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Electronic structure in a Si-doped $(GaP)_1/(InP)_1$ strained-layer superlattice

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Abstract. The electronic structure of lightly and heavily Si-doped (001)-oriented $(GaP)_1/(InP)_1$ strained-layer superlattices (SLSs) is calculated by using a recursion method with a cluster containing about 10 000 atoms. Si-impurity-related states are at $E_c - 0.09$ eV or -0.06 eV in n-type light doping when a Si is substituted for a Ga or an In atom, respectively. In p-type light doping, they are at $E_v + 0.26$ eV. On increase in the Si impurities in the n-type systems, the energy gaps of the density of states decrease from 1.91 to 1.51 eV. A description of the Si influence on electronic occupancy is given. The structural parameters of the stable (001)-oriented $(GaP)_1/(InP)_1$ SLS are determined by the Keating model.

Very recently, the stability and electronic structure of the GaP/InP strained-layer superlattice (SLS) have been studied by Nelson and Batra [1], by Kurimoto and Hamada [2] and by the present authors [3, 4] using different theoretical methods. As is known, the doping of semiconducting materials is a basic step in the fabrication of electronic and optoelectronic devices. Therefore, it is a matter of general interest to study the influence of impurities on the electronic properties of GaP/InP systems. In this paper, we report the impurity-related problems in lightly and heavily silicon-doped [001]-oriented $(GaP)_1/(InP)_1$ SLS using a recursion method for the first time.

The models used in the calculation are schematically drawn in figure 1, in which we use $I_{Si} = 0$ to represent an ideal (001)-oriented $(GaP)_1/(InP)_1$ SLS without impurities. Its stable structural parameters are determined by the Keating [5] method. Because the lattice constant of InP differs by about 7.4% from that of GaP, we find that the deviations of the bond lengths in the stable $(GaP)_1/(InP)_1$ (001) structure are -1.0% (In–P) and 0.8% (Ga–P) of their bulk values. Along the growth direction [001], the distance between In and P or between P and In atomic layers is $b_1 = 1.5475$ Å, and that between Ga and P or between P and Ga atomic layers is $b_2 = 1.3171$ Å. The in-plane lattice constant $a_\perp$ is 5.6086 Å. In the light-doping case, we assume that there is a silicon impurity in the cluster containing about 10 000 atoms, which is taken as an imitation of a real doped $(GaP)_1/(InP)_1$ SLS. The heavily doped model $I_{Si} = \frac{1}{2}$ represents the case where there is a silicon dopant on a gallium site in the unit cell of the $(GaP)_1/(InP)_1$ SLS, and $I_{Si} = \frac{1}{4}$ is the case where one in every four Ga atoms is substituted by Si, shown also in figure 1.

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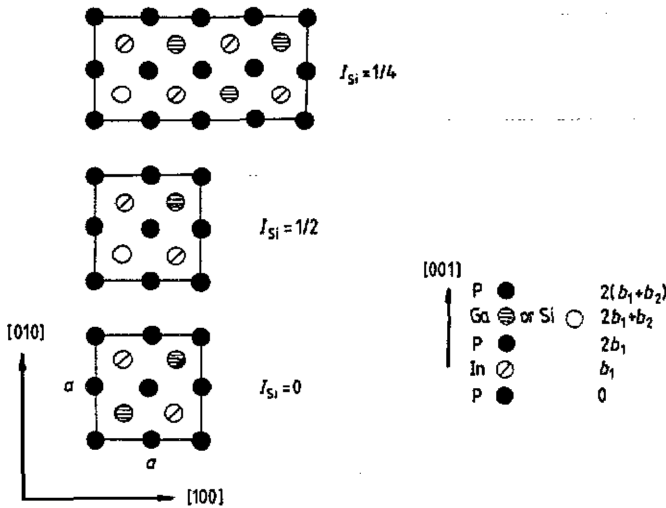

Figure 1. The models used for lightly and heavily silicon-doped (001)-oriented $(GaP)_1/(InP)_1$ SLSs.

A detailed description of a recursion method can be seen in Haydock's [6] work, and the validity of the procedure developed for the semiconductor superlattice is given in earlier papers by the present authors and co-workers [7, 8]. Because this method does not need Bloch's periodic boundary condition, it is especially suitable for discussing the local environment of an imperfect region. In this, we select the recurrence chain length as $L = 30$.

Figure 2 shows the local density of states (LDOS) and the partial density of states (PDOS) of Si dopant on a Ga site in the light-doping model. As references, the LDOS and PDOS of a normal Ga atom before doping are also shown as broken curves. By comparison, we find that the main influence of the Si impurities in n-type light doping is on the conduction band of a (001)-oriented $(GaP)_1/(InP)_1$ SLS, while the valence band is well conserved. The localized shallow state contributed by the s partial wave is at $E_c - 0.09$ eV. A very similar result can be obtained when a Si is substituted for an In atom. In this case, the Si-related impurity level in the lightly doped (001)-oriented $(GaP)_1/(InP)_1$ SLS is located at 0.06 eV below the bottom of the conduction band.

In order to discuss the electronic structure of a p-type, lightly doped (001)-oriented $(GaP)_1/(InP)_1$ SLS, the LDOS of an impurity and its neighbours are shown in figure 3, where n and f, respectively, represent an atom near to or far from the dopant Si. In contrast with the above case, the main influence of Si impurities is on the valence band when a Si is substituted for a P atom at the interface in the (001)-oriented $(GaP)_1/(InP)_1$ SLS. For example, in the density of states there are more peaks in the gaps of the valence bands below the Fermi energy for In(n) and Ga(n) atoms. The acceptor level is at $E_v + 0.26$ eV, which is higher than the experimental result ($E_v + 0.204$ eV) for bulk GaP [9].

The calculated Fermi level for a lightly doped $(GaP)_1/(InP)_1$ SLS is 0.5700 Ryd, which does not change with different types of doping, and the calculated Fermi levels are -0.4982 Ryd and -0.4962 Ryd for n-type, heavily doped models with $I_{Si} = \frac{1}{4}$ and $\frac{1}{2}$, respectively. It is found that the Fermi energy becomes higher on increase in the Si impurities in a GaP/InP strained-monolayer superlattice. For the energy distribution, the valence electron number that an atom possesses can be determined by integrating

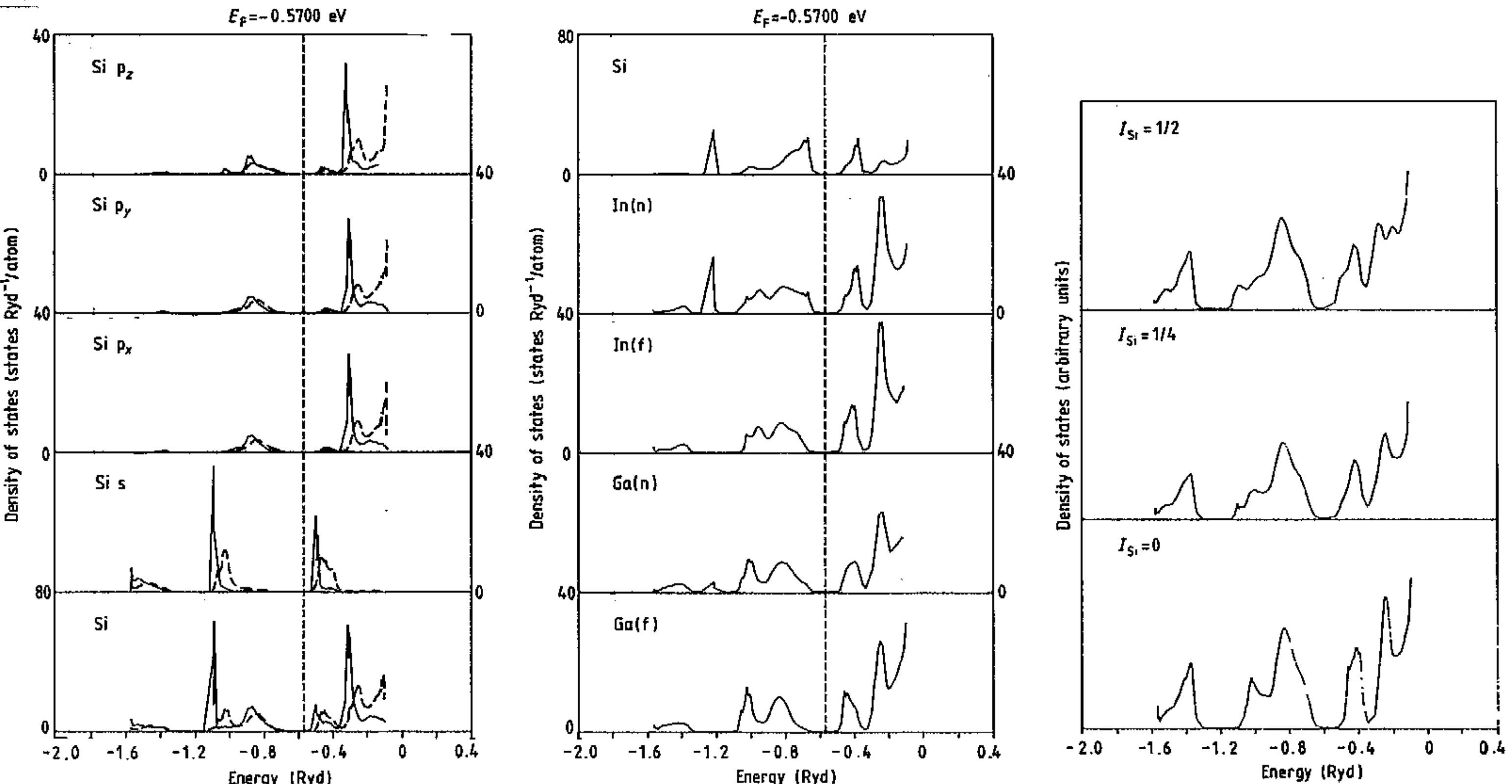

Figure 2. LDOS and PDOS of a Si dopant on a Ga site in the n-type light-doping model: – – –, results for a normal Ga atom in a stable (001)-oriented $(GaP)_1/(InP)_1$ SLS.

Figure 3. LDOSS of an impurity and its neighbouring atoms when a Si dopant is substituted for a P atom in light doping. The notations n and f, respectively, represent the atoms near to or far from the Si impurity.

Figure 4. TDOSS of light- and heavy-doping models given in figure 1.

Table 1. The electronic occupancy and valence (in parentheses) of a Si impurity in lightly and heavily doped (001)-oriented $(GaP)_1/(InP)_1$ SLSs.

Model	Substituting relation	Electronic occupancy (valence)				
		s	p_x	p_y	p_z	Total
$I_{Si} = 0$	Si → Ga	1.415	0.652	0.652	0.626	3.345 (0.655)
$I_{Si} = 0$	Si → In	1.482	0.611	0.611	0.652	3.355 (0.645)
$I_{Si} = 0$	Si → P	1.601	0.978	0.978	0.978	4.535 (−0.535)
$I_{Si} = \frac{1}{4}$	Si → Ga	1.617	0.646	0.646	0.635	3.544 (0.456)
$I_{Si} = \frac{1}{2}$	Si → Ga	1.621	0.654	0.654	0.629	3.559 (0.441)

its LDOS up to the Fermi level [7]. The electronic occupancy of a Si dopant is given in table 1. Because the higher Fermi level of a system will lead to more occupied electrons on an atom, the valence of an impurity decreases from 0.665 to 0.441 in the order $I_{Si} = 0 \rightarrow \frac{1}{4} \rightarrow \frac{1}{2}$ when a Si is substituted for a Ga atom. In all cases, we find that the charge density is highly localized around a positive or negative centre in n- and p-type doped (001)-oriented $(GaP)_1/(InP)_1$ SLSs, respectively.

Finally, we show the total densities of states (TDOSs) of different doping models in figure 4. With increase in the Si impurities in these n-type systems, the occupied band becomes wider and the energy gap becomes narrower because of p-state splitting. The calculated energy gaps are 1.91 eV, 1.77 eV and 1.51 eV for models $I_{Si} = 0$, $\frac{1}{4}$ and $\frac{1}{2}$, respectively.

In conclusion, we have calculated the electronic structures of lightly and heavily doped (001)-oriented $(GaP)_1/(InP)_1$ SLSs. The structural parameters of the stable strained-monolayer superlattice are determined by the Keating method. Our results give a detailed description of the Si dopant influence on the energy gap and electronic occupancy in different assumed models, which is useful to understanding the impurity-related problem in a SLS fabricated from III–V semiconductors.

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