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Manipulating thermal conductance across 3D/1D interface by impedance matching[1] JINGJIE ZHANG, CARLOS POLANCO, AVIK GHOSH, University of Virginia — Self-assembled monolayers (SAMs) are of special interest to nano-electronic and thermal devices, because we can tune their properties by changing the bonding strength that links the SAMs to a thin film layer. We explain how this bonding strength influence heat across this 3D-1D interfaces based on a frequency dependent broadening matrix that acts as a generalization of acoustic impedance. We demonstrate both how to build an equivalent "impedance" broadening matrix that captures the dimensionality mismatch at the 3D-1D transition and the "matching" effect of the end group on an equivalent 1D-1D interface. We calculate thermal boundary conductance (TBC) at metal/polymer interfaces with different terminal groups and polymers. The calculations are done with non-equilibrium Green's function formalism coupled with ab-initio parameters for the chemical group functionalized systems. Our results confirm that in the low frequency spectrum, the stronger the bonding the larger the TBC. Nevertheless, when we consider the whole phonon spectrum, there is a sweet spot in the bonding strength that maximizes TBC.

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