Materials Discovery using Machine Learning and DFT for Interconnects

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As the dimensions of semiconductors in computing technologies continue scaling down, the dimensions of the wires connecting them must scale down as well. Traditional wires have become less viable at the nano-scale because the resistivity of typical conductors such as copper increases dramatically as dimensions scale down. Previous studies show that this effect can be reduced by directional conductors with highly anisotropic Fermi velocities[1]. However, the amount of materials that are able to outperform copper at small dimensions remains low. Using the previous work as a training dataset, we utilize machine learning (ML) models to predict the resistivity scaling for thousands of unseen materials. We validate the ML predictions using DFT and evaluate electron-phonon scattering for the most promising candidates to map their overall resistivity as a function of dimension. We identify 29 new materials that can potentially outperform copper at ~10nm and below.

[1] S. Kumar, C. Multunas, B. Defay, D. Gall and R. Sundararaman, "Ultralow electron-surface scattering in nanoscale metals leveraging Fermi-surface anisotropy", *Phys. Rev. Mater.* **6**, 085002 (2022)