Finite-Difference Time-Domain Study of Phonon Dynamics and Rough-Interface Scattering in Nanostructures

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The advancements in the growth of heterostructures with high-quality interfaces arise from the need for high-performance electronic devices. However, systems with multiple interfaces suffer from low thermal conductivity owing to a complex and still insufficiently understood interplay of interface scattering and phonon-dispersion modification. In this work, we introduce a finite-difference time-domain (FDTD) simulation technique for the analysis of elastic-wave scattering at a rough interface between dissimilar elastic solids [1]. We tease out the effects of interface morphology (rms roughness and correlation length) and the mismatch between the materials' elastic properties on the refraction/transmission and mode localization near the interface.

The model system is a lateral interface between single-layer graphene and hBN [3]. In Figs. 1 and 2, we present the time progression of the energy-density profile for a normally incident longitudinal wave packet. The rms roughness is 1.23 nm, the wavelength equals 10 rms, and the autocorrelation length equals rms roughness in Figure 1 and is 1/2 of the rms roughness in Figure 2. The smaller correlation length leads to more transmitted energy and less reflection. Moreover, at a smaller correlation length, more energy remains localized at the interface. The results of this study on phonon transport across junctions between dissimilar materials can be used to develop simplified interface-scattering models to be used in the design of functional nanomaterials with desired thermal properties.

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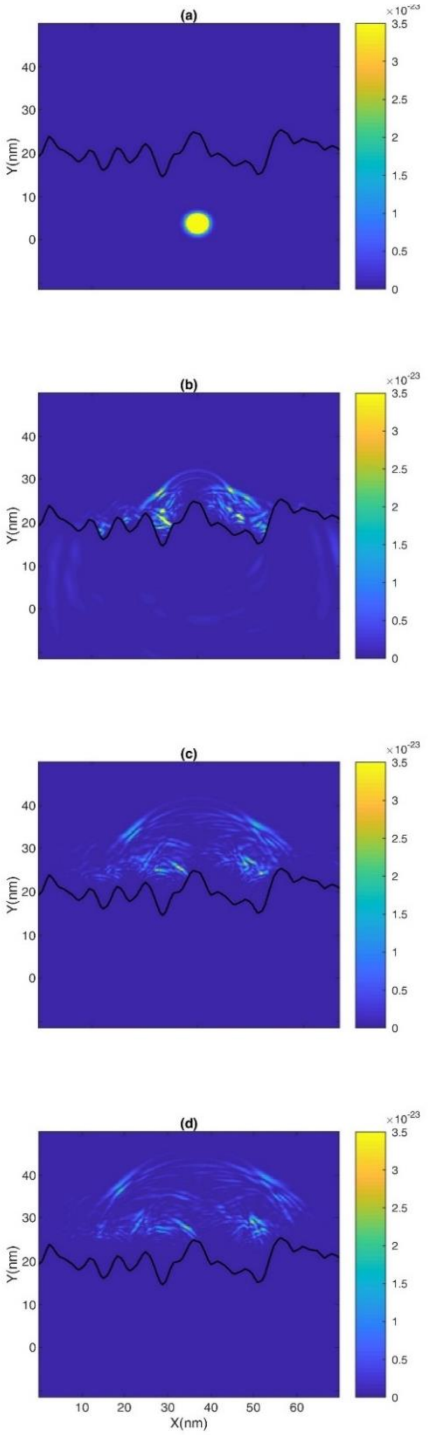

Fig.1: Energy-density profile (yellow: high; blue: low) after a scattering event at the interface between graphene and hBN. A longitudinal wave packet was injected toward the interface from the bottom and center with normal incidence. The rms roughness of 1.23 nm, autocorrelation length equals rms roughness, and the wavelength is 10 times the rms roughness. The results are plotted at a) 0, b) 2, c) 4 and d) 5 ps.

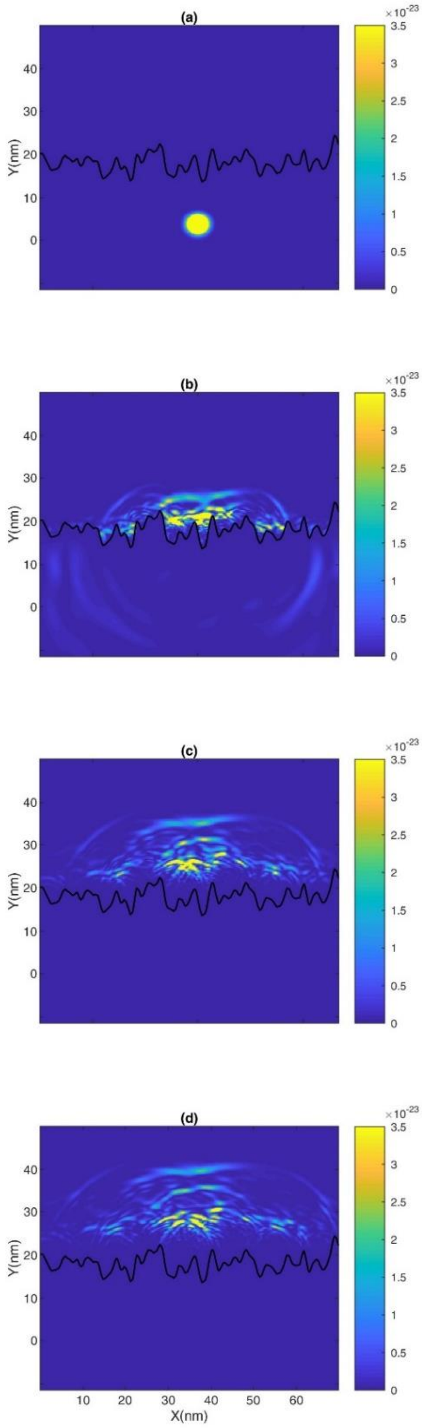

Fig.2: Energy-density profile (yellow: high; blue: low) after a scattering event at the interface between graphene and hBN. A longitudinal wave packet was injected toward the interface from the bottom and center with normal incidence. The rms roughness of 1.23 nm, autocorrelation length equals half of rms roughness, and the wavelength is 10 times the rms roughness. The results are plotted at a) 0, b) 2, c) 4 and d) 5 ps.