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Large enhancement of the thermoelectric figure of merit in a ridged quantum well

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Abstract

Recently, new quantum features have been observed and studied in the area of ridged quantum wells (RQWs). Periodic ridges on the surface of the quantum well layer impose additional boundary conditions on the electron wavefunction and reduce the quantum state density. As a result, the chemical potential of RQWs increases and becomes ridge-height-dependent. Here, we propose a system composed of RQWs and an additional layer on the top of the ridges forming a periodic series of p^+–n^+ junctions (or metal–n^+ junctions). In such systems, a charge depletion region develops inside the ridges and the effective ridge height reduces, becoming a rather strong function of temperature T. Consequently, the T dependence of chemical potential is magnified and the Seebeck coefficient S increases. We investigate S in the system of semiconductor RQWs having abrupt p^+–n^+ junctions or metal–n^+ junctions on the top of the ridges. Analysis made on the basis of Boltzmann transport equations shows a dramatic increase in S for both cases. At the same time, other transport coefficients remain unaffected by the junctions. Calculations show one order of magnitude increase in the thermoelectric figure of merit ZT relative to the bulk material.

1. Introduction

Quantum wells are considered the most reliable low-dimensional systems for thermoelectrics [1–3]. However, improvements in thermoelectric properties over bulk materials are insufficient for most applications. In this work, we present ridged quantum wells (RQWs) having advanced thermoelectric properties. The RQW layer has periodic ridges on the surface. Its operation is based on the effect of quantum state depression (QSD). Periodic ridges impose additional boundary conditions on the electron wavefunction. Supplementary boundary conditions forbid some quantum states for free electrons, and the quantum state density in the energy $\rho(E)$ reduces. According to Pauli's exclusion principle, electrons rejected from the forbidden quantum states have to occupy the states with higher E. Thus, chemical potential μ increases. In semiconductors, QSD reduces $\rho(E)$ in all energy bands including the conduction band (CB). Electrons rejected from the filled bands occupy the quantum states in the empty bands and the electron concentration in the CB increases [4]. This corresponds to donor doping (we will refer to it as QSD doping). The QSD transfers electrons to higher energy levels. If initially the semiconductor is intrinsic, then the QSD doping will modify it to n-type. It is comparable with conventional donor doping from the point of increase in μ. However, there are no donor atoms. QSD doping does not introduce scattering centres and consequently allows high electron mobility. There are distinctions and similarities between the QSD forbidden quantum state and a hole. The state is forbidden by the boundary conditions and cannot be occupied. However, it is not forbidden in an irreversible way. If the boundary conditions change (e.g. owing to charge depletion), then it can recombine with the electron (like the hole recombines with the electron). As the QSD forbidden state is confined to the boundary conditions (macroscopic geometry), it is not localized in the lattice and cannot move like a hole.

The density of states in RQW (figure 1) reduces G times $\rho(E) = \rho_0(E)/G$, where $\rho_0(E)$ is the density of states in a conventional quantum well layer of thickness L ($a = 0$) and G is the geometry factor introduced in [5]. In the first approximation, for the case $L, w \gg a$ and within the range $5 < G < 10$, the following simple expression (obtained in [4]) can be used:

$$G \approx L/a \tag{1}$$

where a is the ridge height and L is the RQW layer thickness (figure 1). The density of QSD forbidden quantum states is

$$\rho_{\mathrm{FOR}}(E) = \rho_0(E) - \rho_0(E)/G = \rho_0(E)\,(1 - G^{-1}). \tag{2}$$

