Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Heat flow and δ-layers in Si nanowires MEHMET B. BEBEK, T. MICHAEL GIBBONS, STEFAN K. ESTREICHER, Texas Tech — Modern semiconductor growth techniques allow the use of heterostructures in semiconductor devices such as δ-layers or superlattices, and their behavior regarding heat flow is generating considerable interest. However, there is no fully 'first-principles' theoretical description of the interactions between heat flow and the interface between two dissimilar materials. In this contribution, we present the result of ongoing ab-initio, microcanonical, non-equilibrium MD simulations on Si/Ge or Si/C interfaces in a Si nanowire. We show that the 'spatially-localized vibrational modes' (SLMs) associated with the interface trap incoming bulk phonons for lengths of time ranging from dozens to hundreds of periods of oscillation. Then, the trapped phonons decay into lower frequency bulk phonons. This decay depends on the availability of receiving modes on either side of the interface rather than on the origin of the incoming flow of heat.

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Date submitted: 14 Nov 2014 Electronic form version 1.4