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An analysis of the effect of nitrogen and a screened (by free carriers) Coulomb field on the binding energy of hydrogenic shallow donors in GaInAsN

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ABSTRACT

The effect of nitrogen concentration on the screening with free carriers and binding energy of hydrogenic shallow donors in GaInAsN alloys is investigated. The binding energy is calculated using a novel algebraic model which was proposed recently by Gönül et al. (2006) [16], in order to find an analytical solution to the screened Coulomb potential. The results show that the nitrogen concentration is a strong factor in producing a screening field of free carriers and in affecting the binding energy of hydrogenic shallow donors.

1. Introduction

The introduction of nitrogen, N, into III–V alloys leads to very important and unusual changes of alloy properties. Even a small magnitude of N results in a significant reduction of the band gap. For example, the band gap of GaAs decreases by approximately 0.1 eV when 1% of N is added into the system [1]. This behaviour is different from that of usual semiconductors. Band anticrossing model (BAC) is proposed to explain this unusual behaviour. It has been reported that the BAC model [2] can be used to describe the composition dependence of the band gap energy of GaInAsN on GaAs

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substrates [3]. According to the model, there is an interaction between localized nitrogen states and the extended conduction band (CB) states which leads to a splitting of the CB into two states. The non-parabolic dispersion relationship for the lower E_- and upper E_+ conduction subbands is given by

$$E_\pm(k,y) = \frac{1}{2}\left(E_N + E_M(k) \pm \sqrt{(E_N - E_M(k))^2 + 4C_{NM}^2 y}\right) \tag{1}$$

where E_N is the energy position of the nitrogen-related level, $E_M(k)$ is the energy of the CB of the semiconductor matrix, C_{NM} is the interaction parameter and y is nitrogen molar fraction. The E_N, C_{NM} and $E_M(k)$ values are 1.65 eV, 2.7 eV and E_g(*interpolated band gap of* GaInAsN) $+ \hbar^2 k^2/2m^*$ [4], respectively.

The investigation of impurities in semiconductors is very important because they have a very special role in controlling the conductivity of semiconductors [5]. When an impurity is added into the lattice, its mobility and transport properties change. With doping, one can observe impurity states which have a bearing on the electronic and optical properties of semiconductor heterostructures. In particular, the hydrogenic shallow donor state of an electron bound by the Coulombic electrostatic force of the excess charge of the impurity is used to construct semiconductor diodes, transistors and numerous kinds of semiconductor electronic and optoelectronic devices, including lasers [6]. The dielectric constant of the crystal and the screening effect of the free carriers are the important factors which determine the Coulombic force.

Screening occurs due to the free carriers in the semiconductor. The electrostatic interaction is shielded by the carriers which exist between the ionized shallow donor and its bound electron. In this study, we aim to investigate the effect of screening on the electrostatic force of a shallow donor impurity and its binding energy in the GaInAsN heterostructure. Furthermore, we aim to present the relationship of the screening factor and the nitrogen and free carrier densities for GaInAsN alloys.

In GaInAsN, Si is a typical donor and sits at the Ga site [7]. Si being a group IV element gives an electron to the crystal as a shallow donor. The binding energy of this electron will be calculated by solving the screened Coulomb potential. When we consider GaInAsN as a bulk semiconductor, the electron effective mass will be proportional to the inverse of the second derivative of the conduction band dispersion relationship for a parabolic band. The non-parabolic dispersion and strong N dependency of the conduction band of GaInAsN cause unusual behaviour of the electron effective mass and the binding energy for the shallow donor. This unusual behaviour of the electron effective mass and the variation of the mass-dependent binding energy will also be presented in this study.

We assume that the interaction between the electron and the ionized donor can be described by the screened Coulomb potential, which is given by

$$V(r) = -\frac{e^2}{4\pi\varepsilon r}\exp(-\alpha r) \tag{2}$$

where α is the screening parameter which is due to free charge carriers in the semiconductor and e is the carrier charge while ε is the dielectric constant. Because the corresponding Schrödinger equation for this potential does not admit exact analytic solutions for non-zero angular momentum, various numerical and approximate methods [8–15] have been developed in the past. More recently, a new methodology [16,17] has been introduced. The results of our calculations in the framework of [16, 17] show that the binding energy is strongly dependent on the temperature, free carrier density and nitrogen concentration of the III–V–N alloy.

We first present this novel formalism, used in our calculations to obtain bound states of the related screened Coulomb interaction. Then we discuss in detail the corresponding screening parameter α in the present work and the related Bohr radius as a function of nitrogen concentration and present the calculated binding energy versus increasing nitrogen content for the ground state. Finally, we outline the results.