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Surface roughness and phonon transport in thin Si nanowires: an atomistic study[1] JESUS CARRETE, LUIS JAVIER GALLEGO, LUIS MIGUEL VARELA, Facultad de Fisica, Universidad de Santiago de Compostela, Spain, NATALIO MINGO, LITEN, CEA-Grenoble, France — Good thermal insulation is much harder to achieve than electrical insulation. Thus, the astonishingly low thermal conductivities recently reported on Si nanowires came as a surprise, since the displayed values were an order of magnitude lower than predicted by the diffuse boundary limit of Casimir's theory. Recent theoretical work has employed the Born approximation to predict a very much enhanced boundary scattering rate that would lead to a thermal conductivity well below the Casimir limit. We present a Green's function calculation that answers the question of whether the Casimir limit to the phonon mean free path can be overcome by roughness. Our results show that the mean free path (MFP) and the thermal conductivity of a nanowire are very close to the Casimir limit for shallow disorder, and can only be pushed below it using very deep surface roughness, well beyond previous estimates. We also explore the limits of the Born approximation in this context using vacancies and isotopic impurities as defects.

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