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Geometry-induced electron doping in periodic semiconductor nanostructures

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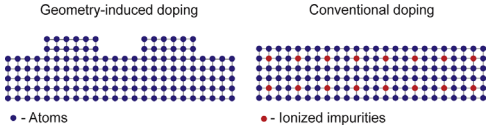
HIGHLIGHTS

- Influence of nanograting on electronic properties of thin semiconductor layer is studied.
- Geometry induced doping or *G*-doping is introduced.
- *G*-doping in the system of homojunction and heterojunction multiple nanograting layers is analyzed.
- Using of *G*-doping for high carrier mobility applications is discussed.
- Methods of growing multiple nanograting layers are discussed.

GRAPHICAL ABSTRACT



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ABSTRACT

Recently, new quantum features have been observed and studied in the area of nanostructured layers. Nanograting on the surface of the thin layer imposes additional boundary conditions on the electron wave function and induces *G*-doping or geometry doping. *G*-doping is equivalent to donor doping from the point of view of the increase in electron concentration *n*. However, there are no ionized impurities. This preserves charge carrier scattering to the intrinsic semiconductor level and increases carrier mobility with respect to the donor-doped layer. *G*-doping involves electron confinement to the nanograting layer. Here, we investigate the system of multiple nanograting layers forming a series of hetero- or homojunctions. The system includes main and barrier layers. In the case of heterojunctions, both types of layers were *G*-doped. In the case of homojunctions, main layers were *G*-doped and barrier layers were donor-doped. In such systems, the dependence of *n* on layer geometry and material parameters was analysed. Si and GaAs homojunctions and GaAs/AlGaAs, Si/SiGe, GaInP/AlGAs, and InP/InAlAs heterojunctions were studied. *G*-doping levels of 10^{18}–10^{19} cm^{-3} were obtained in homojunctions and type II heterojunctions. High *G*-doping levels were attained only when the difference between band gap values was low.

1. Introduction

Developments in nanotechnology allow the fabrication of densely packed, periodic structures [1–4]. Recently, ultra short period nanopore arrays and nanogratings have been obtained by block copolymer lithography [1,2]. Another method for nanograting fabrication is a multi-beam interference lithography. Using these techniques, gratings with 10-nm (Ref. [3]) and even sub-10 nm pitch [4] have been fabricated. At the same time, nanograting (NG) has been shown to dramatically improve thermoelectric [5] and electron emission properties [6] when the grating pitch becomes comparable with the electron's de Broglie wavelength. This is due to the special boundary conditions imposed by NG on the electron wave function. Supplementary boundary conditions forbid some quantum states, and the density of quantum states (DOS) is reduced (in all bands). Electrons rejected from NG-forbidden quantum states have to occupy empty

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states with a higher energy E Fermi energy E_F increases, and the electronic properties of the NG layer change. In the case of semiconductor materials, electrons rejected from the valence band (VB) occupy empty quantum states in the conduction band (CB). Electron concentration n in the CB increases, which can be termed as geometry-induced electron doping or G-doping. G-doping is equivalent to donor doping from the point of view of the increase in n and Fermi energy E_F. However, there are no ionized impurities. This maintains charge carrier scattering to the intrinsic semiconductor level and increases carrier mobility with respect to the donor-doped layer of the same electron concentration. G-doping is temperature independent because it originates from layer geometry and no ionized impurities are involved.

Other methods of doping without impurities include the well-known modulation doping and the recently introduced polarization doping [7]. Both are 2D in nature. However, a 3D approach to modulation doping was introduced in Ref. [8] to improve the thermoelelectric characteristics of nanocomposites [9,10]. The influence of periodic structures on electronic properties has been studied in related geometries, such as periodic curved surfaces [11,12], nanotubes [13], cylindrical surfaces with nonconstant diameter [14], and strain-driven nanostructures [15].

Electron confinement to the NG layer is needed to obtain G-doping. The layer can be made freestanding, but in practice it is usually sandwiched between wide bandgap layers. The NG layer thickness is fundamentally limited by the requirement of having quantum properties. However, thin layers have low optical absorption. The layer thickness also limits the lateral charge and heat transport.

Here, we investigate G-doping in multiple nanograting layers. Such layers are quasi-3D and have improved optoelectronic [16] and thermoelectric characteristics with respect to a single layer. Multiple nanograting layers consist of a replicated structure including main and barrier layers, forming a series of hetero- or homojunctions. The main layer is thicker than the barrier layer and plays a leading role in carrier transport and optical absorption. The barrier layer forms electron confinement energy regions. It also contributes to carrier transport and optical absorption. Both the main and barrier layers have NG geometry.

The objectives of this work are to calculate n and E_F in multiple nanograting layers and to find out how they are dependent on layer thicknesses and material properties. First, we introduce G-doping in a single nanograting layer (Section 2). Next, we calculate n and E_F in a homojunction multilayer structure (Section 3). Subsequently, we calculate the same for a heterojunction multilayer structure (Section 4). Finally, the possibility of realizing such structures and their advantages for optoelectronic and thermoelectric devices are discussed (Section 4.4). In Section 5, our conclusions are summarized briefly. An analysis is made within the limits of a parabolic band, a wide quantum well, and degenerate electron gas approximations. A parabolic band approximation can be used as we consider only band edges. Wide quantum well is a good approximation as we regard relatively thick layers with better optical absorption and lateral transport properties. Degenerate electron gas approximation is suitable as we consider only high electron concentrations (high G-doping levels).

2. DOS and electron concentration in a single nanograting layer

Fig. 1 shows a cross section of a single NG layer. The grating has depth a and period $2w$. To make a comparison, we set the reference layer as a plain layer with thickness H such that it has the same cross-section area. Nanograting imposes additional boundary conditions on the electron wave function and forbids some quantum states. The DOS in energy $\rho(E)$ is reduced [17] with respect to the reference well

$$\rho(E) = \rho_0(E)/G, \tag{1}$$

where $\rho_0(E)$ is the DOS (number of quantum states within the unit energy region and in the unit volume) in a reference well, and $G = G(H, w, a) > 1$ is the geometry factor.

The geometry factor or DOS calculation requires solving the time-independent Schrödinger equation in NG geometry. Mathematically, there is no difference between DOS reduction and electromagnetic (TM) mode depression [18,19]. The Helmholtz equation and Dirichlet boundary conditions are used in both cases. Unfortunately, there is no exact analytical solution for NG geometry. The approximate analytical expression known as Weyl's formula [20,21] allows the calculation of DOS by using a ratio of layer surface area and volume. The perturbation method [22] has been used to find an approximate analytical expression for G in NG geometry. The DOS for electromagnetic modes in resembling geometries has been numerically calculated in the literature related to the Casimir effect [23].

Nanograting reduces the DOS in all bands. Electrons rejected from NG-forbidden quantum states have to occupy empty quantum states with higher E. In a semiconductor, electrons rejected from the VB have to occupy empty (and not forbidden by NG) energy levels in the CB (Fig. 2). Electrons are rejected from low energy levels and occupy high energy ones. During this process, the Fermi energy increases from $E_F^{(0)}$ to E_F. To simplify the presentation, in Fig. 2, we presume that $T=0$ (T is the absolute temperature) and the energy levels are equidistant on the energy scale (the geometry-induced energy level shift is also ignored). We use Eq. (1) to calculate the DOS and investigate the G-dependence

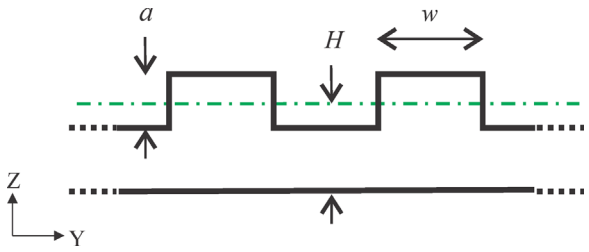

Fig. 1. Cross section of nanograting layer.

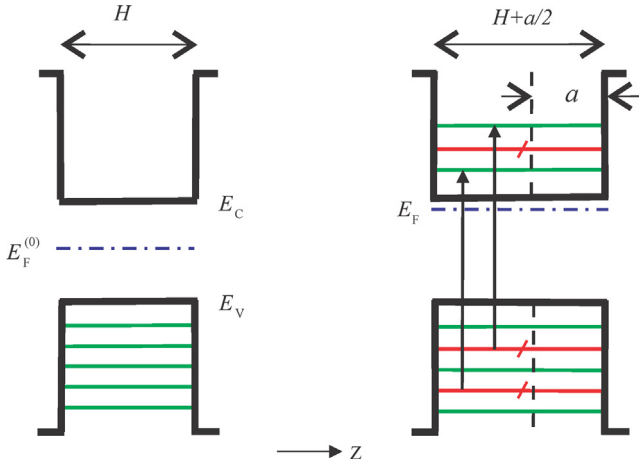

Fig. 2. Energy diagrams of (a) the reference semiconductor quantum well and (b) the NG layer. The horizontal (green) lines indicate occupied energy levels; the crossed (red) lines indicate NG-forbidden energy levels. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)