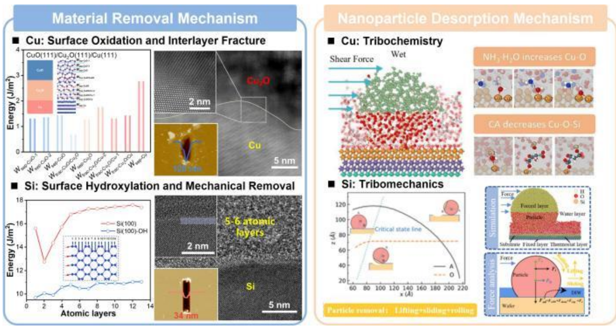

Figure 1: The material removal mechanisms and the particle desorption mechanisms of Cu and Si.

Conclusions

ⅰ. During CMP, Cu removal is governed by interfacial fracture, whereas Si removal relies on bond weakening by *OH adsorption.

ⅱ. During post-CMP cleaning, particle desorption follows a tribochemical mechanism on Cu and a tribomechanical mechanism on Si.

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References

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