CORA Cork Open Research Archive
Cartlann Taighde Oscailte Chorcaí

Title	First-principles calculation of P-type alloy scattering in Si1-xGex
Authors	Joyce, S.;Murphy-Armando, Felipe;Fahy, Stephen B.
Publication date	2007-04-01
Original Citation	JOYCE, S., MURPHY-ARMANDO, F. & FAHY, S. 2007. 'First-principles calculation of P-type alloy scattering in Si1-xGex'. Physical Review B, 75, 155201. doi:10.1103/PhysRevB.75.155201
Type of publication	Article (peer-reviewed)
Link to publisher's version	http://link.aps.org/doi/10.1103/PhysRevB.75.155201 - 10.1103/PhysRevB.75.155201
Rights	©2007 The American Physical Society
Download date	2026-11-17 03:37:51
Item downloaded from	https://hdl.handle.net/10468/2669



UCC
University College Cork, Ireland
Coláiste na hOllscoile Corcaigh

First-principles calculation of *p*-type alloy scattering in $Si_{1-x}Ge_x$

S. Joyce,[1] F. Murphy-Armando,[1] and S. Fahy[2]
[1]*Tyndall National Institute, Lee Maltings, Prospect Row, Cork, Ireland*
[2]*Tyndall National Institute and Department of Physics, University College, Cork, Ireland*
(Received 26 July 2006; revised manuscript received 16 February 2007; published 5 April 2007)

The *p*-type carrier scattering rate due to alloy disorder in $Si_{1-x}Ge_x$ alloys is obtained from first principles. The required alloy scattering matrix elements are calculated from the energy splitting of the valence bands, which arise when one average host atom is replaced by a Ge or Si atom in supercells containing up to 128 atoms. Alloy scattering within the valence bands is found to be characterized by a single scattering parameter. The hole mobility is calculated from the scattering rate using the Boltzmann transport equation in the relaxation time approximation. The results are in good agreement with experiments on bulk, unstrained alloys.

DOI: 10.1103/PhysRevB.75.155201 PACS number(s): 71.55.Cn, 72.80.Cw, 72.10.−d, 72.80.Ng

The emergence of SiGe alloys as an important material in the development of strained heterostructure devices has led to an increased interest in understanding and exploiting its physical properties.[1] One of the key properties of concern is the carrier mobility. In particular, increasing the hole mobility through strain engineering has become a significant factor in device design.[2–4]

Calculations relating the band structure and the transport properties of SiGe alloys have so far been performed using empirical methods,[5–8] where the effects of inelastic phonon and elastic alloy scattering have been considered. These calculations have often been frustrated by the lack of good quality experimental data, particularly in the case of the holes. This provides strong motivation for an examination of these properties from first principles.

In this paper, we calculate the scattering matrix elements for *p*-type carriers due to alloy disorder from first principles using a supercell approach. This work is based on our recently developed technique, which was applied to *n*-type carrier[9] scattering in $Si_{1-x}Ge_x$ and can be extended to a wide range of semiconductor alloys. We apply the method to extract the individual matrix elements that characterize the light-hole and heavy-hole scattering within the valence bands from the single-particle wave functions and energies which are obtained from first-principles calculations of random SiGe alloys. The scattering matrix elements are found to be given by a single scattering parameter which depends weakly on the alloy composition and can be approximated by 0.81 eV. We calculate the *p*-type carrier scattering rate, which is then used in the Boltzmann transport equation, in the relaxation time approximation, to give the carrier mobility. We find good agreement with the available mobility measurements in bulk, unstrained alloys.

The scattering rate for carriers in band α due to alloy disorder in the random binary substitutional alloy is given by

$$R_A(\mathbf{k},\alpha) = \frac{2\pi}{\hbar}x(1-x)\frac{a_0^3}{8}\sum_\beta \int \frac{d\mathbf{k}'}{(2\pi)^3}|\langle V_{\alpha\beta}(\mathbf{k},\mathbf{k}')\rangle|^2 \times \delta[E(\mathbf{k},\alpha) - E(\mathbf{k}',\beta)], \quad (1)$$

where x is the Ge content, a_0 is the cubic lattice constant, β labels the bands into which scattering occurs, δ is the Dirac delta function, E are the energy eigenvalues, and the scattering matrix is

$$\langle V_{\alpha\beta}(\mathbf{k},\mathbf{k}')\rangle = \langle V^{\mathrm{Ge}}_{\alpha\beta}(\mathbf{k},\mathbf{k}')\rangle - \langle V^{\mathrm{Si}}_{\alpha\beta}(\mathbf{k},\mathbf{k}')\rangle = N\langle\psi_{\mathbf{k}\alpha}|\Delta V^{\mathrm{Ge}}|\phi_{\mathbf{k}'\beta}\rangle - N\langle\psi_{\mathbf{k}\alpha}|\Delta V^{\mathrm{Si}}|\phi_{\mathbf{k}'\beta}\rangle. \quad (2)$$

In Eq. (2), ΔV^A is the perturbing potential caused by the substitution of one atom in the periodic host by a type-*A* atom, ψ is the Bloch state of the periodic host lattice, and ϕ is the exact eigenstate in the presence of the perturbing potential, with the boundary condition $\phi_{\mathbf{k}\beta}(\vec{r}) = \psi_{\mathbf{k}\beta}(\vec{r})$ when $\vec{r}$ is far from the type-*A* atom. The wave functions ψ and ϕ are normalized in a large region containing N host atoms. We assume that each atom scatters independently of others and that the alloy is a truly random substitutional alloy. The periodic host is represented in the virtual crystal approximation (VCA) in which the ionic potential at each atomic site is taken to be $V_x^{\mathrm{VCA}} = (1-x)V^{\mathrm{Si}} + xV^{\mathrm{Ge}}$. The potential ΔV^A (with A=Si or Ge) is found by placing one *A*-type atom as a substitutional defect in a supercell of $N-1$ VCA host atoms. Structural relaxation around the defect atom and the supercell single-particle electronic states, $|\phi\rangle$, are calculated in density-functional theory (DFT).

To calculate the *p*-type scattering rate, we consider carriers in the light-hole and heavy-hole bands only. The split-off band is neglected as the majority of the carrier population is contained within the upper two valence bands at room temperature. The total scattering rate of band α is therefore obtained by varying β over the four light-hole and heavy-hole states.

Spin-orbit coupling introduces an angular dependence in the scattering matrix between the initial Bloch state wave vector $\mathbf{k}$ in band α and the final state wave vector $\mathbf{k}'$ in band β. Near the valence-band maximum the periodic part of the Bloch functions, $u_{\mathbf{k}\alpha}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}\alpha}(\mathbf{r})$, can be approximated by $j=\frac{3}{2}$ angular momentum eigenstates with quantization of the angular momentum component along $\mathbf{k}$. For the light holes, $\mathbf{k}\cdot\mathbf{J}/(\hbar k) = \pm\frac{1}{2}$, and for the heavy holes, $\mathbf{k}\cdot\mathbf{J}/(\hbar k) = \pm\frac{3}{2}$. Using band indices, α and $\beta = \mathbf{k}\cdot\mathbf{J}/(\hbar k)$, the scattering matrix for an *A*-type defect can now be written as

 ©2007 The American Physical Society

$$\langle V^A_{\alpha\beta}(\mathbf{k},\mathbf{k}')\rangle = dV^A(k,k')\mathcal{D}^{3/2}_{\alpha,\beta}(\theta,0), \tag{3}$$

where $\mathcal{D}^{3/2}_{\alpha,\beta}(\theta,0)$ is the Wigner rotation matrix for angular momentum $j=\frac{3}{2}$ and θ is the angle between $\mathbf{k}$ and $\mathbf{k}'$. Since the defect potential is short ranged compared with $2\pi/k$, $dV^A(k,k')$ is approximately independent of k and k',[10] and

$$dV^A \approx N dE^A \langle \psi_{0\alpha}|\phi_{0\alpha}\rangle, \tag{4}$$

where dE^A is the shift of the valence-band maximum energy caused by the introduction of an A-type substitutional defect in a host supercell of N atoms. $|\psi_0\rangle$ is the Γ-point Bloch state and $|\phi_0\rangle$ is the Γ-point defect state. For a sufficiently large supercell, far from the defect,[10] $\langle \psi_{0\alpha}|\phi_{0\alpha}\rangle \approx 1$.

We account for the warping of the valence bands in Si and Ge by using the approach of Baldereschi and Lipari,[11,12] in which the light-hole and heavy-hole dispersion relations, indexed by "+" and "−," respectively, are given by

$$E_\pm = \frac{\hbar^2\gamma_1}{2m_0}\left\{k^2 \pm \left[\left(\mu - \frac{6}{5}\delta\right)^2 k^4 + \frac{12}{5}\delta(5\mu-\delta)(k_x^2k_y^2 + k_z^2k_y^2 + k_x^2k_z^2)\right]^{1/2}\right\}. \tag{5}$$

The constants γ_1 and μ preserve the spherical symmetry, and δ governs the strength of the cubic terms. To obtain the scattering rate, we combine Eqs. (1), (3), and (5), and expand the scattering rate in terms of δ. The expansion results in an analytic form, which includes the effect of the nonparabolicity of the valence bands on the scattering rate. This derivation is detailed in the Appendix. The total scattering rate from a lighthole or a heavyhole as a function of the nonparabolicity δ is

$$R^A(E_\pm) = \frac{\pi}{\hbar}x(1-x)\frac{a_0^3}{8}|dV|^2[\rho^+(E,\delta) + \rho^-(E,\delta)], \tag{6}$$

where $dV = dV^{\mathrm{Ge}} - dV^{\mathrm{Si}}$. $\rho^\pm(E,\delta)$ is the density of states of the lightholes or heavyholes per unit volume per spin expanded to third order in δ,

$$\rho^\pm(E,\delta) = \frac{m_0^{3/2}\sqrt{E_v - E}}{\sqrt{2}\pi^2\hbar^3(\gamma_1 \pm \gamma_1\mu)^{3/2}}\left\{1 \mp \frac{18\delta^2}{35\mu(\mu\pm1)^2} \mp \frac{36\delta^3(\mp 11\mu^2 + 9\mu \mp 2)}{3575\mu^2(\mu\pm1)^3} + O[\delta^4]\right\}. \tag{7}$$

E_v is the valence-band maximum. In the parabolic approximation, $\delta=0$ and Eq. (7) reduces to the familiar expression. From Eq. (6) it is clear that the scattering rate is dominated by scattering into the heavy-hole states due to their large density of states.

The scattering parameter dV was obtained from total energy calculations using ABINIT,[13] a plane-wave electronic structure code. The exchange and correlation was treated within the local-density approximation and the pseudopotentials[14] of Hartwigsen *et al.* were used for all calculations. Spin-orbit coupling effects were included in the ABINIT computations through the code's existing fully relativistic implementation. Large supercells of up to 128 atoms were used to accurately represent the full structural relaxation of the host alloy in the presence of the Si or Ge substitutional atom. The single-particle wave functions and energy eigenvalues required to evaluate dV were calculated in supercells of sizes $N=16$, 64, and 128. A Monkhorst-Pack[15] grid of $4\times4\times4$ k points was used for the 16-atom cell. This was reduced to $2\times2\times2$ for the larger supercells. All results were converged at a plane-wave cutoff of 25 hartree. The difference between the values of dV obtained from the 16-atom and 64-atom calculations was small. Increasing the cell size to 128 atoms produced a negligible effect.

The evaluation of $\langle\psi_\alpha|\Delta V|\phi_\beta\rangle$ from finite supercell calculations poses a difficulty as the zero of potential is arbitrary in the supercell. To compare the potentials arising from the N host atom calculations with the $N-1$ host atom calculations, the average of the local DFT potential over points in the supercell far from the defect, $V^A_{loc}(r)$, is compared with the same average from the periodic host, $V^{\mathrm{VCA}}_{loc}(r)$. This provides a reference shift in the potentials, given by $\Delta V_{loc}(r) = V^A_{loc}(r) - V^{\mathrm{VCA}}_{loc}(r)$, which fixes the comparison of the potentials and energy eigenvalues obtained from the two supercell calculations. At large r, $\Delta V_{loc}(r)$ tends to a constant value which is subtracted from the valence-band eigenvalue shift dE.

We have calculated the scattering parameters from first principles with the method described above at Ge compositions of $x=0$, 0.25, 0.5, 0.75, and 1. We find that the scattering matrix element, including the effects of spin-obit coupling and interpolated in x, is $dV=0.1662x^2-0.1061x+0.8049$ eV (neglecting spin-orbit effects yields $dV=0.1250x^2-0.0787x+0.6992$ eV). We note that the scattering parameter has only a weak x dependence and, to a first approximation, could be considered as independent of the host lattice. The best constant fit yields a value of 0.8141 eV for dV. Atomic relaxation near the Si or Ge atom in the supercell is found to have an important effect on the scattering; the scattering intensity is almost twice as large as that calculated keeping all atoms in their ideal diamond lattice positions. The effect of the spin-orbit coupling is small and, to a good approximation, corresponds to a constant shift of 0.107 eV in the value of dV for all x calculated without spin-orbit effects.

The effective masses were calculated from the DFT band structure of the VCA crystal. A diamond primitive unit cell was used with a $14\times14\times14$ k-point grid and a plane-wave energy cutoff of 25 hartree. Spin-orbit coupling was included in these calculations, the results of which are presented in Table I. The band parameters were obtained by fitting the light-hole and heavy-hole bands with a second-order polynomial around Γ along the [100] and [111] axes. The values obtained for Si were remarkably well reproduced given the well-known failure of DFT to predict accurately the direct band gap. However, the germanium light-hole masses were underestimated by 50%.

Figure 1 shows the scattering rate from a heavy hole or a light hole into either of the valence bands. This was obtained by evaluating Eq. (6) at the thermal energy, $E=\frac{3}{2}k_BT$, using three different effective mass schemes. The scattering rate into the heavy holes is approximately ten times greater than that into the light holes.

TABLE I. Calculated and experimental properties of Si and Ge used in this work. The experimental values were taken from Ref. 16. $m_{\pm}^{111}=1/\{\gamma_1[1\pm(\mu+\frac{4}{5}\delta)]\}$, $m_{\pm}^{100}=1/\{\gamma_1[1\pm(\mu-\frac{6}{5}\delta)]\}$, and the spherical mass is $m_{\pm}^{*}=1/[\gamma_1(1\pm\mu)]$ (Ref. 17).

		Silicon		Germanium	
Quantity	Units	Expt.	Calc.	Expt.	Calc.
E_{direct}	eV	3.34	2.53	0.90	0.22
Δ_{SO}	eV	0.04	0.05	0.30	0.31
a_0	a.u.	10.26	10.17	10.69	10.55
γ_1		4.27	4.44	13.30	26.71
μ		0.47	0.46	0.77	0.88
δ		0.27	0.26	0.10	0.03
m_{+}^{100}		0.20	0.19	0.05	0.02
m_{-}^{100}		0.28	0.26	0.21	0.20
m_{+}^{111}		0.14	0.14	0.04	0.02
m_{-}^{111}		0.75	0.67	0.50	0.54
m_{+}^{*}		0.16	0.15	0.04	0.02
m_{-}^{*}		0.44	0.42	0.33	0.31

The mobility due to alloy disorder, μ_A, was calculated using the Boltzmann transport equation in the relaxation time approximation. The derivation for the mobility as a function of the non parabolicity is detailed in the Appendix. Within the isotropic, parabolic band approximation, the mobility is given by

$$\mu_A = \frac{32e\hbar^4\sqrt{2\pi}(m_+^{*1/2}+m_-^{*1/2})}{3x(1-x)\sqrt{k_BT}a_0^3|dV|^2(m_+^{*3/2}+m_-^{*3/2})^2}, \tag{8}$$

where $m_{\pm}^{*}$ are the spherical effective masses. This expression suggests that the overall trend in the mobility is largely governed by the heavy-hole effective masses. We have calculated the mobility numerically and verified that an expansion up to third order in δ is sufficient to accurately describe the effects of nonparabolicity on the valence band.

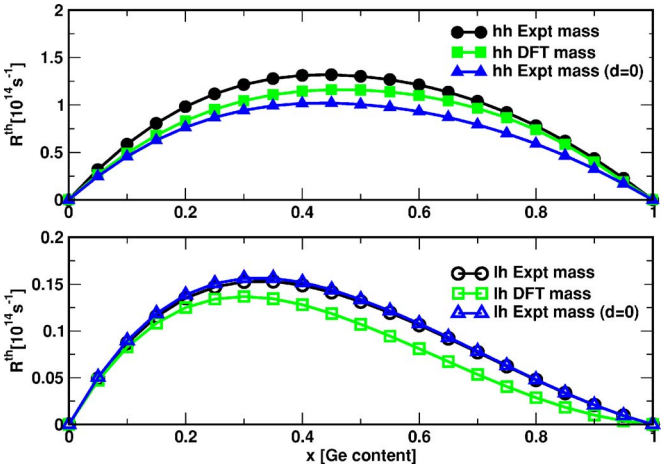


FIG. 1. (Color online) Scattering rate obtained by evaluating Eq. (6) at thermal energy, $E=\frac{3}{2}k_BT$. The top graph illustrates the scattering rate from a light hole or a heavy hole into a heavy-hole state for experimentally determined masses (circles), calculated masses (squares), and experimental masses in the spherical approximation (triangles). The bottom graph shows the scattering rate into light-hole states.

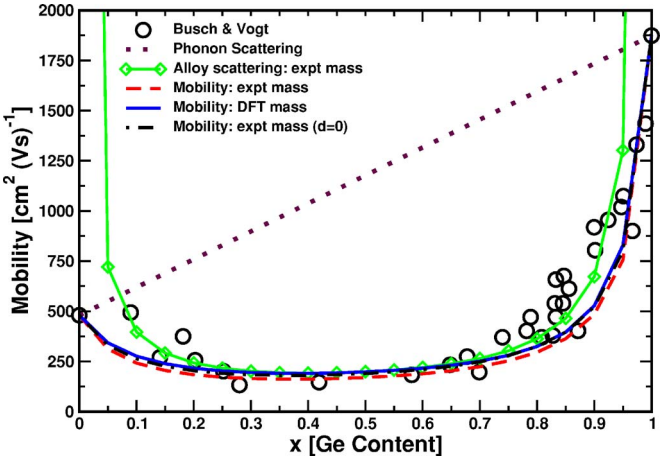


FIG. 2. (Color online) Calculated *p*-type carrier mobility in $Si_{1-x}Ge_x$ at 300 K with experimental effective masses (dashed line) and calculated effective masses (solid line). The linearly interpolated phonon-limited mobility is shown (dotted line), as is the mobility due to alloy disorder alone (diamond). Experimental data are from Ref. 18 (circles). The mobility in the spherical approximation is also shown (dash-dotted line).

In order to compare the calculated mobility with experiment, we must account for the phonon-limited mobility, μ_P. We obtained a reasonable approximation of this from a linear interpolation in x between the experimental values for germanium and silicon.[18] This approach yields values which do not differ significantly from the values calculated using the empirical method of Fischetti and Laux.[5] The final mobility is then approximated by Matthiessen's rule, $\frac{1}{\mu}=\frac{1}{\mu_A}+\frac{1}{\mu_P}$, and the results are shown in Fig. 2 in comparison with experiment.[18]

The experimental values were obtained from polycrystalline samples, and the variation in the data is quite large. However, the overall agreement between the calculated values and experiment is good. We note that the difference between the results calculated with the DFT effective masses and the experimental masses is small, which reflects the dominance of the heavy-hole contribution to the alloy scattering. The effect of valence-band warping on the alloy-limited mobility is larger in the silicon-rich alloy. Comparing μ_A calculated with both the nonparabolic and parabolic effective masses at $x=0.05$ shows a reduction of 13% in the alloy-limited mobility due to the nonparabolicity, while a reduction of 8% is found at $x=0.95$.

In summary, we have calculated *p*-type alloy scattering for SiGe alloys as a function of alloy composition, using *ab initio* supercell methods to numerically represent the alloy scattering problem. We have shown that the scattering can be characterized by a single scattering parameter which is associated with the shift of the valence-band maximum due to the substitution of one Si or Ge atom in the host alloy. We have used this to determine the *p*-type mobility at room temperature and to investigate the effect of band warping on the

mobility. The resulting mobilities are in good agreement with experiment.

ACKNOWLEDGMENTS

This work has been supported by the Science Foundation of Ireland. We thank Jim Greer for stimulating discussions.

APPENDIX

1. Scattering rate

The scattering rate of a carrier with an initial Bloch state wave vector of $\mathbf{k}(E_\alpha,\theta,\phi)$ into a final state of $\mathbf{k}'(E_\beta,\theta',\phi')$ is obtained by combining Eqs. (1), (3), and (5) to give

$$R^A(E_\alpha,\theta,\phi) = \frac{2\pi}{\hbar}x(1-x)\frac{a_0^3}{16(2\pi)^3}|dV|^2 \times\sqrt{E_v-E}\sum_\beta\int_0^{2\pi}\int_0^{\pi}M_\beta^{3/2}(\theta',\phi') \times|\mathcal{D}_{\alpha\beta}^{3/2}(\theta,\phi,\theta',\phi')|^2\sin\phi'\,d\phi'\,d\theta', \tag{A1}$$

where β sums over the four light-hole and heavy-hole states. $\mathcal{D}_{\alpha\beta}^{3/2}(\theta,\phi,\theta',\phi')$ is the Wigner rotation matrix for angular momentum $j=\frac{3}{2}$ in terms of the angular coordinates of $\mathbf{k}$ and $\mathbf{k}'$. E_v is the valence-band maximum and $M_\beta^{3/2}(\theta',\phi')$ is an angle-dependent mass term, obtained by rewriting Eq. (5) for the light-hole and heavy-hole states in spherical coordinates. If we replace the index β with "+" for the two light holes and "−" two for the heavy holes, where each band is spin degenerate, we obtain the following expression:

$$M_\pm^{-1}(\theta',\phi') = \frac{\hbar\gamma_1}{2m_0}\left[1\pm\sqrt{\left(\mu-\frac{6}{5}\delta\right)^2+\frac{12}{5}\delta(5\mu-\delta)\mathcal{F}(\theta',\phi')}\right], \tag{A2}$$

with $\mathcal{F}(\theta',\phi')=\sin^2\phi'(\sin^2\theta'\cos^2\theta'\sin^2\phi'+\cos^2\phi')$. Instead of integrating Eq. (A1) numerically, expanding the integrand in powers of δ yields a compact analytic form where

$$R^A(E_\alpha,\theta,\phi) = \frac{\pi}{2\hbar}x(1-x)\frac{a_0^3}{8}|dV|^2\frac{m_0^{3/2}\sqrt{E_v-E}}{\sqrt{2}\pi^2\hbar^3(\gamma_1\pm\gamma_1\mu)^{3/2}}\Delta^\pm(\delta) \tag{A3}$$

is the scattering rate into a light-hole (+) or a heavy-hole (−) state, with

$$\Delta^\pm = 1\mp\frac{18\delta^2}{35\mu(\mu\pm1)^2}\mp\frac{36\delta^3(\mp11\mu^2+9\mu\mp2)}{3575\mu^2(\mu\pm1)^3}+O[\delta^4]. \tag{A4}$$

The total scattering rate from a light-hole or heavy-hole state is given by

$$R^A(E_\pm,\theta,\phi) = \frac{\pi}{\hbar}x(1-x)\frac{a_0^3}{8}|dV^A|^2[\rho^+(E,\delta)+\rho^-(E,\delta)]. \tag{A5}$$

Here $\rho^\pm(E,\delta)$ is the density of final states in terms of δ such that

$$\rho^\pm(E,\delta) = \frac{m_0^{3/2}\sqrt{E_v-E}}{\sqrt{2}\pi^2\hbar^3(\gamma_1\pm\gamma_1\mu)^{3/2}}\Delta^\pm(\delta). \tag{A6}$$

2. Current density

The current density of carriers in band α of charge e is given by the Boltzmann transport equation, formulated within the relaxation time approximation, as

$$\mathbf{j}^\alpha = -\frac{e}{(2\pi)^3\hbar^2}\int\frac{\mathbf{v}^\alpha\mathbf{F}\cdot\nabla_\mathbf{k}f_0(\mathbf{k})}{R(\mathbf{k})}d\mathbf{k}. \tag{A7}$$

Here $\mathbf{v}(\mathbf{k})$ is the group velocity, f_0 is the distribution function at equilibrium, $1/R(\mathbf{k})$ is the relaxation time, and $\mathbf{F}$ is the applied force. In the case of an applied electric field, $\mathbf{F}=e\mathcal{E}$ for a carrier of charge e. In an isotropic material, an electric field in the λ direction will induce a current in the same direction, giving

$$\mathbf{j}_\lambda^\alpha = -\frac{e^2E_\lambda}{(2\pi)^3\hbar^2}\int\frac{|\mathbf{v}_\lambda^\alpha|^2}{R(\mathbf{k})}\frac{\partial f_0}{\partial E}d\mathbf{k}. \tag{A8}$$

For simplicity, choosing $\lambda=x$ and rewriting Eqs. (5) and (A8) in spherical coordinates give

$$\mathbf{j}_x^\pm = -\frac{e^2E_x}{2(2\pi)^3\hbar^2}\int_{-\infty}^{E_v}\frac{(E_v-E)^{3/2}}{R(E_\pm)}\frac{\partial f_0}{\partial E}dE\int_0^{2\pi}\int_0^{\pi} \times|v_x^\pm(\theta,\phi)|^2M_\pm^{5/2}(\theta,\phi)\sin\phi\,d\theta\,d\phi, \tag{A9}$$

where $\pm$ indicates a light-hole or heavy-hole state, $M_\pm^{5/2}(\theta,\phi)$ is defined in Eq. (A2), and

$$v_x^\pm(\theta,\phi) = 2\frac{\hbar^2\gamma_1}{2m_0}\left[1\pm\frac{\left(\mu-\frac{6}{5}\delta\right)^2+\frac{6}{5}\delta(5\mu-\delta)\mathcal{G}(\theta,\phi)}{\sqrt{\left(\mu-\frac{6}{5}\delta\right)^2+\frac{12}{5}\delta(5\mu-\delta)F(\theta,\phi)}}\right] \tag{A10}$$

is the angle-dependent group velocity, where $\mathcal{G}(\theta,\phi)=\sin^2\theta\sin^2\phi+\cos^2\phi$. Expanding Eq. (A8) to third order in δ and accounting for spin degeneracy give

$$\mathbf{j}_x^\pm = -\frac{4e^2E_xm_0^{1/2}}{3\sqrt{2}\pi^2\hbar^3}\Sigma^\pm(\delta)\int_{-\infty}^{E_v}\frac{(E_v-E)^{3/2}}{R(E_\pm)}\frac{\partial f_0}{\partial E}dE \tag{A11}$$

for the light-hole or heavy-hole current density. The expansion is given by

$$\Sigma^{\pm}(\delta) = 1 \pm \frac{6\delta^2(\pm 5 + 23\mu \mp 99\mu^2 + 109\mu^3 \pm 38\mu^4)}{175\mu(\mu \pm 1)^5} + \frac{12\delta^3(\pm 2 - 53\mu \mp 30\mu^2 + 208\mu^3 \pm 304\mu^4 + 117\mu^5)}{3575\mu^2(\mu \pm 1)^6} + O[\delta^4]. \quad \text{(A12)}$$

3. Mobility

The mobility in a light-hole or a heavy-hole band is

$$\mu^{\pm} = \frac{j^{\pm}}{n_{\pm} e \mathcal{E}}, \quad \text{(A13)}$$

where $n_{\pm}$ is the number of carriers in either band and is given by

$$n_{\pm} = 2\frac{\Delta^{\pm}}{(\gamma_1 \pm \gamma_1\mu)^{3/2}}\left(\frac{m_0 k_B T}{2\pi\hbar^2}\right)^{3/2} e^{(E_v - E_F)/k_B T}. \quad \text{(A14)}$$

$\Delta^{\pm}$ is defined in Eq. (A4), k_B is the Boltzmann constant, T is the temperature, E_F is the Fermi energy, and the factor of 2 accounts for spin degeneracy. By combining Eqs. (A11), (A13), and (A14), and integrating over the energy, we obtain the mobility in a light-hole or heavy-hole band as a function of δ, giving

$$\mu^{\pm} = \frac{32e\sqrt{2\pi}\hbar^4}{3m_0^{5/2}(k_B T)^{1/2}x(1-x)a_0^3|dV|^2} \times \frac{\Sigma^{\pm}(\gamma_1 \pm \gamma_1\mu)}{\Delta^{\pm}\left(\frac{\Delta^+}{(\gamma_1 + \gamma_1\mu)^{3/2}} + \frac{\Delta^-}{(\gamma_1 - \gamma_1\mu)^{3/2}}\right)}. \quad \text{(A15)}$$

The total mobility, limited by alloy scattering, is calculated by summing over the per band contributions with $\mu_A = \frac{n_+}{n}\mu_+ + \frac{n_-}{n}\mu_-$. The total carrier density is $n = n_+ + n_-$. Applying this to Eq. (A15) yields the expression

$$\mu_A = \frac{32e\sqrt{2\pi}\hbar^4}{3m_0^{5/2}(k_B T)^{1/2}x(1-x)a_0^3|dV|^2} \times \left[\frac{\Sigma^+}{(\gamma_1 + \gamma_1\mu)^{1/2}} + \frac{\Sigma^-}{(\gamma_1 - \gamma_1\mu)^{1/2}}\right] \times \frac{1}{\left(\frac{\Delta^+}{(\gamma_1 + \gamma_1\mu)^{3/2}} + \frac{\Delta_m^-}{(\gamma_1 - \gamma_1\mu)^{3/2}}\right)^2} \quad \text{(A16)}$$

for the total mobility.

In the parabolic effective mass approximation, with $\delta = 0$, Eq. (A16) takes a simple form,

$$\mu_{AS} = \frac{32e\sqrt{2\pi}\hbar^4(m_+^{*1/2} + m_-^{*1/2})}{(k_B T)^{1/2}x(1-x)a_0^3|dV|^2(m_+^{*3/2} + m_-^{*3/2})^2}, \quad \text{(A17)}$$

where m^* are the parabolic effective masses.

[1] D. Paul, Semicond. Sci. Technol. **19**, R75 (2004).
[2] D. Nayak, J. Woo, J. Park, K. Wang, and K. MacWilliams, Appl. Phys. Lett. **62**, 2853 (1993).
[3] D. Nayak and S. Chun, Appl. Phys. Lett. **64**, 2514 (1994).
[4] K. Ismail, J. Chu, and B. Meyerson, Appl. Phys. Lett. **64**, 3124 (1994).
[5] M. Fischetti and S. Laux, J. Appl. Phys. **80**, 2234 (1996).
[6] S. Krishnamurthy, A. Sher, and A.-B. Chen, Appl. Phys. Lett. **47**, 160 (1985).
[7] S. Krishnamurthy, A. Sher, and A.-B. Chen, Phys. Rev. B **33**, 1026 (1986).
[8] T. Manku and A. Nathan, IEEE Trans. Electron Devices **39**, 2082 (1992).
[9] F. Murphy-Armando and S. Fahy, Phys. Rev. Lett. **97**, 096606 (2006).
[10] S. Fahy and E. O'Reilly, Appl. Phys. Lett. **83**, 3731 (2003).
[11] A. Baldereschi and N. Lipari, Phys. Rev. B **8**, 2697 (1973).
[12] A. Baldereschi and N. Lipari, Phys. Rev. B **9**, 1525 (1974).
[13] The ABINIT code is a common project of the Université Catholique de Louvain, Corning Incorporated, and other contributors (http://www.abinit.org).
[14] C. Hartwigsen, S. Goedecker, and J. Hutter, Phys. Rev. B **58**, 3641 (1998).
[15] H. Monkhorst and J. Pack, Phys. Rev. B **13**, 5188 (1976).
[16] O. Madelung, *Semiconductors: Data Handbook*, 3rd ed. (Springer, New York, 2004).
[17] N. Binggeli and A. Baldereschi, Phys. Rev. B **43**, 14734 (1991).
[18] G. Busch and O. Vogt, Helv. Phys. Acta **33**, 437 (1960).