Effects of Surface Roughness on Nanophononic Metamaterial Performance

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The roughness of surfaces is a characteristic that is relevant to a wide range of problems in physics, spanning a wide range of length scales, from the geological scale for planetary surfaces down to the atomic scale for material surfaces. In this work, we extend the state-of-the art in roughness studies pertaining to nanoscale phonon transport and apply it to nanophononic metamaterials in the form of suspended single-crystal silicon membranes with nanopillars standing on their surfaces [1]. In this set up, we introduce statistically characterized surfaces using several techniques and explore the impact of phonon-boundary scattering from these surfaces on the thermal conduvity. In particlar, we examine cases where only the membrane surface is roughned and cases where only the nanopillar surfaces are roughened. In all cases, the roughness is measued by metrics that characterize a power spectral density function for the surface profile; these metrics include the Hurst component and root mean square. We then run a series of equilibrium molecular dynamics simulations and compute the in-plane thernal conductivity using the Green-Kubo method. Our results reveal a competition towards reducing the thermal conductivity between the effects of the local resonances and the effect of boundary scattering from the rough surfaces. This competiton is analyzed in terms of the roughness parameters.

References

1. B.L. Davis and M.I. Hussein, *Phys. Rev. Lett*. **112**, 055505, (2014).