Determination of Phononic Bandgap and Phonon Anomalies in Epitaxial Metal/Semiconductor Superlattices with Inelastic X-ray Scattering

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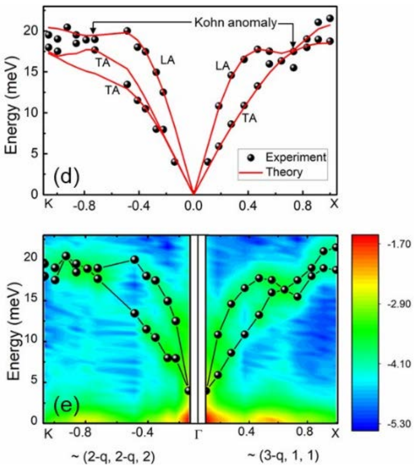
Epitaxial metal/semiconductor superlattice heterostructures with lattice-matched abrupt interfaces and suitable Schottky barrier heights are attractive for thermionic emission-based waste-heat to electrical energy conversion, hot electron-based solar-to-electrical energy conversion and for the demonstration of the thermal hyper-conductivity in solid-state devices. HfN/ScN is one of the earliest demonstrations of epitaxial single-crystalline metal/semiconductor heterostructures and has attracted significant interest in recent years to harness its excellent properties into device applications. Though the understanding of the mechanism of thermal transport in HfN/ScN superlattices is extremely important for practical applications, not much attention has been devoted to measure their phonon dispersion and related properties.

In this work, we employ non-resonant meV-resolution inelastic X-ray scattering to determine the momentum-dependent phonon modes in epitaxial metallic HfN and lattice-matched HfN/ScN metal/semiconductor superlattices. HfN exhibits a large phononic bandgap (~ 40 meV) and Kohn anomaly in the longitudinal and transverse acoustic phonon modes at q~0.73 along the [100] and [110] directions of the Brillouin zone due to the nesting of the Fermi surface by the wave vector (q). The in-plane [100] acoustic phonon dispersion of the HfN/ScN superlattices is found to be dominated by the HfN phonons, while the optical phonons exhibit both ScN and HfN characteristics. First-principles density functional perturbation theory modeling is performed to explain the experimental phonon spectra and temperature-dependent thermal conductivity are measured with a pump-probe spectroscopic technique. These results will help understand the phonons in HfN and HfN/ScN metal/semiconductor superlattices for thermionic energy conversion.



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