Modeling of Electron Mobility in Semi-metallic $Hg_{1-x}Cd_xTe$ Quantum Wells at T = 77 K: Application to THz Detection

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In this work transport properties of electrons in $Hg_{0.32}Cd_{0.68}Te/Hg_{1-x}Cd_xTe$ quantum well (QW) were modeled at the liquid nitrogen temperature (T=77 K). Energy spectra and wave-functions are calculated in terms of full 8-band k·p method, which allows describing the onset of semi-metallic or semiconducting phases in QW depending on its growth parameters.

Two main scattering mechanisms, making the largest impact on the electron mobility in the bulk – scattering on longitudinal optical (LO) phonons and background charged impurities – are considered in the mobility calculations. In our case, the LO phonon scattering is strongly inelastic because the LO phonon energy (17 meV) is several times larger than k_BT (6.7 meV). Thus, the approximation of a single relaxation time for mobility calculations is inapplicable. Linear Boltzmann equation, which allows one to calculate of electron distribution function perturbation for in-plane electric field, was solved directly by the iterative technique. The electron mobility is calculated by averaging velocities of all electrons in the conduction band. Hence our numerical results incorporate the inelasticity of LO phonon scattering, band mixing, nonparabolicity of the energy dispersion, and degeneracy of the 2D electron gas. For the background concentration of charged impurities in the well of 10^{14} cm^{-3}, the calculated mobility varies from $1.5\cdot10^5$ to $1\cdot10^6$ $cm^2/(V\cdot s)$, depending on the QW width. For charged impurity concentration 10^{15} cm^{-3}, the mobility varies from $7.3\cdot10^4$ to $1.6\cdot10^5$ $cm^2/(V\cdot s)$. Our results are consistent with available experimental data.

We also estimate the impact of the interface scattering, modeling roughness by $5\cdot10^{10}$ cm^{-2} concentration of interface defects with the average lateral size of 3x3 lattice constants and height of 1 monolayer. In the QW of 20 nm width and x=0, the corresponding relaxation time is of the order of $\tau\sim10^{-7}$ s, and for a 12 nm wide well with x=0.06, it is about $\tau\sim6\cdot10^{-10}$ s. This relaxation time is much greater than those corresponding to main scattering mechanisms, so the interface roughness scattering for our problem can be safely neglected.

These calculations are applied to model the resistivity and resistance of semi-metallic $Hg_{1-x}Cd_xTe$ QW used as a channel for THz hot-electron bolometer. At low concentration of background charged impurities (10^{14} cm^{-3}), variation of the channel composition x and thickness (which corresponds to the QW width) allows one to tune the resistance in the range of 220-340 Ohm/□. For higher concentration of charged impurities (10^{15} cm^{-3}), this resistance varies in the range of 715-1690 Ohm/□. Thus, the resistance of the channel can be efficiently tuned to match the impedance of the antenna.

Comparing to real graphene devices, $Hg_{1-x}Cd_xTe$ heterostructures can provide an order of magnitude higher mobility. This is explained by the fact that the mobility in graphene placed on the substrate, is considerably deteriorated to values of the order of $(1\ldots5)\cdot10^4$ $cm^2/(V\cdot s)$ at T=77 K. Thus, $Hg_{1-x}Cd_xTe$ heterostructures are prospective for various applications where high mobility is important.

Our estimates show that properties of semi-metallic $Hg_{1-x}Cd_xTe$ QWs could be sufficiently tuned to meet specific requirements of sub-THz and THz hot-electron bolometric detectors and field-effect transistors on their base utilizing plasma waves.