

Effect of strain on the deformation potentials in Ge-like SiGe

F. Murphy-Armando^{1,*} and S. Fahy¹

¹*Tyndall National Institute, University College Cork, Ireland*

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We calculate the effects of strain on the intra- and intervalley electronphonon matrix elements of Ge-like SiGe. Second-order terms of the strain are added to the intravalley deformation potentials and calculated by the frozen-phonon approach using first-principles electronic structure methods. The intervalley matrix elements of the strained crystal are calculated using density functional perturbation theory. The effects of the change in these elements with strain prove to be negligible compared to the boost brought about by the loss of intervalley scattering.

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I. INTRODUCTION

When strain is applied to SiGe alloys, the degeneracy of the 6-fold Δ (in Si like alloys) and 4-fold L (in Ge-like alloys) valleys is lifted, eliminating major sources of intervalley scattering (both from alloy and phonon scattering). Furthermore, it opens the possibility of enhancing the mobility by limiting transport through a reduced effective mass direction. In a previous work [1], we found the strength of intervalley scattering to be more influential to the mobility than previously considered by phenomenological models [2]. In this study, we use methods similar to those in Ref. [3] to study the effects of strain on the electron-phonon matrix elements, to determine whether deformation potential theory needs a revision or not, and to calculate strained systems. The contribution of strain to the intravalley deformation potentials is considered by adding a second-order term to the shift in the energy due to strain. The parameters of this second term are then calculated from electronic structure theory. Likewise, the change to the intervalley matrix elements are calculated directly from density functional perturbation theory calculations in the strained system.

II. THEORY

We will consider the effects of strain on the electronic interaction with both acoustic, intervalley phonons and optical phonons. The interaction with acoustic phonons is described by the deformation potential approach of Refs. [3] and [4], plus a second-order term due to the strain.

The effects of strain on the deformation potentials can be obtained by perturbation theory from the second term in the following expansion of the conduction-band energy shift

in terms of the strain,

$$\delta E = \sum_{i=1}^6 \left(\frac{\partial E}{\partial e_i} e_i + \sum_{j=1}^6 \frac{\partial^2 E}{\partial e_i \partial e_j} e_i e_j \right), \quad (1)$$

where the strain components are defined as

$$\begin{aligned} e_1 &= \epsilon_{xx}; & e_2 &= \epsilon_{yy}; & e_3 &= \epsilon_{zz}; \\ e_4 &= \epsilon_{xy} + \epsilon_{yx}; & e_5 &= \epsilon_{zy} + \epsilon_{yz}; & e_6 &= \epsilon_{zx} + \epsilon_{xz}. \end{aligned} \quad (2)$$

The first term contains the deformation potentials. There are, in principle 6 deformation potentials and 21 elements in the second-order term. However, symmetry arguments reduce this number to the number of irreducible representations compatible with the particular bands under consideration. For the Δ and L valleys of SiGe, these numbers are reduced to two deformation potentials, and six second-order terms. Thus, the energy shift for the L valley in terms of strain can be expressed in terms of

$$\begin{aligned} \delta E_L &= \Xi_1(e_1 + e_2 + e_3) + \Xi_2(e_4 k_x k_y + e_5 k_z k_y + e_6 k_x k_z) \\ &+ A(e_1^2 + e_2^2 + e_3^2) \\ &+ B(e_1 e_2 + e_1 e_3 + e_2 e_3) \\ &+ C(e_1 e_4 k_x k_y + e_2 e_5 k_z k_y + e_3 e_6 k_x k_z + e_1 e_6 k_x k_z + e_2 e_4 k_x k_y + e_3 e_5 k_z k_y) \\ &+ D(e_1 e_5 k_z k_y + e_2 e_6 k_x k_z + e_3 e_4 k_x k_y) \\ &+ E(e_4^2 + e_5^2 + e_6^2) \\ &+ F(e_4 e_6 k_y k_z + e_4 e_5 k_x k_z + e_5 e_6 k_x k_y) \end{aligned} \quad (3)$$

where $\Xi_1 = \Xi_d + 1/3\Xi_u$ and $\Xi_2 = 1/3\Xi_u$, are the deformation potentials; A, B, C, D, E , and F are the second-order deformation potentials; and k_x, k_y , and k_z are the Cartesian components of the unitary vector in the direction of the L conduction valley in question. These are all calculated using the DFT frozen phonon method described in Ref. [3], with the addition of 0.5% and 1% strains along the $\langle 100 \rangle$, $\langle 110 \rangle$, $\langle 111 \rangle$, and equivalent directions. The results are shown in Table I.

The case of the intervalley deformation potentials is rather simpler since the matrix elements are momentum independent. The matrix elements are calculated as in Ref. [3] using density functional perturbation theory and applying a strain of 1% along the required direction. We have only calculated the parameter values for Ge since we expect them to change little with Si composition. Table II shows the percentage of change for the matrix elements per percent strain.

III. FROZEN PHONON

In the deformation potential approach, the effect of a long-wavelength phonon on the electronic bands is assumed to be equivalent to a slowly varying potential, given by

Deformation potential	Value	Units
Ξ_1	-0.61^a	eV
Ξ_2	5.66^a	eV
A	17	eV
B	-11.7	eV
C	3	eV
D	-13	eV
E	2	eV
F	-3	eV

^aCalculated in Ref. [3].

TABLE I: Second-order deformation potentials calculated for the L valley of Ge.

$\Delta H_{kk'}$	$\langle 100 \rangle$	$\langle 111 \rangle$
$\Delta g[100]$	-1%	0.2%
$\Delta g[010]$	0.1%	0.2%
Δf	-0.5%	-1.3%
$LL[100]$	24%	19%
$LL[010]$	-12%	19%
opL	0.5%	3%
$\Delta L[100]$	2%	-6%
$\Delta L[010]$	-1%	-6%

TABLE II: Percentage change in the intervalley electron-phonon matrix element due to 1% positive strain in the $\langle 100 \rangle$ and $\langle 111 \rangle$ directions. The numbers in brackets indicate the general direction of the phonon momentum, which becomes inequivalent under strain.

the displacements of the atoms from their equilibrium positions due to the presence of a phonon of momentum \mathbf{q} ,

$$\delta \mathbf{R}(\mathbf{r}) = \delta \mathbf{R}_0 \sin(\mathbf{q} \cdot \mathbf{r} - \omega t). \quad (4)$$

The strain produced by this displacement is given by

$$\epsilon_{ij}(\mathbf{r}) = \frac{1}{2} \left(\frac{\partial \delta R_i}{\partial r_j} + \frac{\partial \delta R_j}{\partial r_i} \right), \quad (5)$$

where δR_i is the i^{th} Cartesian component of the atomic displacement vector at \mathbf{r} . More explicitly, eq. (5) becomes

$$\epsilon_{ij}(\mathbf{r}) = \frac{1}{2} (q_i \delta R_{0j} + q_j \delta R_{0i}) \cos(\mathbf{q} \cdot \mathbf{r} - \omega t). \quad (6)$$

Inserting eq. (6) in eq. (3), the matrix element of $\langle \mathbf{k} | \delta E_L | \mathbf{k}' \rangle$ with electron states $|\mathbf{k}\rangle$ and $|\mathbf{k}'\rangle$ at $t = 0$ will contain terms with

$$\langle \mathbf{k} | \cos(\mathbf{q} \cdot \mathbf{r}) | \mathbf{k}' \rangle = \frac{\delta_{\mathbf{k}-\mathbf{k}',\mathbf{q}} + \delta_{\mathbf{k}'-\mathbf{k},\mathbf{q}}}{2} \quad (7)$$

and

$$\langle \mathbf{k} | \cos^2(\mathbf{q} \cdot \mathbf{r}) | \mathbf{k}' \rangle = \frac{\delta_{\mathbf{k}-\mathbf{k}',2\mathbf{q}} + \delta_{\mathbf{k}'-\mathbf{k},2\mathbf{q}}}{4} + \frac{\delta_{\mathbf{k}',\mathbf{k}}}{2}. \quad (8)$$

If we were to calculate, for example, the effect on the bands of a longitudinal phonon in the x direction, which introduces a strain $e_1 = \delta R_0 q \cos(qx)$, the matrix element of the shift of band E_L between states $|\mathbf{k}\rangle$ and $|\mathbf{k} + \mathbf{q}\rangle$ becomes

$$\langle \mathbf{k} | \delta E_{111} | \mathbf{k} + \mathbf{q} \rangle = \frac{1}{2} \Xi_1 \delta R_0 q, \quad (9)$$

yielding as a result the deformation potential Ξ_1 . In a similar manner, by introducing a uniform strain e'_1 in the x direction, the total strain becomes

$$e_1 = \delta R_0 q \cos(qx) + e'_1, \quad (10)$$

and hence, the matrix element becomes

$$\langle \mathbf{k} | \delta E_{111} | \mathbf{k} + \mathbf{q} \rangle = \left(\frac{1}{2} \Xi_1 + A e'_1 \right) \delta R_0 q, \quad (11)$$

We notice in eq. (11) that the effect of uniform strain on the crystal is to introduce a change in the deformation potential proportional to that strain.

To see what effects do these changes in the deformation potentials have on the mobility, we must evaluate the expression for the inverse of the relaxation time, given by

$$\frac{1}{\tau_{\mathbf{k}}} = \int \frac{d\mathbf{k}'}{(2\pi)^3} R_{\mathbf{k},\mathbf{k}'} \left(1 - \frac{v_{\mathbf{k}'}}{v_{\mathbf{k}}} \right), \quad (12)$$

where $v_{\mathbf{k}}$ is the group velocity, and the scattering rate is, summing over the three phonon branches η ,

$$R_{\mathbf{k},\mathbf{k}'} = \sum_{\eta} \frac{2\pi}{\hbar} \langle \mathbf{k} | \delta E_L^{\eta} | \mathbf{k}' \rangle \delta(E_{\mathbf{k}'} - E_{\mathbf{k}}) \quad (13)$$

Eq. (12) has been evaluated numerically, in the same fashion as eqs. (23), (24), (25), and (26) of Ref. [2], with the exception of the interpolation of the matrix element in \mathbf{q} , performed in Ref. [2] as in Ref. [4], while we have calculated it exactly. The resulting change in the inverse relaxation time of the strained crystal with respect to the unstrained case is shown in Table III, separated into the contributions of the different phonon branches, and transport direction relative to the direction of the strain. Since the results are similar for strain in the $\langle 111 \rangle$ and $\langle 100 \rangle$ directions, we only show results for the former.

TABLE III: Percentage change in the intravalley electron–phonon relaxation time due to 1% positive strain in the $\langle 111 \rangle$ direction. The transport direction is relative to the direction of strain, l along $\langle 111 \rangle$ and t transverse to it. The phonon longitudinal and two transverse branches are labeled L, T1, and T2, respectively. “Total” refers to the relaxation time calculated by summing over all phonon branches.

Transport Direction	L	T1	T2	Total
l	0.24%	1.28%	−1.74%	0.21%
t, \parallel	−4%	0.66%	−0.5%	−2.5%
t, \perp	−1.5%	1.1%	−1.1%	−1.1%

IV. DISCUSSION

As we can gather from Table III, strain has a relatively mild effect on the overall relaxation time due to the scattering of electrons by acoustic phonons, although the individual components of the matrix elements can be rather large (Table I). What occurs is that the integration over the momentum cancels out most of the contributions of opposite sign. This might not be the case for confined structures, where the integration on momentum is restricted.

Some of the changes due to strain on the intervalley scattering parameters are also quite considerable, especially bearing in mind that the change of its contribution to the mobility would be twice the values shown in Table II since the square of this matrix element enters the scattering rate. In particular, the contribution of the L to L intervalley matrix element would increase by 40%. However, this contribution is negligible next to that of the intravalley phonon scattering [3], and its effect will not be noticeable in the mobility. For the Δ valley, while the contribution of intervalley scattering is comparable to the intravalley scattering, the change produced by strain on the matrix elements is minuscule.

V. CONCLUSIONS

Using first-principles electronic structure theory methods, we have calculated the effects of strain on the intra- and intervalley electron-phonon matrix elements. We find that while the change in individual matrix elements due to strain can be large, the overall integrated quantities cancel these out, having little influence on the overall mobility.

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- * Electronic address: Philip.murphy@tyndall.ie
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