Metastability in Periodically δ-doped GaAs

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Ab initio calculation of periodically δ-doped GaAs was performed in the regime of high donor concentration. We investigated two structural configurations the clustering formation Si_{Ga}-Si_{As} and off-center-Si, DX^- like. Both defects could explain why the donor density in GaAs: Si-δ doping does not increase proportionally to dopand donor density.

I. Introduction

Recently, several works in semiconductors physics have been devoted to understand electron-gas confinement in systems as quantum-wells (2D), quantum-wires (1D) and quantum-dots (OD)[1]. In this work we are interested in a periodic sheet doping in GaAs doped by Si impurities (δ-GaAs:Si)[2]. Experimentally, Si-atoms doped GaAs during the growth by molecular beam epitaxy or metal-organic vapor phase epitaxy in (001) direction. Recently, Liu *et al*[3] have observed δ-GaAs: Si by high resolution transmission electron microscopy in very high dopant concentration, higher than 10^{13} cm^2. In high density doses, when the Si-concentration exceeds $\sim 10^{13}$ cm^{-2}, the carrier density decreases. The reason for this behavior is yet[4] an open question. The aim of this work is devoted to understand this question, using a microscopic model based on an *ab initio* theoretical calculation.

II. Theoretical Procedure

The conventional theoretical approaches for δ-doping systems are done on the basis of the effective-mass theory[5], where to obtain the band structure one solves the one-dimensional Schröedinger equation. In contrast, here, we solved the Schröedinger equation for a real 3D system in the local Density Approximation (LDA). Our calculations were carried out using a cubic super cell with 54 atoms and a tetragonal supercell with 64 atoms[6], with appropriate plane wave expansion up to 12 Ry in kinetic energy and ab initio nonlocal pseudopotential[7]. The total energy and the total charge are calculated with a special set of k-points.

III. Results and Discussion

The substitutional single Si-atom at Ga site, as expected, introduces a a_1-antibonding state in the gap region. We show in Fig. 1a (for cubic supercell) the charge contour plot for this level. If we continue doping with Si-atoms in the Ga-site at the (001) plane, more levels related with the Si-atom appear, and the δ level spreads around the impurity atoms. In Figs. 1b and 1c we plot the charge contour for Si-line doping and Si-sheet doping (Si-δ) respectivelly, at Γ point. From the figure we can see that the wave function spread between the Si atoms (Fig. 1c). In Fig. 2, using the tetragonal supercell, we plotted the charge density for (a) the conduction band minimum, (b) the δ-band and (c) the top of valence band (this results correspond to the case with superlattice period, $d = 45\text{Å}$ and donor dopand, $n = 3.12 \times 10^{14}$ cm^{-2}). For the conduction band and valence band there are large delocalization in charge; however for the δ-band we have a very strong charge confinement in the layer. To understand the decrease of the carrier density for the high donor concentration, we study two possibles cases (i) the clustering formation (Si_{Ga}-Si_{As}), i. e., the Silicon atom occupying also the As site (Si_{Ga}). From our calculation we obtain for this complex configuration (Si_{Ga}- Si_{As}) no electronic levels in the gap, leaving the center electrically inactive. In Fig. 3a we plotted the local charge distribution for the Si_{Ga}-Si_{As} system. There are strong chemical bonds

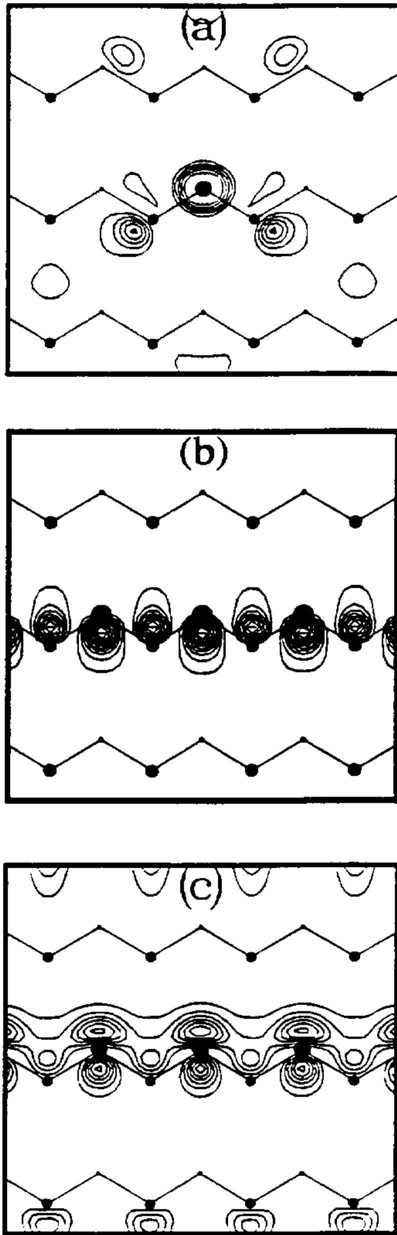

Figure 1: Charge density in (110) plane for (a) high occupied single Si_{Ga} defect; (b) orbital for Si-line doping at Γ point; and (c) the Si-δ-band, the larger full-circles are the positions of the Si atoms.

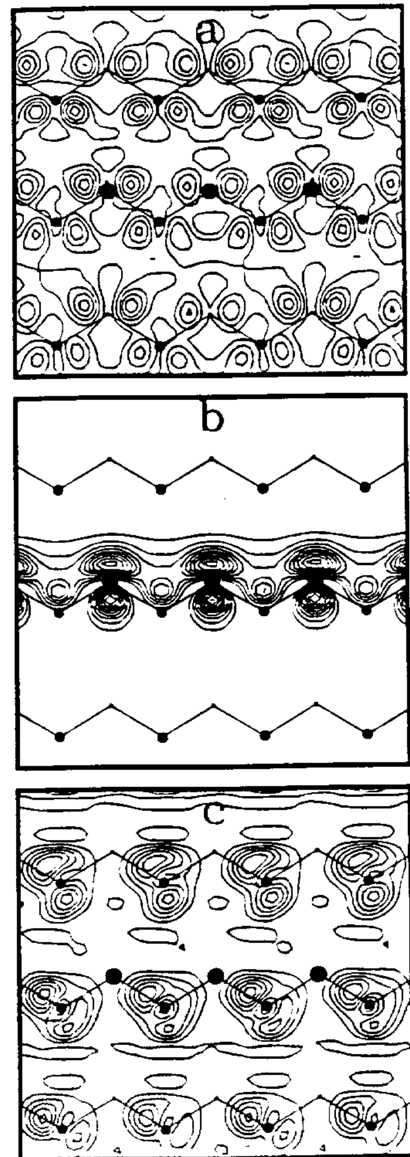

Figure 2: Calculated squared single-particle wave functions at the Γ point in the (a) bottom of the conduction band, (b) Si-δ band, and (c) top of the valence band. The larger full circles represent the Si atoms.

between pair of Silicon atoms. The electronic charge distribution over the two Si atoms is almost the same, which could explain the lack of observation of the vibronic modes, induced by electric dipole moment[4]. In Fig. 3b we show the first unoccupied impurity level for the Si_{Ga}-Si_{As} pair. The squared single-particle wave function is very similar to the single Si-δ (compare with Fig. 2). We also investigated the displacement of the single-Si atom, located initially at the δ-sheet, along the (111) direction towards the interstitial site. In Fig. 4 we present our total energy results versus displacement. The results clearly show a metastable configuration around 1.3Å from the substitutional site. It is known that in the case of Si_{Ga} (single impurity in GaAs), the neutral state (Si) does not present metastable configuration. In the case of Si-δ, we have a plane of Si-atom, and when a isolated Si-atom is displaced, there is a charge transference from δ-sheet region to the Si-atom displaced, i.e. the Si in the metastable configuration works-like DX^-.

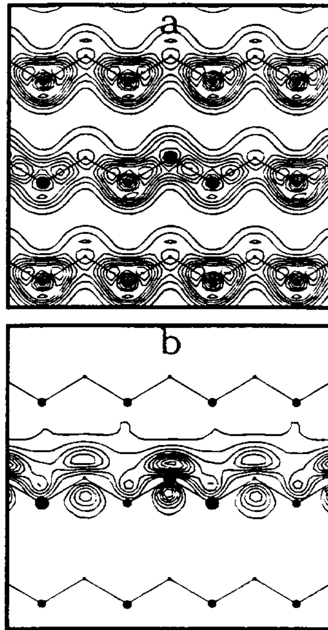

Figure 3: Results for complex configuration Si_{Ga}-Si_{As} (a) total valence band charge density; (b) the squared single-particle wave function for the unoccupied Si-δ level at the Γ point; The larger full-circles are the Si-atoms.

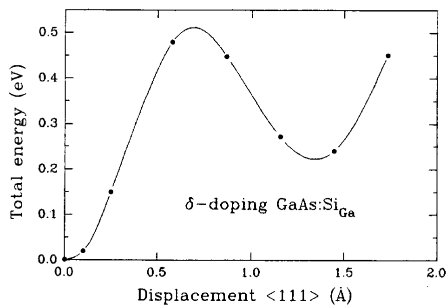

Figure 4: Total energy curve for the displacement of the Si-atom along the (111) direction towards the cation interstitial site in the δ-GaAs systems.

IV. Summary

From our *ab initio* calculation we show that (i) the Si_{Ga}-Si_{As} clustering is an electrically inactive center, and there are a very strong bond between Si-Si atoms and (ii) we obtained from total energy calculation a metastable configuration for Si-atom displaced along the (111) direction, working-like DX^- center. This metastable configuration could explain why the donor density does not increase proportionally to dopant density in GaAs: Si-δ, in the high donor concentration regime. This work was supported by FAPEMIG and FAPESP Brazilian Agencies.

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