Intrinsic mobility modulation of transition metal dichalcogenides via thickness-dependent deformation of the electron wave function

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We study the intrinsic phonon scattering contribution to the transport properties of a two-dimensional transition-metal dichalcogenide. Analytical expressions are derived for scattering by acoustic phonons, nonpolar and polar optical phonons based on a full Boltzmann transport theory formalism. Taking into account of various electron wave functions induced by spatial quantum confinements, we calculate the mobility (μ) as a function of thickness (d). Our work encompasses two physically distinct thickness ranges with respect to electron wave function: the growth μ_{UP} and saturation μ_{SAT} regimes. In the μ_{UP} regime, the electron wave function is given by quantum well model, which produces an intimate linearly $\mu-d$ relation in all three phonon modes. In the μ_{SAT} regime, however, the result is determined by variational-subband-wave-function model, leading to a thickness-independent mobility. Importantly, we show that a single assumption of spatial correlation, defined through a variational parameter b, is sufficient to bridge the results in both μ_{UP} and μ_{SAT} regimes. In addition, we investigate in detail the carrier density and temperature dependence of high-temperature mobility and find excellent agreement with experimental data for the coefficient γ from $\mu \sim T^{-\gamma}$. We also compare these results with externally accessible knobs, such as deformation potential (strain), carrier screening, and conduction valley degeneracy, and check their level of validity.