Understanding and predicting interconnect metal deposition and morphology from atomic scale simulations

Cara-Lena Nies[a*], Karl Ronnby[a], Samuel Delgado Aldana[a] and Michael Nolan[a]
[a] *Tyndall National Institute, University College Cork, Cork T12 R5CP, Ireland*
[*] *corresponding author e-mail: caralena.nies@tyndall.ie*

Optimising the deposition process and morphology of interconnect metals is essential to successful metallisation processes. Atomic scale simulations provide a powerful tool to understand the underlying mechanisms of metal deposition and growth processes, as well as the dependence of their morphology on the substrate. We have developed a screening approach based on multiscale first principles simulations to predict the morphology of a metal on a given substrate. This way, promising material candidates can be pre-selected, thus reducing the time and cost of experimental development.

Growth of advanced metal interconnects is particularly impacted by the issue of metal morphology. At small scales, *ca* < 10 nm, copper preferentially forms non-conducting islands, leading to defects and poor quality of the deposited metal. To prevent this, a liner material that promotes 2D Cu morphology is deposited onto the diffusion barrier, which itself prevents migration of Cu into the surrounding dielectric. However, the lowest, and smallest, levels of interconnects have extremely high aspect ratios and the diffusion barrier and liner bilayer takes up too much volume to allow depositing sufficient Cu.

To tackle this significant technology bottleneck, we use density functional theory (DFT), ab initio molecular dynamics and kinetic Monte Carlo to investigate the morphology of copper and other possible interconnect metals on TaN, the state of the art diffusion barrier.

In particular, the competition between the metal-substrate and metal-metal interaction tends to be the key to controlling the final morphology [1], see Fig. 1. These interaction energies change based on the substrate and metal combination. By altering the properties of TaN through doping and defects we can optimize these interaction energies to drive 2D, horizontal growth of the interconnect metal.

With this methodology, we have developed promising TaN-based materials to promote deposition of high quality interconnects made from Cu for the higher metallization levels and Co and Ru for the lowest and smallest interconnect levels. Our kinetic Monte Carlo approach provides further insight into the metal deposition process for these materials, providing quantitative information on the depositedmetal, and highlighting the effect of substrate, deposition temperature and annealing on the film morphology and quality [2].

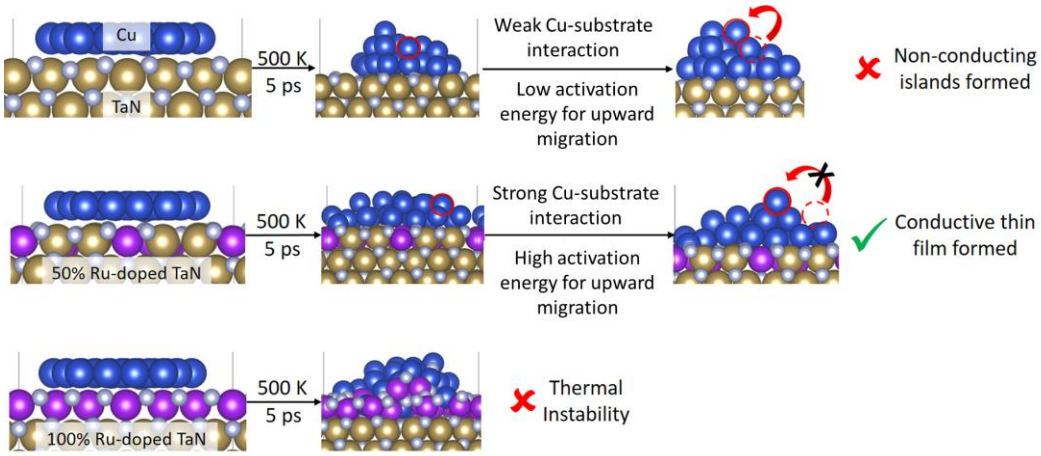

Figure 1: Examples of Cu morphologies on different TaN substrates. Cu = blue, Ru = purple, Ta = gold, N = silver

References:

1. C.-L. Nies, S. K. Natarajan and M. Nolan, Chem. Sci. **13**, 713-725 (2022).
2. S. D. Aldana, C.-L. Nies and M. Nolan, arXiv, (2024) https://doi.org/10.48550/arXiv.2410.06133