

First principles calculations of the scattering cross section of substitutional carbon in silicon

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2010 J. Phys.: Conf. Ser. 242 012003

(<http://iopscience.iop.org/1742-6596/242/1/012003>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 143.239.130.12

The article was downloaded on 06/08/2013 at 11:30

Please note that [terms and conditions apply](#).

First principles calculations of the scattering cross section of substitutional carbon in silicon

M.P. Vaughan¹ and S. Fahy^{1,2}

¹Tyndall National Institute, Lee Maltings, Cork, Ireland; ²Department of Physics, University College Cork, Cork, Ireland

E-mail: martin.vaughan@tyndall.ie

Abstract. A method of calculating scattering cross-sections based on first principles electronic structure calculations, previously used for alloy scattering in SiGe is presented and applied to substitutional carbon in silicon. It is found that the intravalley scattering is the predominant scattering mechanism with a contribution to the scattering rate around a factor of 4 greater than intravalley alloy scattering in SiGe.

1. Introduction

The introduction of carbon into SiGe/Ge heterostructures is of technological interest due the dual effects of strain-compensation in the SiGe layers [1] and suppression of the out-diffusion of p-type acceptors, in particular boron [2] and indium [3], during wafer fabrication. Transport measurements of tensile strained $\text{Si}_{1-y}\text{C}_y$ and compressive strained $\text{Si}_{1-x-y}\text{Ge}_x\text{C}_y$ show a degradation of the n and p -type Hall mobility respectively as the carbon concentration is increased [4].

We investigate n -type scattering using a model of alloy scattering based on first principles electronic structure calculations [5]. The model has previously been used to calculate both n -type [5, 6] and p -type mobility [7] in SiGe alloys. The methodology is presented in section 2 and the details of the self-consistent calculations and extracted scattering parameters are given in section 3.

2. Theory

The method of calculating the scattering cross-section described here [5, 6] is based on *ab initio* electronic structure calculations in large supercells. Initially, a supercell is constructed for the unperturbed material, which, due to the periodic boundary conditions, will often have degenerate eigenvalues at points where high symmetry points in the primitive Brillouin zone (BZ) have been folded back into the supercell BZ. Next, a similar supercell is constructed with one of the original (in our case silicon) atoms replaced with a defect (substitutional carbon). This introduces a perturbing potential that causes the degenerate eigenvalues to split. The scattering cross-section is then proportional to the square of these splittings multiplied by the density of states.

The folding back of \mathbf{k} -points occurs when the smaller reciprocal lattice vectors of the supercell map a \mathbf{k} -point within the supercell BZ to another \mathbf{k} -point outside of it but still within the primitive cell BZ. For instance, for a crystal with a face-centred cubic (FCC) primitive cell

such as silicon, a 64-atom supercell may be constructed with simple cubic (SC) symmetry with reciprocal lattice vectors (in Cartesian coordinates) $\mathbf{g}_1 = (2\pi/a)(1/2, 0, 0)$, $\mathbf{g}_2 = (2\pi/a)(0, 1/2, 0)$ and $\mathbf{g}_3 = (2\pi/a)(0, 0, 1/2)$, where a is the lattice constant. Each $\pm\mathbf{g}_i$ maps the Γ point to one of the 6 equivalent points halfway along the Δ line (which we shall denote by $X/2$) of the primitive BZ. Similarly, the vectors $\pm 2\mathbf{g}_i$ map the Γ point to the 6 X points. Since a translation of the supercell BZ by its reciprocal lattice vectors must leave the physics unchanged, these points must be folded back to the Γ point. Thus, when we carry out first principles calculations for the bandstructure of the pure material, we obtain two sets of 6-fold degenerate states at $\mathbf{k} = 0$ (as well as the original Γ states and other states folded back to this point).

Consider the ways in which carriers in the 6 equivalent Δ valleys may scatter due a perturbing potential $\Delta V = H - H_0$, where H and H_0 are the Hamiltonians of the perturbed and unperturbed system respectively. Denoting the unperturbed states by $|\psi_\beta\rangle$, where β labels the band, the scattering matrix in the Born approximation is $\langle\psi_\alpha|\Delta V|\psi_\beta\rangle$. When $\alpha = \beta$, we have intravalley scattering. For intervalley scattering, only two types of scattering are distinguishable by symmetry considerations: g -type, where the scattering is from one valley to its mirror image along the same Cartesian coordinate, and f -type, where the scattering is to a valley in an orthogonal direction. The matrix elements for g -type, f -type and intravalley scattering may be denoted respectively by V_g , V_f and V_Δ . Diagonalisation of the matrix yields one non-degenerate and 2 and 3-fold degenerate eigenvalues ΔE_1 , ΔE_2 and ΔE_3 respectively. Writing the original scattering matrix elements in terms of these, we find [6]

$$V_\Delta = \frac{1}{6} (\Delta E_1 + 2\Delta E_2 + 3\Delta E_3), \quad (1)$$

$$V_g = \frac{1}{6} (\Delta E_1 + 2\Delta E_2 - 3\Delta E_3), \quad (2)$$

$$V_f = \frac{1}{6} (\Delta E_1 - \Delta E_2), \quad (3)$$

In the more general situation, where we go beyond the Born approximation using the results of supercell calculations, the construction of the scattering matrix with the exact states $|\phi_\beta\rangle$, requires that far from the impurity site $|\phi_\beta\rangle \rightarrow |\psi_\beta\rangle$. However, this condition cannot be satisfied for any eigenstate $|\phi_i\rangle$ within the confines of the supercell, so instead we construct $|\phi_\beta\rangle$ from the projection of the unperturbed states onto a subset of the $|\phi_i\rangle$ giving the greatest overlap according to $|\phi_\beta\rangle = \sum_{i=1}^M |\phi_i\rangle \langle\phi_i|\psi_\beta\rangle$. The scattering matrix element is then

$$\langle\psi_\alpha|\Delta V|\phi_\beta\rangle = \langle\psi_\alpha|\Delta V \sum_{i=1}^M |\phi_i\rangle \langle\phi_i|\psi_\beta\rangle = \sum_{i=1}^M \Delta E_i^\alpha \langle\psi_\alpha|\phi_i\rangle \langle\phi_i|\psi_\beta\rangle, \quad (4)$$

where $\Delta E_i^\alpha = E_i - E_\alpha$ is the difference between the perturbed and unperturbed eigenvalues E_i and E_α respectively. Putting $dV_\alpha^{red} = \sum_{i=1}^M \Delta E_i^\alpha |\phi_i\rangle \langle\phi_i|$, Eq. (4) may be written as

$$\langle\psi_\alpha|\Delta V|\phi_\beta\rangle = \langle\psi_\alpha|dV_\alpha^{red}|\psi_\beta\rangle. \quad (5)$$

For electron scattering, this matrix may then be constructed from, say, the n lowest lying conduction band states using Eq. (4), giving an $n \times n$ matrix. To calculate the scattering parameters given in Eqs (1) - (3), we must extract from this $n \times n$ matrix the 6×6 submatrices corresponding to the originally 6-fold degenerate states (for a 64-atom cell, the X and $X/2$ states).

When calculating the scattering due to a localised impurity, large supercells are required to ensure that the perturbed system has converged to the original system far from the impurity site and that the artificially imposed boundary conditions on the supercell are not giving rise

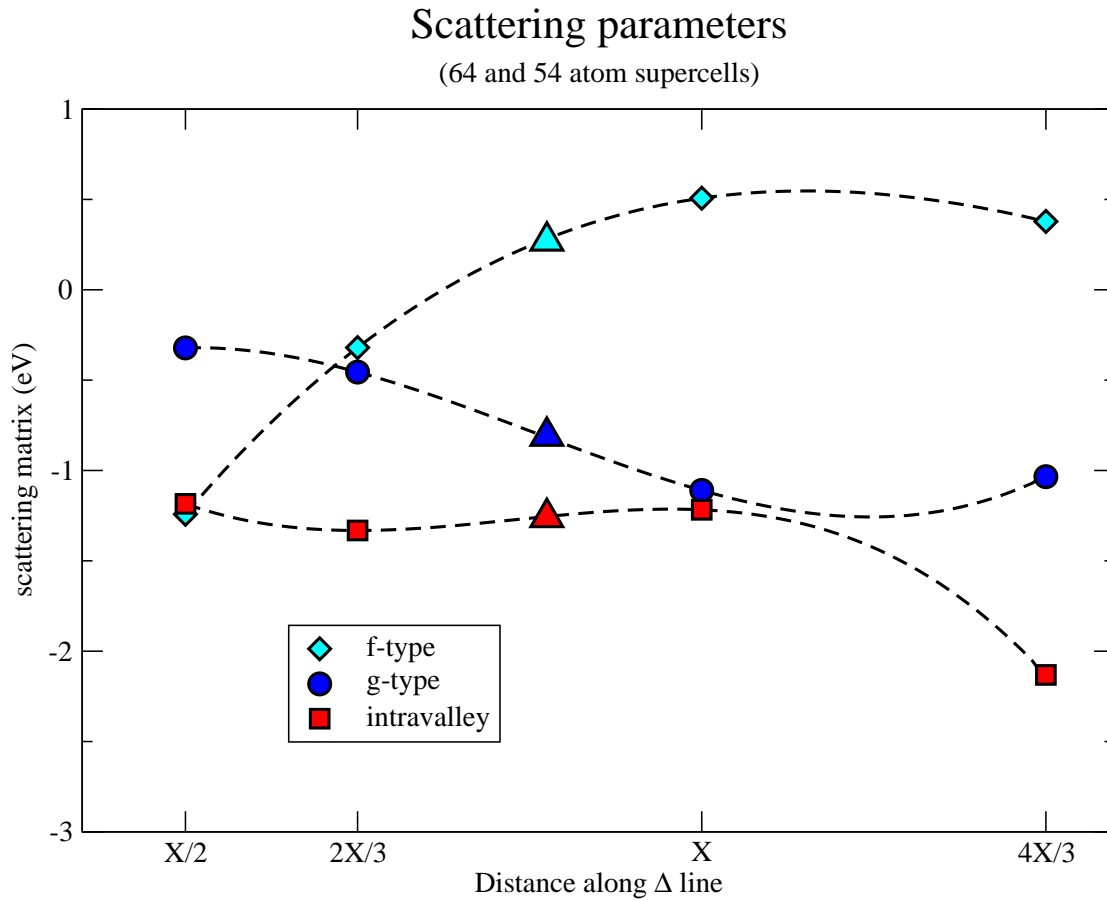


Figure 1. The parameters for intravalley and *f*-type and *g*-type intervalley scattering. The $X/2$ and X points are found from calculations of a 64-atom supercell calculations; the $2X/3$ and $4X/3$ points from a 54-atom supercell. The values at the Δ valley minimum (shown as triangles) are calculated from the polynomial interpolation of these points.

to spurious results. However, unless the impurity forms a bound state, the splitting of the degenerate energy levels will be inversely proportional to the supercell volume. Hence, the scattering parameters must be multiplied by the cell size, N , to give a consistent scattering matrix to be used in mobility calculations [5, 6].

Another important point that needs to be addressed is that the zero of the potential in a supercell is arbitrary. However, Eqs. (1) - (3) show that whilst intervalley scattering depends only on the relative shifts in the eigenvalues, intravalley scattering requires knowledge of the absolute values of the energy shifts. The approach used here is to take the atomic position of the Si atom furthest away from the repeated C atoms at the vertices of the supercell that remains fixed on ionic relaxation. For the 64-atom cubic supercell, this is the atom at the centre of the cell; for the 54 atom FCC supercell, this is the atom at $(4/9)a(1,1,1)$. The differences in the total potential of the pure Si supercell and relaxed Si($N-1$)C(1) structure are then averaged over increasing radii from this atomic centre. The value of the averaged difference Where the derivative with respect to radius is zero is taken as the energy offset to correct the relaxed eigenvalues.

3. Results

3.1. Details of electronic structure calculations

The electronic structure calculations were performed using the ABINIT software [8] using the local density approximation (LDA) for the exchange and correlation functional. Troullier-Martins pseudopotentials [9] were used with an energy cutoff of 40 Hartree, chosen on the basis of convergence tests for 8-atom supercells. The ionic positions were relaxed using modified Broyden-Fletcher-Goldfarb-Shanno (BFGS) minimisation [10–12], which takes into account both the total energy as well as the energy gradients [13].

3.2. Scattering parameters

Calculations for 54 and 64 supercells were carried out and the scattering parameters (multiplied by cell size) extracted. Note that these values need to be squared and multiplied by the density of states to obtain the actual scattering cross-section via Fermi's Golden Rule. The results are plotted in Fig. 1 at different points along the Δ line between the Γ and X points. These points indicate the real variation of the scattering parameters with \mathbf{k} -vector. Interpolating these data at the conduction band minimum in Si gives us the values, $V_f = 0.27$ eV, $V_g = -0.81$ eV and $V_{\Delta} = -1.26$ eV, shown as triangles in the figure.

4. Conclusions

The results indicate that the dominant scattering mechanism will be intravalley scattering, with $|V_{\Delta}|^2$ being about a factor of 6 greater than intravalley alloy scattering in SiGe [5, 6]. In SiGe alloys, each scattering parameter is of comparable magnitude at around 0.5 eV. In the present case, f -type scattering is around 4 times weaker and g -type around 3 times stronger than in SiGe. Thus the application of strain, which would lift the degeneracy of perpendicular valleys, will have little effect on the carrier mobility. It is interesting to compare these present results to the much higher scattering due to substitutional nitrogen in GaInAs alloys [14]. Both C and N have much smaller covalent radii and much larger electronegativities than the atoms they substitute for, so in both case may be thought of as forming 'extreme alloys'. However, the results presented here suggest that extremely high carrier scattering, as observed in GaAs:N, is not necessarily a signature of such alloys.

Acknowledgments

The authors would like to thank Philip Murphy-Armando for many useful discussions. This work was supported by the Science Foundation Ireland.

References

- [1] Jain S, Osten H, Dietrich B and Rücker H 1995 *Semicond. Sci. Tech.* **10** 1289–1302
- [2] Osten H, Rücker H, Liu J and Heinemann B 2001 *Microelectron. Eng.* **56** 209–212
- [3] Tan C, Chor E, Liu J, Lee H, Quek E and Chan L 2003 *Appl. Phys. Lett.* **83** 4169
- [4] Osten H and Gaworzewski P 1997 *J. Appl. Phys.* **82** 4977–4981
- [5] Murphy-Armando F and Fahy S 2006 *Phys. Rev. Lett.* **97** 96606
- [6] Murphy-Armando F and Fahy S 2008 *Phys. Rev. B* **78** 35202
- [7] Joyce S, Murphy-Armando F and Fahy S 2007 *Phys. Rev. B* **75** 155201
- [8] Gonze X, Beuken J, Caracas R, Detraux F, Fuchs M, Rignanese G, Sindic L, Verstraete M, Zerah G, Jollet F *et al.* 2002 *Computational Materials Science* **25** 478–492
- [9] Troullier N and Martins J 1991 *Physical Review B* **43** 1993–2006
- [10] Broyden C 1967 *Math. Comput.* **21** 368–381
- [11] Goldfarb D 1970 *Math. Comput.* **24** 23–26
- [12] Shanno D 1970 *Mathematics of Computation* **24** 647–656
- [13] Schlegel H 1982 *J. Comput. Chem.* **3** 214–218
- [14] Skierbiszewski C, Perlin P, Wisniewski P, Suski T, Walukiewicz W, Shan W, Ager J, Haller E, Geisz J, Friedman D *et al.* 1999 *physica status solidi(b)* **216** 135–139