Kinetic Monte Carlo Simulation of Filling High-Aspect-Ratio Through Silicon Via - II

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Through silicon via (TSV) [1] is a key technology for the success of high density 3D packaging in microelectronics. The crucial point for this process is to fill high-aspect-ratio via holes completely without voids by copper electrodeposition. The purpose of this work is to study the mechanism of TSV filling with use of a Kinetic Monte Carlo (KMC) simulation.

The simulation system is the two-dimensional square lattice which is described in detail in our previous report.[2] Four kinds of additives are included in solution; Cl^-, PEG (inhibitor), SPS (accelerator) and SDDACC (leveler).[3] PEG is combined with Cu^+ and Cl^- (CuClPEG) and suppresses the copper deposition on the surface. SPS is decomposed into two MPS molecules. MPS is combined with Cu^+ to produce Cu(I)thiolate. Cu(I)thiolate has a catalytic effect to enhance Cu deposition (accelerant). SDDACC is included as a leveler, which has weak suppressing effect. We also assume a synergistic effect of SDDACC and PEG, i.e. the suppressing effect of PEG is enhanced in the presence of SDDACC.

For the dissolved oxygen molecules, following reactions are taken into account.

$$4\,Cu^+ + O_2 + 4H^+ \rightarrow 4Cu^{2+} + 2H_2O$$

$$4\text{Cu(I)thiolate} + O_2 + 8H^+ \rightarrow 4Cu^{2+} + 4\text{MPS} + 2H_2O$$

Since the accelerants are oxidized by the dissolved O_2 molecules, the filling mechanism depends on the distribution of O_2 in solution.

In order to improve the filling efficiency, we applied the pulse reverse current. The waveform is illustrated in Fig.1.

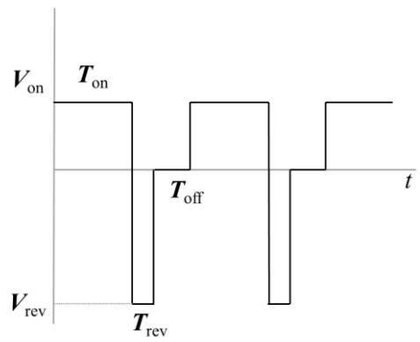

Fig. 1

The waveform is characterized by T_{on}, T_{rev}, T_{off} (time periods of forward current, reverse current and off-time, respectively) and V_{on}, V_{rev}.

Figure 2 shows the result of the simulation of via filling with the pulse reverse current of $T_{on} : T_{rev} : T_{off} = 20 : 1 : 9$. The via width is 10 μm and the aspect ratio is 7. It is clearly observed that large void does not appear in the hole and superfilling is achieved. A typical V-shape of the surface is observed during the filling. The growth of the upper part is strongly suppressed by PEG and the Cu(I)thiolate is deposited around the bottom and the sidewall of the via, which realized the bottom-up process.

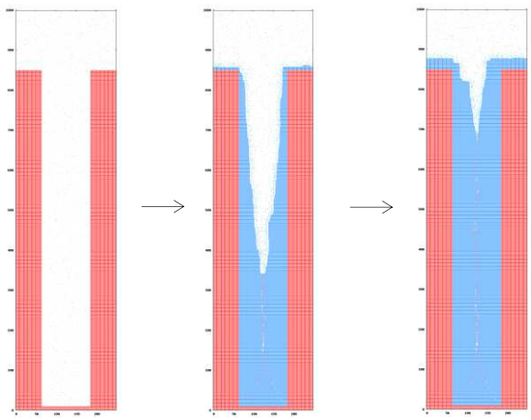

Fig. 2

In this work, we study the dependence of the filling efficiency on the combination of (T_{on}, T_{rev}, T_{off}) and (V_{on}, V_{rev}). We pay attention to the distribution of Cu^+ produced by the reverse current. The influence of dissolved oxygen which oxidizes Cu^+ and Cu(I)thiolate is also discussed.

References

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3. T. Hayashi, K. Kondo, T. Saito, T. Takeuchi and N. Okamoto, J. Electrochem. Soc. 158, D715 (2011) .