Acoustic phonon limited mobility in two-dimensional semiconductors: Deformation potential and piezoelectric scattering in monolayer MoS2 from first principles - DTU Orbit (13/01/2019)

Acoustic phonon limited mobility in two-dimensional semiconductors: Deformation potential and piezoelectric scattering in monolayer MoS2 from first principles

We theoretically study the acoustic phonon limited mobility in n-doped two-dimensional MoS2 for temperatures T<100 K and high carrier densities using the Boltzmann equation and first-principles calculations of the acoustic electron-phonon (el-ph) interaction. In combination with a continuum elastic model, analytic expressions and the coupling strengths for the deformation potential and piezoelectric interactions are established. We furthermore show that the deformation potential interaction has contributions from both normal and umklapp processes and that the latter contribution is only weakly affected by carrier screening. Consequently, the calculated mobilities show a transition from a high-temperature $\mu \sim T^{-1}$ behavior to a stronger $\mu \sim T^{-4}$ behavior in the low-temperature Bloch-Grüneisen regime characteristic of unscreened deformation potential scattering. Intrinsic mobilities in excess of 105 cm² V⁻¹ s⁻¹ are predicted at T<10 K and high carrier densities (n>10¹¹ cm⁻²). At 100 K, the mobility does not exceed ~7×10³ cm² V⁻¹ s⁻¹. Our findings provide new and important understanding of the acoustic el-ph interaction and its screening by free carriers, and is of high relevance for the understanding of acoustic phonon-limited mobilities in general.

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