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LETTER TO THE EDITOR

Electronic structure of n–i–p–i Si superlattices

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Abstract. The electronic structure of n–i–p–i Si superlattices is investigated by the tight-binding renormalization method. Strong anisotropy of the hole masses in the in-plane direction is found and strong localization of the electron and hole wave-functions in the growth direction is reported. For the structure studied, a type-II configuration is found with nearly zero overlap between electron and hole wave-functions. The latter property is discussed in view of its possible device applications.

Silicon is certainly the most widely used material in semiconductor devices. The reason for this lies essentially in the well controlled way of introducing both n-type and p-type dopants during the epitaxial growth [1]. This has opened the way to novel and improved device geometries for both fundamental and applied research. One of the simplest yet most important geometries consists in alternated n-type and p-type doped regions in an otherwise homogeneous (intrinsic) structure. The outcome is a doped structure known as an n–i–p–i Si superlattice. The carriers in this device are subject to a sawtooth potential, whose strength and shape are determined by the doping concentrations and extension of the intrinsic region [2, 3]. This results in a type-II confinement, where electrons and holes are confined in spatially separated regions. Such an electronic configuration thus allows very low radiative recombination rates and in-plane high mobilities due to reduced electron–hole scattering mechanisms. Moreover, under certain conditions, dictated by the doping concentrations, n–i–p–i Si superlattices could be very good candidates to investigate fundamental phenomena such as thermodynamically stable excitonic condensate phases [4, 5].

In this letter, we investigate theoretically, with the tight-binding renormalization method [6, 7], the electronic structure of thick n–i–p–i Si superlattices. The atomistic character of the approach allows us a detailed study of all the bulk Si band structure effects on the carrier properties, thus giving more insight into the possibilities of this device for real applications. We first give here a brief presentation of the theoretical apparatus used in these calculations and discuss the range of validity of the approximations made in order to describe the sawtooth potential. We then show the in-plane dispersions of both types of carrier and correlate them with the bulk Si band structure. Finally, the electron and hole wave-functions are presented to show the extreme type-II band configuration that can be attained in a real structure.

We start from a localized basis representation of the bulk silicon crystal Hamiltonian $H(\mathbf{k})$. This is obtained by using a Slater–Köster [8] tight-binding model with an orthogonal

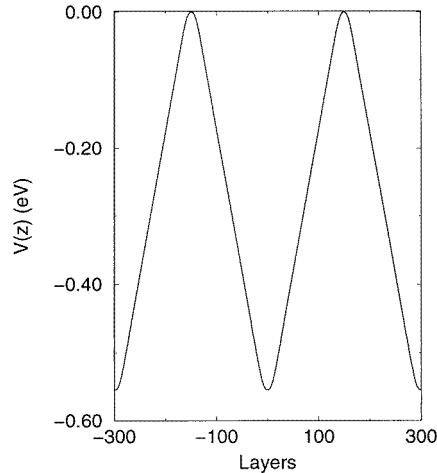


Figure 1. Periodic potential $V(z)$ generated by the n–i–p–i charge distribution. We have assumed $d_n = 40 \text{ \AA}$, $d_i = 160 \text{ \AA}$ and $d_p = 40 \text{ \AA}$. The interlayer separation is $d = 1.35 \text{ \AA}$.

basis built from s and p atomic orbitals. In this approach, the Hamiltonian matrix elements are given in terms of the Slater–Köster parameters. We use a recently obtained [9] accurate parametrization which includes only first- and a few selected second-neighbour interactions. This parametrization includes spin–orbit coupling and gives an accurate description of the energy bands and effective masses near the fundamental gap.

The effect of doping on the electronic structure is considered by superimposing on the (100) silicon superlattice a suitable potential $V(z)$ along the growth direction as shown below. This potential is caused by the positively charged ionized donors in the n-type layers and the negatively charged acceptors in the p-type layers. The n–i–p–i superlattice is thus represented as a multilayer structure, and the dimension of the supercell along the growth direction is given by the spatial period of the doping profile. We focus our attention on the particular structure of the n–i–p–i superlattice potential (figure 1), generated by n-doped, p-doped and intrinsic regions of lengths $d_n = 40 \text{ \AA}$, $d_i = 160 \text{ \AA}$ and $d_p = 40 \text{ \AA}$ respectively; the corresponding supercell contains more than 1200 atoms, and a huge matrix for $H(\mathbf{k})$ results. However, since we restrict ourselves only to first- and second-neighbour interaction, we can handle this matrix by the renormalization procedure. Let us briefly summarize the steps followed in this procedure. We begin by writing the Green function of a given isolated layer: this Green function is represented by a matrix much smaller than the $H(\mathbf{k})$ matrix. Then we add on either side of our initial layer two new layers, and we consider the corresponding interlayer interactions. The presence of the two new layers is taken into account by a self-energy term in the original isolated layer Green function. In this way, the system of three layers is represented by a new single effective layer with a renormalized Green matrix and renormalized interlayer interactions. This procedure can be iterated until all the layers in the supercell are added, and the final renormalized Green matrix is the Green matrix of the whole superlattice. At each step of the iteration, the dimension of the matrices involved does not change, and only inversion of small matrices is required in the numerical calculation. Furthermore, in order to take into account also the second-neighbour interactions we have to consider pairs of layers and not single layers in the procedure. Further details on the renormalization procedure and a discussion of its

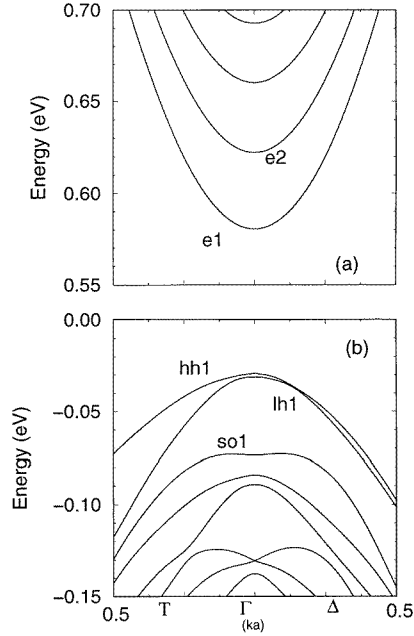


Figure 2. In-plane conduction (a), and valence (b), band structure of the n-i-p-i silicon superlattice, for the parameters chosen in figure 1.

applicability to several semiconductor systems can be found in [6] and [7].

We consider here the impurity band regime only [2], i.e. doping concentrations for which the band merging condition is not reached. For silicon this corresponds to concentrations of no more than $N \approx 2 \times 10^{19} \text{ cm}^{-3}$ dopants [10]. In this regime a simple space-charge model can be used to calculate the potential shape induced by the dopant distributions. We use a doping concentration of $n = 10^{19} \text{ cm}^{-3}$ for donors and $p = 10^{19} \text{ cm}^{-3}$ for acceptors. The resulting sawtooth potential obtained by integration of the Poisson equation is plotted in figure 1. We have assumed that the doping concentration is homogeneous, i.e. the doping concentrations n and p are constant in the respective doping layers. Doping profiles are also assumed to be abrupt and potential fluctuations are neglected. Thus the periodic space charge potential $V(z)$ is parabolic in the ionized impurity regions and linearly varying in the intrinsic layers.

Table 1. In-plane effective masses, around Γ , for the silicon n-i-p-i superlattice, for two different doping concentrations. The masses are given in units of the bare electron mass; doping concentrations are given in cm^{-3} .

	m_{HH}^{Δ}	m_{LH}^{Δ}	m_{HH}^T	m_{LH}^T	m_{e1}
Bulk	0.284	0.245	0.473	0.184	0.200
$N_{A,D} = 10^{18}$	0.322	0.389	0.904	0.226	0.211
$N_{A,D} = 10^{19}$	0.365	0.420	0.905	0.260	0.205

We report in figure 2 the calculated electronic structure for the conduction and valence bands of n-i-p-i superlattices with the parameters defined above. The electronic levels

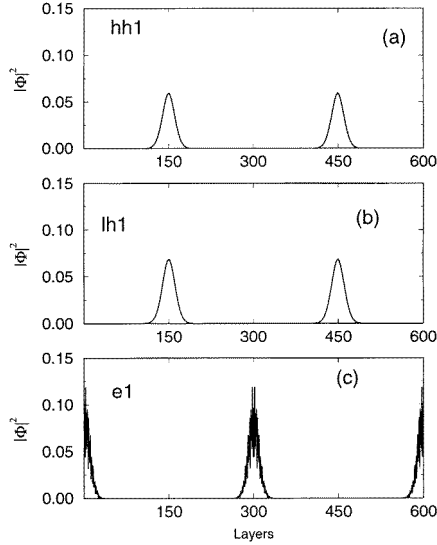


Figure 3. Wave-function amplitude, as a function of the superlattice layer index, for (a) heavy and (b) light holes, and for the lowest conduction electron (c). We can see that electrons are localized in the n layers and holes in the p layers.

in the conduction band approach the spectrum of a harmonic oscillator due to the almost parabolic form of the confining potential. In the valence band the confinement produces strong mass anisotropy. This effect is known as mass inversion: at the Γ point, the HH mass is confined at lower energy with respect to the LH, thus producing the characteristic anticrossing behaviour in the in-plane Brillouin zone. The effect of doping on the mass is analysed in table 1. We report the value of the HH and LH masses calculated at the Γ point along the Δ and T directions of the in-plane Brillouin zone; the electronic bulk value refers to the transversal mass in the Δ valley. Two different doping concentrations are considered. We see that mass anisotropy does not strongly depend on the doping concentration, and that the electronic mass is almost independent of the confinement.

In figure 3 we show the spatial localization, at Γ , of the wavefunctions of the heavy-hole and of the light-hole subbands and of the lowest electron conduction band. We can see that electrons and holes are clearly localized in separated regions. We also detect typical oscillations in the electron wave-function due to the valley interference [7]. We wish to stress that our treatment allows us to overcome the difficulties encountered by effective mass approaches when dealing with intervalley interactions in the evaluation of electronic states. We properly consider, from the beginning, all the equivalent valleys on the same footing through the microscopic interactions in the Hamiltonian $H(\mathbf{k})$. These interactions enter also when the superimposed modulating n-i-p-i periodic potential generates the superlattice. The oscillations of the d.o.s. corresponding to the lowest longitudinal e_1 electronic level at Γ are a fingerprint of the interference between the silicon valleys along (001) and (00 $\bar{1}$) directions. In fact they indicate that this level is indeed a doublet generated by the superlattice potential. With the same procedure we can also evaluate the conduction bands originated from the fourfold degenerate valleys orthogonal to the (001) direction; as well known [11], they lie at higher energies with respect to the electronic longitudinal bands shown in figure 2(a), due to the lower value of the electron transverse mass.

We finally note that, along the same lines shown before, we can handle any shape of superimposed doping profile, thus the method is well suited to study realistic situations in compensated and uncompensated superlattices.

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References

- [1] See, e.g., Gossmann H J and Schubert E F 1993 *Crit. Rev. Solid State Mater. Sci.* **18** 1
- [2] Priester C, Allan G, Lannoo M and Fishman G 1987 *Phys. Rev. B* **35** 2904
- [3] Metzner C, Schrüfer K, Wieser U, Lubber M, Kneissl M and Döhler G H 1995 *Phys. Rev. B* **51** 5106
- [4] Zhu X, Littlewood P B, Hybertsen M S and Rice T M 1995 *Phys. Rev. Lett.* **74** 1633
- [5] Naveh Y and Laikhtman B 1996 *Phys. Rev. Lett.* **77** 900
- [6] Moroni S, Grosso G and Pastori Parravicini G 1989 *Phys. Rev. B* **40** 12328
- [7] Grosso G, Pastori Parravicini G and Piermarocchi C 1996 *Phys. Rev. B* **54** 16393
- [8] Slater J C and Köster G F 1954 *Phys. Rev.* **94** 1498
- [9] Grosso G and Piermarocchi C 1995 *Phys. Rev. B* **51** 16772
- [10] Beregren K F 1973 *Phil. Mag.* **27** 1027
- [11] Stern F and Howard W E 1967 *Phys. Rev.* **163** 816