Ab Initio Calculation of High-Rate Deposition of Copper Film by Low-Pressure Chemical Vapor Deposition with CuI on Ru Substrate

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We have studied low-pressure chemical vapor deposition of Cu on Ru substrate using CuI [1] using VASP program package (MPI parallelization with multiple threads). This year, we focused on the molecular mechanism of adsorption, migration and desorption. This is a collaborative work with the experimentalist [2] (Prof. Satoshi Yamauchi at Ibaraki University), who conducted the LPCVD experiment.

In this study, we elucidated the molecular mechanism of Cu deposition using copper(I) iodide (CuI) on Ru substrate by low-pressure chemical vapor deposition through electronic structure calculations. Using density functional theory calculations, we show that CuI molecules adsorb and decompose exothermically due to a strong adsorption of iodine atoms onto the Ru(001) surface. The rate-limiting step of the Cu deposition is found to be the desorption of iodine molecules from the Cu(111) surface, suggesting that the removal of iodine species is necessary to achieve the high-rate deposition of highly-conductive copper films for ultra large scale integration metallization.

Based on this study, we are now extending our calculations to analyze the dynamical properties in more detail. In addition, new sets of precursor and substrate are explored for ultra large scale integration metallization together with experiment.

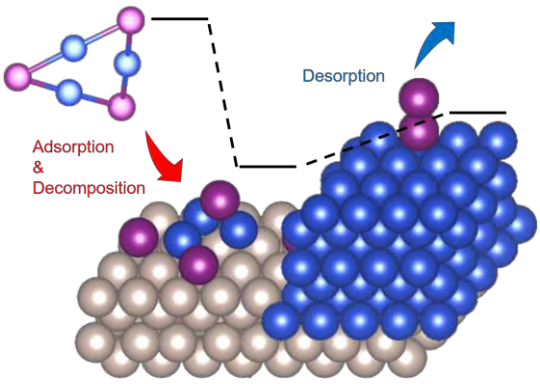

Fig. 1: Molecular mechanism of LPCVD of Cu.

References

[1] T. Joutsuka, S. Yamauchi: Chem. Phys. Lett. **741** (2020) 137108.

[2] T. Nishikawa, K. Horiuchi, T. Joutsuka and S. Yamauchi: submitted.