CPPP 47 P THERMOELECTRIC FIGURE OF MERIT OF (111) ORIENTED PbTe/Pb $_{1-x}$Eu $_x$Te DOUBLE QUANTUM WELL STRUCTURE

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The search of materials of improved thermoelectric properties retains important and interesting activity. Quantum wells with thin internal barriers (DQW) attract the attention due the possibility to enhance carrier mobility [1-3] using the effect of wave function modulation in such structures. In present report, the thermoelectric opportunities of n - PbTe/Pb1-x Eu$_x$ Te DQW were estimated theoretically. The model of DQW with rectangular confinement potential oriented parallel to (111) plane, was considered. Dimensional quantization lifts the valley degeneracy and two sets of subbands arising from different valley appear. One set is from longitudinal (*l*) ellipsoid perpendicular to QW, and second set of three times degenerated subbands arises from oblique (*ob*) ellipsoids of constant energy. The energies E_α^l, E_α^{ob} of levels of dimensional quantization, dispersion law and subbands populations were calculated as a function of inner barrier width b. Due to the coupling of wells energy levels double at some b^* when b increase. The energy of second new level reduces from energy of top of QW to values character for isolated quantum well at large distance between the wells. The considered structure with quantum well thickness $d_1 = d_2 = 20$Å, contains two levels E_1^l and E_2^l at $b > 10$Å. In oblique ellipsoids new level E_2^{ob} appear at $b_{ob}^* \approx 30$Å.

Carrier transport along wells had been considered on the base of Boltzmann equations, which were solved by iterations. The scattering on bulk acoustical and optical phonons, the carrier intrasubband and intersubband transitions, the multivalley character of bulk materials and nonparabolicity of electron dispersion law were taken into account. The electron mobility μ, Seebeck coefficient, electron thermal conductivity k^e, and thermoelectric figure of merit ZT were calculated as a functions of inner barrier width. As in [2, 3], the dependence $\mu(b)$ contains the maximum connected with the appearance of new level E_2^{ob} at $b = b_{ob}^*$. Despite its small population (~10%), contribution of that subband to mobility is essential. In considered structure, maximal value of mobility exceeds, on 15%, the mobility in single quantum well. The dependence $k^e(b)$ contains the maximum, too. However, maximum electron thermal conductivity is smaller than lattice thermal conductivity, and thermoelectric figure of merit increases at $b \sim b^*$. Maximum value of $ZT = 0.93$exceeds the corresponding $ZT^{SW} = 0.84$ in single well calculated at the same parameters [4]. Note, however, the range of b, where $ZT > ZT^{SW}$, is of order ten angstrom.

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