Screening effects on phonon scattering at interfaces

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Nanoscale heat transport is a key parameter affecting the ultimate performance of semiconductor devices (transistors). Thus, a fundamental understanding of thermal transport near active, atomically-sized device structures such as interfaces and defects will be valuable for future design. Recently, developments of highly monochromatic atom-wide electron beams have promised to allow exploration of phonon excitations in nanomaterials with high spatial resolution [1]. The experimental data, however, can present enormous interpretation challenges, requiring a much deeper understanding of probe screening effects, scattering *f*-sum rules, localized and delocalized phonon excitations, and symmetry selection rules, etc. In this work, we suggest that the local dielectric response of the specimen can screen the long-range coulomb behavior of a probe electron. This screening can cause the dipole vibrational signal to be weak or be nearly absent in some materials, revealing short wavelength vibrational behavior associated with the local structure.

We performed spatially-resolved studies across a SiC/SiO_2 interface (a core component of MOSFET transistors) using a 0.15 nm probe with about 9 meV of energy resolution. We found that the vibrational response is strongly dependent on the probe position (Fig. 1). To evaluate the effects of the screening of each material, we also studied independently SiO_2 and SiC wedges. For these nanostructures, we found that bulk silica films (~100 meV) can be excited with a probe parked 10's of nanometers away from the film (aloof excitation). This probably occurs due to the low ionic behavior (~50%) of the glass. In contrast, in the SiC wedge we do not observe bulk behavior without actually linking the bulk material by the electron beam. Therefore, we believe that higher energy - electronic, phononic - modes associated with the bulk/surface or with adjacent materials, shield the external field of the swift electron, preventing excitation of bulk phonon modes in the SiC. For the intersecting geometry, bulk and surface polaritons modes can both be excited in those finite films [2]. For the composite system SiC/SiO_2, we found spectral changes as function of the probe location (Fig.1). When the probe intersects the SiC (Fig.1a), most of bulk longitudinal phonon modes of SiC (~40, 65, 110 meV) are excited due to the efficient coupling between the lattice vibrations and the fast electron, including surface polaritons at ~104 meV. These long wavelength optical surface modes play an important role in the heat dissipation by radiative mechanisms. In addition, the prominent resonance at ~40 meV corresponds to the excitation of the short-wavelength acoustic modes. In this probe configuration the SiC response shields the electric field preventing surface excitation of the silica. When the probe impinges SiO_2 layer (Fig.1b), however, one can excite surface phonon excitations from both the SiO_2 (~50, 135 meV)[2] and SiC (~104 meV). Also, the bulk phonon mode (~100 meV) of silica is excited.

Our results bring further understanding of the screening effects on the phonon scattering and highlight the importance of accounting for this effect on vibrational data interpretation. Angle-resolved experiments are in progress in order to investigate short-wavelength phonon modes near the interface, which are responsible for heat diffusion on the bulk.

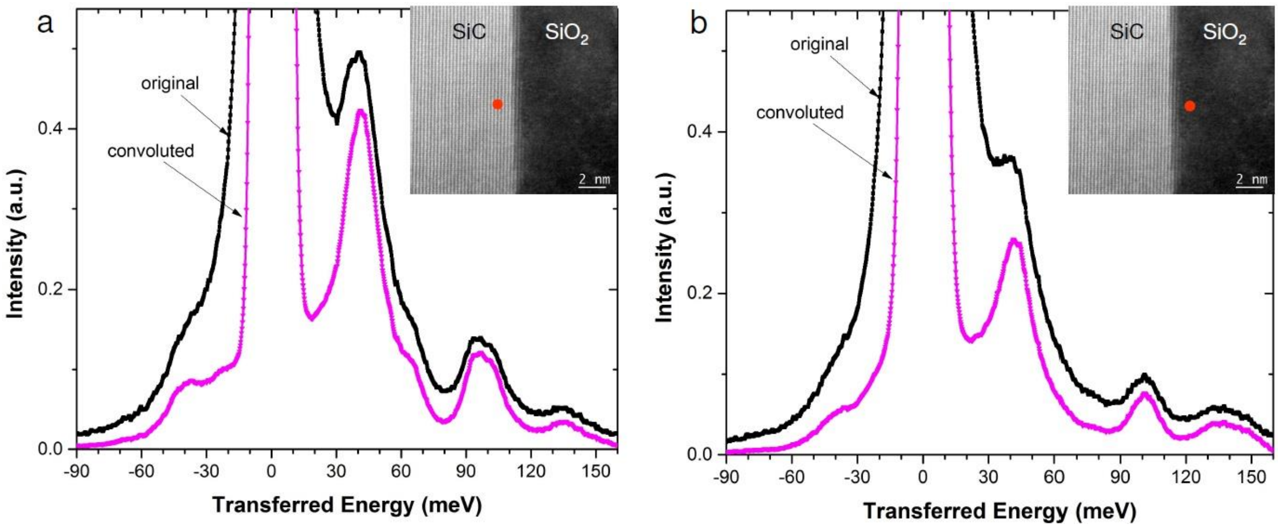

Fig.1. Vibrational spectroscopic spectra (black curves) acquired in both sides of the SiC/SiO_2 interface (inset). Note variations in the shape and amplitude of the resonances. Probe position is indicated by a red circle (~1 nm from the interface) in the inset. Deconvoluted spectra (magenta curve) using a Richardson-Lucy method [3] are also shown (3 iterations). We found the FWHM of the ZLP is reduced down to ~5 meV.

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