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ELECTRONIC STRUCTURE OF SILICON SUPERLATTICES†

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Utilizing a new complex-band-structure technique, the electronic structure of model $\text{Si-Si}_{1-x}\text{Ge}_x$ and MOS superlattices have been obtained over a wide range of layer thickness d ($11 \leq d \leq 110$ Å). For $d \geq 44$ Å, it is found that these systems exhibit a direct fundamental band gap. Further calculations of band-edge effective masses and impurity scattering rates suggest the possibility of a band-structure-driven enhancement in electron mobility over bulk silicon.

I. INTRODUCTION

The device-application potential of semiconductor superlattices has attracted a great deal of attention in recent years. In contrast to the mainstream of work on III-V materials, our interest in semiconductor superlattices has focused on the possibilities offered by creating such structures in silicon, still the most technologically important electronic material. Within the confines of silicon materials technology (i.e., excluding III-V and II-VI materials), of course, the number of feasible superlattice structures is greatly limited. With regard to conventional layered structures, the $\text{Si-Si}_{1-x}\text{Ge}_x$ system is the prototype silicon superlattice. In addition to our theoretical work on this system,¹ an increasing experimental interest in fabricating and studying $\text{Si-Si}_{1-x}\text{Ge}_x$ superlattices has also emerged.^{2,3}

Beyond the $\text{Si-Si}_{1-x}\text{Ge}_x$ system, silicon materials technology offers some other novel possibilities for superlattice structures. One is an MOS (metal-oxide-silicon) configuration with a grided metal electrode made up of fine parallel metal lines uniformly spaced on the oxide layer.⁴ In this system, it is envisioned that an extra periodic electron potential could be extended into the silicon by holding alternate metal lines in the grid at different voltages. A third possible silicon superlattice structure could be one consisting of alternately *n*- and *p*-doped silicon layers, the so-called *nipi* superlattice.⁵

In a previous paper,¹ we formulated a realistic, but simplified, tight-binding model of the electronic structure of silicon superlattices that could be applied to all of the above cases. Straight-forward application of the method, however, was limited to systems with layer thickness $d \leq 11 \text{ \AA}$, because the size of the Hamiltonian matrix increases linearly with

d. We have now combined this model with a new complex band-structure technique, based on that developed by Schulman and Chang for III-V systems,⁶ in which the size of the Hamiltonian matrix does not increase with layer thickness. We report here results obtained for silicon superlattices over the complementary range $11 \leq d \leq 110$ Å, using this new technique.

II. SUPERLATTICE BAND STRUCTURE

We consider a [100]-oriented silicon superlattice of alternating A and B layers with an underlying tetrahedral symmetry of the bulk diamond lattice, as illustrated in Fig. 1. We envisage that layer A consists of pure Si atoms, while layer B either contains a second species (Ge in $\text{Si}_{1-x}\text{Ge}_x$) or represents Si atoms where the electron potential has been rigidly raised or lowered by some amount (as in an MOS or *nipi* superlattice). For convenience, we assume equal A and B layer thicknesses and a common bulk bond length, so that the superlattice repeats in the x direction with a period

$$s = 2d = n_s a / 2, \quad (1)$$

where a is the lattice constant of pure silicon. In a minimal basis tight-binding description, consisting of one s and three p atomic orbitals per site, the interatomic matrix elements coupling one atom to another are primarily a function of bond length.⁷ We assume, therefore, that these quantities remain the same in the superlattice as in bulk silicon, for which we have obtained carefully fitted nearest and second-nearest neighbor values.¹ The silicon intra-atomic energies ϵ_s and ϵ_p of layer A, on the other hand, are modified in layer B to some values $\epsilon_s + V_s(s)$ and $\epsilon_p + V_s(p)$. The case

$$V_s = V_s(s) = V_s(p) \quad (2)$$

corresponds to an MOS or *nipi* superlattice in which the electron potential is raised

by an amount V_s in layer B. We designate this as type-I behavior. The opposite limiting case

$$V_s = -V_s^{(s)} = V_s^{(p)}, \quad (3)$$

in which s and p electrons effectively see equal and opposite potentials, turns out to be an appropriate model, within the virtual-crystal approximation, for the alloy component in the $\text{Si-Si}_{1-x}\text{Ge}_x$ superlattice.¹ We designate this as type-II behavior. In this case, we have further derived an approximate empirical relationship between V_s and the Ge concentration x of the form

$$V_s \approx (0.5 \pm 0.1)x \quad (\text{in eV}). \quad (4)$$

In both the type-I and type-II models, therefore, we are left with two free parameters: n_s , representing layer thickness and V_s , representing the physical or chemical strength of the superlattice potential.

A primitive unit cell of the superlattice contains $2n_s$ atoms, so that with four orbitals per site the tight-binding Hamiltonian matrix is $8n_s \times 8n_s$ in size. For $n_s \approx 8$ (corresponding to $d = 11 \text{ \AA}$), the matrix is already 64×64 , and hence the calculation of the electronic structure in this manner becomes intractable for even modestly thick layers. The complex band-structure technique of Schulman and Chang⁶ nicely overcomes this difficulty. In this method, one views the superlattice as being composed of bulk regions in each layer separated by interface planes, as shown in Fig. 1. The number of atomic interface planes is taken such that the atoms in bulk regions I and II are not directly coupled: for second-neighbor interactions two planes at each interface are required. One then capitalizes on the fact that the solutions to Schrödinger's equation are local and hence in the bulk regions must be some linear combination of bulk states including

both extended Bloch states (real $\underline{k}$) and evanescent states (complex $\underline{k}$). For a given energy E , there are in our case 16 possible $\underline{k}$ states in each bulk region. These states, together with two-dimensional Bloch sums of atomic orbitals centered on the interface-plane atoms, can be used to expand the superlattice wavefunction in the form

$$\Psi_{\underline{q}}(\underline{r}, E) = \frac{1}{\sqrt{N_L}} \sum_{\underline{L}} e^{i\underline{q} \cdot \underline{L}} \left[\sum_{\sigma, i} A_{\underline{k}_i}^{\sigma}(\underline{q}) \psi_{\underline{k}_i}^{\sigma}(\underline{r} - \underline{L}, E) + \sum_{j, m} B_m^j(\underline{q}) \phi_{\underline{k}_i, m}^j(\underline{r} - \underline{L}) \right], \quad (5)$$

where $\underline{q} = q_x \underline{x} + k_{\parallel}$ is the superlattice wavevector, $\underline{L} = l s \underline{x}$, with l an integer, $\underline{k}_i = k_x^i \underline{x} + k_{\parallel}$ is a bulk wavevector ($i = 1, 13$), $\psi_{\underline{k}_i}^{\sigma}$ is the corresponding bulk wavefunction for region σ ($\sigma = I, II$ in Fig. 1), and $\phi_{\underline{k}_i, m}^j$ is a two-dimensional Bloch state for interface plane j ($j = S_1, S_2, S_3, S_4$ in Fig. 1) and atomic orbital m ($m = s, p_x, p_y, p_z$). The resulting Hamiltonian matrix is of size 48×48 independent of layer thickness.

The price that must be paid for a fixed Hamiltonian-matrix size is an energy dependent basis, requiring an iteration procedure to calculate the superlattice band structure self-consistently. For given values of n_s and V_s , one fixes the superlattice wavevector $\underline{q}$ and selects a trial energy $E = E_t$ to be used in Eq. (5). For the chosen E_t , the 16 bulk states for each region are obtained. This information is contained in the complex band structure of the bulk material,^{8,9} which need only be generated once for each layer. The 48×48 superlattice Hamiltonian is then set up and diagonalized to obtain the true superlattice energy E_s for the assumed basis. One iterates this procedure until $E_s = E_t$ to some acceptable

tolerance. In our procedure, an accuracy of 10^{-5} eV in energy is achieved with typically 5 iterations in less than 1 minute of cpu time. By varying q , the complete superlattice band structure may be mapped out in this way.

Our technique improves upon that of Schulman and Chang^e in two important ways. First, our tight-binding model includes second-neighbor interactions as well as the first-neighbor interactions considered by them. Second, in constructing the superlattice Hamiltonian from the basis (5), we have included finite-layer corrections to the bulk regions that are necessary to make the method exact and were neglected by Schulman and Chang. These corrections become vanishingly small as $n_s \rightarrow \infty$, but significantly affect fine details of the band structure such as effective masses for the range of n_s considered here.

Calculations of the silicon superlattice band structure have now been carried out for $8 \leq n_s \leq 80$ ($11 \leq d \leq 110$ Å) and $0 \leq V_s \leq 1.0$ eV for both the type-I and type-II cases. In particular, the magnitude of the fundamental band gap, conduction band-edge positions, and band-edge effective masses have been obtained over these parameter ranges. The variation of the band gap magnitude E_g with V_s and n_s is shown in Figs. 2 and 3 for the type-I and type-II superlattices, respectively. In both cases, E_g decreases with increasing V_s and n_s , but the E_g vs. V_s curve quickly saturates for large n_s . Extrapolation of the $n_s = 80$ curves in Figs. 2 and 3 suggests that the band gap will close for $V_s = 1.11$ eV, the bulk silicon band gap, in the limit $n_s \rightarrow \infty$, as required in the type-I case.

The position of the conduction band edge(s) also changes as n_s is increased. In general, the effective six-fold degeneracy of the bulk band edges is lifted in the superlattice, with the [100] and [T00] edges folded back towards the

Brillouin-zone center (Γ point) and lowered in energy relative to the remaining [010], [010], [001], and [001] edges, which remain stationary near the zone-boundary (X point). For $n_s \geq 32$ ($d \geq 44$ Å) the former two edges become degenerate at Γ and a direct band gap results. This situation is illustrated in Fig. 4, where the complete longitudinal [100] and transverse [001] band structure $E(q)$ in the vicinity of the fundamental gap is plotted in a typical case. The energy difference Δ between the X and Γ conduction band edges always remains small (≤ 0.0065 eV ≈ 75 K) and eventually declines back to zero as $n_s \rightarrow \infty$, as shown in Fig. 5.

III. ELECTRON MOBILITY

The possibility of enhanced carrier mobilities in semiconductor superlattices is a subject of fundamental as well as applied interest. It is well known that for III-V superlattices, such as GaAs-Ga_{1-x}Al_xAs, the preparation technique of modulation doping can reduce impurity scattering and raise carrier mobility dramatically at low temperatures.^{10,11} Previously,¹ we suggested that a quite different enhancement mechanism, one driven by reduced transverse conductivity effective masses associated with the superlattice band structure, also appeared to be possible in silicon superlattices. We have now addressed this question more fully in the case of impurity scattering by doing actual transport calculations, based on the above band structure results, to obtain realistic upper limits on electron mobility at low temperature.

In the superlattice, the usual isotropic conductivity effective mass for electrons in bulk silicon,

$$m_c^* = \frac{3}{[(1/m_l^*) + (2/m_t^*)]}, \quad (6)$$

is replaced by separate values perpendicular (i.e., longitudinal) and parallel (i.e., transverse) to the layers. For a single conduction band at Γ , for example, one can write for these latter quantities

$$m_{eL}^* = \beta_L m_L^* \quad (7)$$

and

$$m_{eT}^* = \beta_t m_t^* \quad (8)$$

respectively, where β_L and β_t are enhancement factors of the bulk longitudinal and transverse band masses m_L^* and m_t^* . Typically, $\beta_L \gg 1$, due to the band flattening in the longitudinal direction (see Fig. 4), while $\beta_t \approx 1$. Because of the more favorable averaging of the relatively small transverse band mass m_t^* in the superlattice than the bulk, however, the effective transverse conductivity mass is reduced by a factor

$$\gamma_T = m_{eT}^*/m_c^* = 0.73 \beta_t \quad (9)$$

using the known bulk values of $m_L^* = 0.97m$ and $m_t^* = 0.19m$.¹² Ideally, for ionized impurity scattering the mobility should be enhanced by a factor of $\gamma_T^{-1/2}$ and for acoustic phonon scattering by a factor of $\gamma_T^{-5/2}$, if these are the only energy bands involved in the transport.

Of course, additional considerations enter the picture beyond band-edge effective masses. For example, the bulk conduction-band edges which split away and above in energy in the superlattice will always be accessible at a high enough temperature. In practice, a thermal average of the scattering over a number of bands is necessary to establish the effective carrier mobility. Moreover, a different thermal average, which weights the low energy states more heavily in the superlattice than in the bulk, is usually appropriate. In the bulk, the conduction-band-edge constant-energy surfaces are

ellipsoidal in shape and the density of states for a single band has the familiar form

$$N_c(E) = \frac{1}{\hbar^3 \pi^2} m_t^* (2m_l^*)^{1/2} (E - E_c)^{1/2}, \quad (10)$$

where E_c is the conduction-band edge. In the superlattice, on the other hand, the band flattening mentioned above makes the constant-energy surfaces more nearly cylindrical in shape, so that the corresponding density of states is proportional to that of a two-dimensional electron gas. For a single conduction band at Γ :

$$N_c(E) = \frac{1}{\hbar^2 \pi s} \beta_t m_t^*, \quad (11)$$

which is independent of energy.

In our present studies, we have considered ionized impurity scattering of electrons from the screened Coulomb potential

$$v_I(r) = - \frac{e^2}{\kappa} \frac{e^{-\lambda r}}{r}, \quad (12)$$

where κ is the dielectric constant of the host and λ^{-1} is the Debye length, $\lambda^2 = (4\pi n_I e^2 / \kappa k_B T)$, for uniform doping to a concentration n_I . In bulk silicon, where the density of states (10) is operative for each conduction band edge, the corresponding mobility of nondegenerate electrons is well approximated by the standard form¹³

$$\mu_B = \frac{32\kappa^2}{\sqrt{8}\pi^3 e^3} \frac{(k_B T)^{3/2}}{n_I (m_c^*)^{1/2}} G_B(n_I, T, m_c^*), \quad (13)$$

where G_B is a slowly varying function of n_I , T , and m_c^* . In the superlattice, a similar calculation, but with a constant density of states like (11), yields for the i th conduction band

$$\mu_{SL}^i = \frac{15\pi\kappa^{3/2}}{4\pi\sqrt{2}e^2} \frac{k_B T}{(n_I m_{eT}^*)^{1/2}} G_{SL}(n_I, T, m_{eT}^*), \quad (14)$$

neglecting interband scattering. Here G_{SL} is also a slowly varying function and m_{eT}^* is the appropriate transverse conductivity mass for the i th band. The inverse-square-root effective-mass dependence of the bulk is recovered, as expected, but the temperature and impurity concentration dependencies now reflect the two-dimensional nature of the transport. Summing contributions from all thermally accessible conduction bands, the average electron drift mobility in the superlattice is given by

$$\mu_{SL} = \sum_i n_i \mu_{SL}^i / n_I, \quad (15)$$

where n_i is the electron concentration in the i th band. For $T \leq 300$ K, the conduction bands which must be included in Eq. (15) are shown in Fig. 4.

For a typical silicon superlattice, the calculated relative mobility μ_{SL}/μ_B based on Eqs. (13)-(15) is plotted in Fig. 6 as a function of n_I and T . It can be seen that at low temperatures, where impurity scattering dominates other scattering mechanisms, an enhancement in electron mobility is indeed possible for sufficiently high carrier concentrations. The qualitative variations found with n_I and T are most easily understood by considering the high temperature limits of Eqs. (13) and (14), from which one finds

$$\mu_{SL}/\mu_B = C_1 \left(\frac{n_I}{T} \right)^{1/2} \ln \left(\frac{C_2 T^2}{n_I} \right), \quad (16)$$

where C_1 and C_2 are constants. For a fixed T in the range of interest, this function increases to a maximum for some n_I and then decreases monotonically. Similarly, for a fixed n_I , this function increases to a maximum for some T and then decreases.

The corresponding Hall mobility in the superlattice may be calculated by replacing Eq. (15) by the average

$$\sum_i r_i n_i (\mu_{SL}^i)^2 / \sum_i n_i \mu_{SL}^i. \quad (17)$$

where r_i is a weighting factor reflecting the energy dependence and anisotropy of the scattering. Our calculated relative Hall mobility is plotted in Fig. 7 as a function of n_I and T for the same superlattice parameters as in Fig. 6. Similar magnitudes and trends are clearly seen.

The results presented in Figs. 6 and 7 should be considered as upper limits to what could be expected in real systems. Neglected factors will tend to reduce the actual mobility, in particular, interband scattering at high carrier concentrations and alloy scattering in the case of a Si-Si_{1-x}Ge_x superlattice. At the same time, these results take only partial advantage of the unique reduced-effective-mass enhancement mechanism in silicon superlattices, which should be much more effective in the case of phonon scattering.

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FIGURE CAPTIONS

Fig. 1. Schematic diagram of the $n_s = 8$ superlattice geometry, showing the projection of four planes of atoms onto the $z = 0$ plane. The unhatched circles represent the S_i atoms of layer A, while the hatched circles represent the atoms of layer B. Atoms belonging to the planes $z = -a/4$, $a/4$, and $a/2$ are marked $-$, $+$, and $++$, respectively. The bulk regions I and II and interface layers S_1 , S_2 , S_3 , and S_4 apply to the complex band-structure technique discussed in the text.

Fig. 2. Variation of the fundamental energy band gap with V_s for the type-I superlattice at five layer thicknesses.

Fig. 3. Variation of the fundamental energy band gap with V_s for the type-II superlattice at five layer thicknesses.

Fig. 4. Longitudinal [100] and transverse [001] band structures near the fundamental band gap of a type-II superlattice with $n_s = 64$ and $V_s = 0.2$ eV. The bands shown are those thermally accessible to mobile charge carriers at room temperature.

Fig. 5. Energy difference Δ between the X and Γ -point conduction-band minima vs. V_s for various type-I and type-II superlattices. (Solid lines, type-I and dashed lines, type-II.)

Fig. 6. Variation of the impurity-scattering-limited electron drift mobility with donor concentration n_i at various temperatures for a type-II superlattice, where $n_s = 64$ and $V_s = 0.2$ eV, relative to bulk silicon.

Fig. 7. Variation of the impurity-scattering-limited electron Hall mobility with donor concentration n_i at various temperatures for a type-II superlattice, where $n_s = 64$ and $V_s = 0.2$ eV, relative to bulk silicon.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

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