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Electron spectrum of δ-doped quantum wells by the Thomas–Fermi method at finite temperatures

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ABSTRACT

The electron spectrum of δ-doped quantum wells in n-GaAs is investigated by means of the Thomas–Fermi (TF) method at finite temperatures. This method shows rapid convergence and good accuracy. Under two-dimensional (2D) doping concentrations $10^{13}\ldots2\times10^{13}\,\mathrm{cm}^{-2}$, the simplest TF method ($T=0$ K) can be used to calculate the profiles of the potential well up to $T\approx200$ K. The simplest TF method yields correct results for the electron concentrations and the differences of the electron energy sublevels in the quantum well up to room temperature ($T\sim300$ K).

1. Introduction

The doping of semiconductors with atomic resolution (δ-doping) has become possible due to the increasing precision of molecular beam epitaxy (MBE) growth technologies [1–19]. The work on n-type δ-doped structures has primarily been with GaAs semiconductors. If Si atoms occupy the positions of Ga atoms in the direction (1 0 0), then a potential well for electrons is formed [3–11]. Considerable information on the subband structure and the mobilities of these systems through electrical and optical measurements is available [3–5,8–11,13,15,20–31]. Fewer investigations have been conducted on δ-layers in Si, and this is mainly due to the difficulties to incorporate dopants in a well-controlled manner during the MBE growth of Si [12,14,17–19].

Because ionized impurity scattering is the principal factor that determines carrier mobility, the advantage of a field-effect transistor (FET) with a δ-doped channel over uniformly doped materials is the smaller overlap between impurities and carriers [2–4,31]. The electron mobilities within the δ-doped channel have been investigated in numerous papers [3–5,8,11,13,15,17,20–22]. The infrared transitions between electron sublevels within δ-doped quantum wells have potential uses in optoelectronics [3,4,9,10,18,23–31], especially for infrared modulators, detectors, and lasers.

The electron spectrum of δ-doped quantum wells can be calculated by solving the Schrödinger equation jointly with the Poisson equation [25–40]. This direct approach is complicated, and its convergence is slow. To investigate δ-doped quantum wells, a simpler approach based on the statistical Thomas–Fermi (TF) method is possible [41–43]. The main problem with using the direct approach is to find an appropriate initial approximation that can be obtained with the TF method.

This paper investigates the electron spectrum in δ-doped quantum wells in n-GaAs by means of the TF method at finite temperatures. The simplest TF method ($T=0$ K) was found to give correct results for the electron concentrations and the differences in the electron energetic sublevels up to $T\sim300$ K, at which the two-dimensional (2D) doping concentrations are $n_{2d}=10^{13}\ldots2\times10^{13}\,\mathrm{cm}^{-2}$. Non-smoothness of the electron concentrations in the center of the well occurs when the concentrations are computed directly from the TF method. Calculating the electron concentrations from the electron wave functions avoids this peculiarity.

2. Basic equations

Consider a single δ-doped electron quantum well within an n-type semiconductor. Generally, the potential energy for a single electron, $V=-e\varphi$, is given by the Poisson equation (in absolute units):

$$\frac{d^2V}{dz^2}=\frac{4\pi e^2}{\varepsilon}\{-n[V]+n_{2d}\delta(z)+N_d(z)\} \tag{1}$$

n is the electron concentration, which is the functional of V, φ is the electric potential, n_{2d} is the 2D doping concentration, N_d is the three-dimensional (3D) concentration of ionized donors, and ε is the permittivity of the semiconductor. The donors in 2D wells are fully ionized, whereas the volume impurities are partially ionized. The value $E_d\approx0.01$ eV is the donor energetic level, and N_{d0} is the donor doping concentration.

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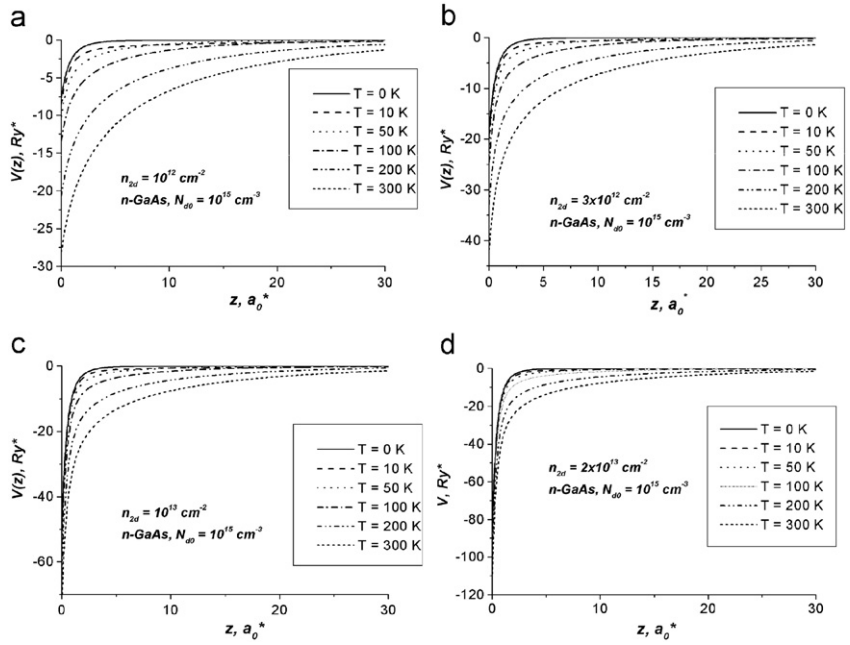

Fig. 1. Profiles of the electron potential energy $V(z)$ at different values of δ-doping n_{2d}. For n-GaAs, the scales are a_0^*=9.14 nm and Ry^*=6.25 meV.

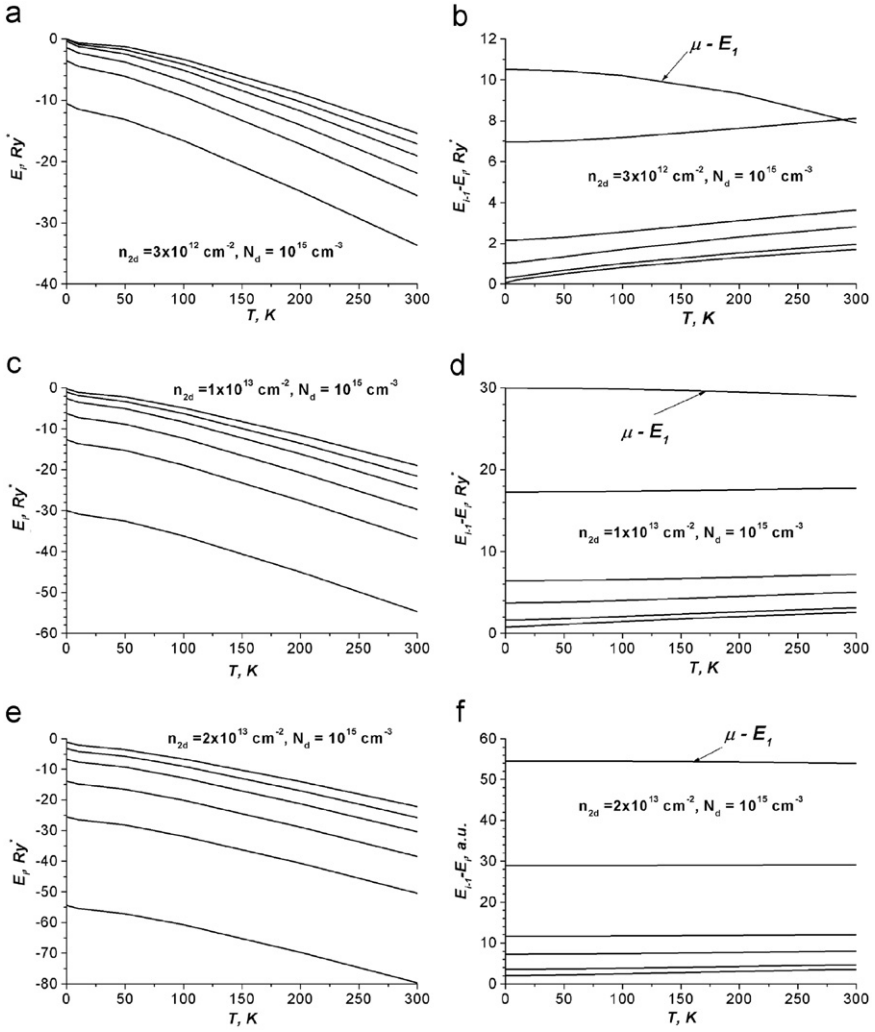

Fig. 2. Dependencies of the energy sublevels of the well (a, c, and e) and differences of the neighboring sublevels (b, d, and f) on the temperature.