Possibility of increased mobility in Ge-Sn alloy system

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We study the effect of strain and alloying with Sn on the band structure of Ge using a combination of *ab initio* and empirical pseudopotential techniques. The properties calculated are used to determine the phonon and alloy scattering contributions to the mobility. Using the dependence of the mobility on strain and alloying Sn, we propose a combination of alloying and biaxial strain to enhance both the electron and hole mobilities of Ge.

I. INTRODUCTION

For more than a decade, silicon microfabrication technology has focused on fabricating smaller and faster integrated circuits (ICs), and this has resulted in an increase of information processing power by almost a factor of 2 per year. However, at the current juncture, the heat generated during the switching of transistors in ICs is beginning to limit the switching rate that can be achieved. Therefore it is attractive to consider higher mobility semiconductors. As a result, there have been several experimental attempts to grow higher mobility semiconductors such as strained GaAs (Ref. 1) and strained Ge.[2,3] Here we extend this approach by suggesting a combination of alloying and straining for Ge.

The mobility of semiconductors is principally determined by their electronic structure and scattering mechanisms. Experimental mobility measurements for Ge and other diamond and zinc-blende semiconductors show a large temperature dependence of the mobility[4] at room temperature indicating that phonon scattering dominates the resistivity of electrons at this temperature. Since both the electronic structure and the electron-phonon couplings in these semiconductors are well understood, a number of calculations of the electron and hole mobilities can be found in the literature.[5] These electronic structure properties can also be calculated from first principles. Recently several calculations of the mobilities of a number of semiconductors such as Ge, Si, GaAs, and SiGe alloys etc. from first principles have been reasonably successful.[6]

A comprehensive study of the temperature and strain dependence of mobility in Ge and Si-Ge alloys was carried out by Fischetti and Laux.[6] In general, even though the effective masses and the position of the valence band edges give an approximate idea of the hole mobility, the actual calculation is complicated by the near degeneracy and warped structure for the valence bands. Therefore these authors solve[6] the Boltzmann transport equations for the holes in the valence band accounting for both interband and intraband phonon scattering to obtain an estimate for the hole mobility as a function of strain. However, as we shall see later, for the case relevant to our current discussion this degeneracy is lifted by strain. So an estimate of trends in mobilities can be made based on trends in density of states and transport effective masses.

There are several ambiguities that arise in theoretical and experimental analysis of the electronic structure of Ge. Therefore, in the following sections we examine some of the above calculations using several theoretical approaches such as empirical pseudopotentials,[7] density functional theory, and the GW method,[8] and explore the possibility of obtaining a high electron and hole mobility semiconductor in a Ge-Sn system.

II. MOBILITY IN DIAMOND AND ZINC-BLENDE SEMICONDUCTORS

The mobility of an electron or a hole in a semiconductor at room temperature is determined by its effective mass m^* and the electron-phonon scattering time τ by the relation

$$\mu = \frac{e\tau}{m^*}. \tag{1}$$

The scattering time τ for phonon scattering is related to the phonon scattering potential, W, and the density of states of electrons, $N(E)$, by Fermi's golden rule.

$$\frac{1}{\tau} \propto |W|^2 N(E). \tag{2}$$

The density of states of electrons for a simple band at Γ is given by

$$N(E) = \frac{1}{2\pi^2}\left(\frac{2m^*_{DOS}}{\hbar^2}\right)^{3/2} E^{1/2}, \tag{3}$$

$$m^*_{DOS} = (m_1 m_2 m_3)^{1/3}, \tag{4}$$

while the phonon scattering potential for an almost classical distribution of phonons scales as $\sqrt{kT}$.

So if we ignore the energy dependence of the scattering matrix elements, the carrier mobility has a scaling given by[9]

$$\mu \propto T^{-3/2} m^{*-5/2}. \tag{5}$$

However, in the above scaling relations we notice that the density of states factor in the scattering contributes $m^{*-3/2}$ while the transport effective mass appears as m^{*-1}. Since these are not directly related in the nonparabolic anisotropic valence bands in Ge, we can define a thermally averaged density of states effective mass by

TABLE I. Semiconductor mobilities.

Semiconductor	μ_e [cm^2/(Vs)]	μ_h [cm^2/(Vs)]
Diamond	1800	1200
Si	1350	480
Si (strained)[a]	2300	3600
Si$_{0.8}$Ge$_{0.2}$[a]	500	250
Si$_{0.8}$Ge$_{0.2}$ (w/o alloy sc)[a]	1000	1000
Ge	3600	1800
GaAs	8000	300

[a]Data from Ref. 6.

$$\left(\frac{m^*}{m_0}\right)_{DOS}^{3/2} = \frac{\int f(E)N(E)dE}{\int f(E)N_0(E)dE},\tag{6}$$

where we have used the free electron density of states for $N_0(E)$, and $f(E)$ is the Boltzmann distribution function defined by $f(E) = \exp[-E/(k_B T)]$.

The transport effective mass is anisotropic in general and is defined through the thermal average of the band curvature as below:

$$\left(\frac{1}{m}\right)_{ab} = \frac{\int N(E)f(E)\frac{\partial^2 E}{\partial k_a \partial k_b}dE}{\int N(E)f(E)dE}.\tag{7}$$

An examination of the mobilities of standard zinc-blende and diamond semiconductors, that are shown in Table I, reveals that GaAs has the highest electron mobility while Ge has the highest hole mobility among unstrained semiconductors with a sizeable band gap that have the zinc-blende symmetry group.

In the table we have also included some strained semiconductors. Strain has been shown to increase mobility significantly in Si. However, in these cases the results we cite[6] are theoretical, which in the case of the Si-Ge alloy compare reasonably to experiment.

According to the $k.p$ expression,[10] the effective masses of the band edge states should decrease with decreasing band gap for direct band gap systems, resulting in increased mobilities. However, decreasing the gap also increases leakage tunneling currents in devices, making semiconductors with small gaps difficult to use for designing devices. We have ignored a number of very high mobility lead compounds for this reason.

Hetero-polar semiconductors such as GaAs have a low hole mobility due to the enhanced scattering from polar phonons.[11] The trend in the hole mobility for elements down column IV of the periodic table is a result of the decreasing hole effective mass and the increasing phonon occupancies due to decreasing phonon frequencies. So, Ge has the largest hole mobility among the unstrained structures. The high electron mobility of GaAs is due to the low effective mass of the conduction band edge minimum which is located at Γ in GaAs.

As noted by Fischetti and Laux,[6] applying a volume tensile strain to Ge results in lowering the Γ_7^- state so that it becomes the bottom of the conduction band and is similar to GaAs. At zero pressure, the minimum of the conduction band of Ge is at the L point. The longitudinal effective mass at the L point is $1.59m_e$ while the transverse effective mass is $0.082m_e$. Application of volume tensile strain results in the Γ point minimum moving below the L point. The conduction band minimum at Γ which is the Γ_7^- state has a small effective mass of about $0.041m_e$.[10] If we assumed that the electron mobility is inversely proportional to the effective mass, this leads to the conclusion that the mobility of the Γ_7^- electrons is about 25 times higher than that of the L electrons. In addition, the scattering times at the Γ and the L points are not necessarily the same. However, a lower bound on the mobility of the Γ_7^- is obtained by observing that the mobility in GaAs, which is a semiconductor with Γ_1 as the bottom of the conduction band, is 8000 [cm^2/(Vs)]. Moreover, the effective mass of the Γ_7^- state in Ge is lower than the corresponding state in GaAs which has an effective mass of $0.066m_e$ and the scattering in GaAs is stronger due to its hetero-polar nature. Therefore for this model, the mobility of the Γ_7^- electrons should be in excess of 25000 [cm^2/(V s)], which is about a factor of 8 higher than the zero pressure electron mobility of Ge.

The hole mobility of group IV and group III-V semiconductors is reduced by the increased scattering between the degenerate valence bands at the valence band edge. This degeneracy also leads to the heavier band occupying the top of the valence band which further reduces the mobility. The valence band degeneracy is a consequence of the symmetry group of the diamond structure, and it can be lifted by using a biaxial strain.[10] Application of a biaxial strain can therefore enhance hole mobility. However, the electron-phonon coupling is stronger in the valence band so the hole mobility continues to be lower than the electron mobility even after the degeneracy has been lifted.

Two ways to apply the equivalent of a tensile volume strain to Ge are to alloy Ge with Sn and to grow Ge on Ge/Sn buffer layers. The former method involving Ge/Sn alloys has been used by Kouvetakis et al.[12] to obtain a direct band gap Ge based semiconductor. They estimate that the transition to a direct gap material occurs at about 15% Sn. However, they do not report any measurement of the electron or hole mobility of this material.

We examine the amount of Sn needed to transform Ge into a direct band gap material for both cases and estimate the mobility gain in the process. Later, using empirical pseudopotential band gap calculations, we show that the amount of Sn that must be alloyed into the material is lower in the case of biaxial strained heterostructures rather than direct alloying of Ge and Sn. In addition to increasing the electron mobility, biaxial strain can also increase the hole mobility by more than a factor of 4.[6]

III. STRAINED Ge-Sn SYSTEMS

Recent advances in experimental techniques have lead to the fabrication of high quality Ge-Sn alloys.[12] These alloys

have been seen to have low levels of segregation of Sn and misfit dislocations. Thus it is possible to speculate that their mobility is limited by more intrinsic phonon and alloy scattering mechanisms.

We consider two approaches for increasing the mobility in Ge-Sn systems. One of them is to biaxially strain Ge by growing it on Ge-Sn alloy substrates. This is similar to the techniques used by Myronov *et al.*[2] for Ge, and Antoniadis *et al.*[3] for Si-Ge systems to obtain a high hole mobility. Since Sn has a lattice constant of 6.49 Å which is higher than the Ge lattice constant of 5.65 Å, the Ge-Sn alloy has a larger lattice constant. The lattice constant of a Ge-Sn alloy is known to be almost linear in the concentration of Sn. Hence a Ge-Sn alloy with 6.72% Sn would have a lattice constant 1% higher than Ge. Ge grown on such a Ge-Sn alloy with an increased lattice constant will be biaxially strained. The resulting biaxial strain on Ge as mentioned above increases the electron and hole mobility.

The other technique is to alloy Sn directly into the Ge transport layer. These alloys have recently been experimentally realized and studied.[12] Alloying Sn in addition to increasing the lattice constant of the material alters the pseudopotential and increases the spin-orbit coupling. Even though the effect of the pseudopotential is not clear without an explicit calculation, one expects the enhanced spin-orbit coupling to lower the conduction band minimum at Γ relative to the other states, and this increases the electron mobility. However, alloying Sn into Ge is expected to create for the most part a uniform volume strain which preserves the symmetry and therefore doesn't alter the valence band properties significantly. Therefore, even in the alloying case one would have to introduce an additional biaxial strain through growing the alloy on a buffer layer in order to increase the hole mobility. However, it must be noted that the mobility in Ge-Sn should also be reduced by alloy scattering.

After studying these techniques we conclude that a combination of the two approaches is possibly the optimal way to create a higher carrier mobility Ge-Sn based semiconductor.

IV. ELECTRON MOBILITY IN DIRECT BAND GAP STRAINED Ge

As has been noted in numerous studies of the effect of strain on Ge, on increasing the unit cell volume the band gaps from the top of the valence band at Γ_8^+ to the Γ_7^- state and the L conduction band minimum decreases. However, the rate of decrease of the Γ_7^- gap is higher than that of the L gap. According to Pollak and Cardona,[10] the experimentally measured pressure coefficients of the gaps in Ge are 13 $\times 10^{-6}$ eV/atm for the direct gap associated with the Γ_7^- state and 5×10^{-6} eV/atm for the indirect gap associated with the L state. The indirect gap of Ge is 0.76 V and the direct gap is 0.9 V.[7] The experimental bulk modulus is 75.03 GPa. From this, the strain coefficients of the direct and indirect gaps are calculated to be

$$\frac{dE(\Gamma_7^-)}{d[\log(a)]} = 32.9 (\text{eV}), \quad \frac{dE(L_6^-)}{d[\log(a)]} = 12.67 (\text{eV}). \quad (8)$$

Using these values and the band gaps from Table II, Ge should make a transition into a direct band gap semiconduc-

TABLE II. Ge and Sn direct and indirect gaps.

Semiconductor	Γ^c (eV)	L (eV)
Ge	0.90	0.76
Sn	−0.42	0.14

tor at a lattice constant which is 0.8% higher than the zero pressure lattice constant. Under this strain, the gap can be estimated to be 0.66 eV.

This could be attained by alloying 5.4% Sn into Ge. The alternative possibility is to biaxially strain the crystal to create an equivalent volume strain. However, because of the elasticity properties of Ge, increasing the in-plane lattice constant by 1% decreases the out of plane lattice constant by 0.7%.[6] So one would have to increase the in-plane lattice constant of the crystal by 1.8%. This can be done in principle by growing Ge on a Ge-Sn alloy with 12.4% Sn.

Since there is a possibility of significant ambiguities in the measurement of band gaps, and the calculation of the band gaps involve some approximations, we have verified this result through several independent calculations. Corkill *et al.*[13] have calculated the pressure dependence of the direct and indirect gaps of Ge using density functional theory in the local density approximation (LDA). Their results are given in Table III.

Using these values we can derive the following strain coefficients for the band gaps.

$$\frac{dE(\Gamma_7^-)}{d[\log(a)]} = 29.7 (\text{eV}), \quad \frac{dE(L)}{d[\log(a)]} = 10.2 (\text{eV}). \quad (9)$$

Our LDA calculations yield similar results. The band gaps of semiconductors are known to be underestimated by density functional theory. In fact, within LDA at zero pressure, Ge has a vanishingly small gap. This makes the calculation of strain dependence at zero pressure problematic within LDA. Quasiparticle corrections introduced through the GW formalism yields gaps in agreement with experiment to less than 0.1 V. However, as has been argued by Louie and Zhu,[14] the GW corrections to the band gaps are independent of strain to a good approximation. So the LDA pressure coefficient should be a reasonable estimate. The LDA calculations that we performed did not include spin-orbit corrections. A first-principles calculation of the strain coefficients of the gaps including spin-orbit and GW is possible in principle, and a calculation of this kind should yield results in close agreement with experiment. However, this is made difficult due to the technical problems associated with the fact that within LDA, which provides the starting point of the

TABLE III. Gap strain coefficients of Ge.

State	E (eV) at a=5.36 Å	E (eV) at a=5.97 Å
Γ_7^-	13.2	7.2
L_6^-	12.0	8.1
Γ_8^+	10.9	8.1

GW calculations, Ge is a metal at volumes slightly larger than at zero pressure. Hence, we perform an empirical pseudopotential calculation which includes the spin-orbit correction. The empirical pseudopotential method (EPM) is not a first-principles method since the three EPM parameters used are fit to experiment. However, the EPM method is known to reproduce the band structures of a large family of semiconductors with a high degree of accuracy. Our EPM calculation resulted in a value of 28.3 eV for the strain co-efficient of the direct gap both with and without spin-orbit coupling. Therefore, even though each of these methods have their limitations and can only reproduce certain aspects of band structure data, all of them yield similar values for the strain coefficients.

V. HIGH ELECTRON MOBILITY IN Ge-Sn ALLOY

Heavy elements like Sn have large spin-orbit couplings which are expected to raise the energy of conduction band states other than those at the Γ point. Therefore it is expected that if one were to alloy Sn into Ge, then the direct gap would be decreased relative to the indirect gap due to spin-orbit coupling, in addition to the decrease due to the in-creased lattice constant. Therefore one expects the fraction of Sn needed to attain a direct band gap semiconductor to be less than our previous estimate of 5%. However, Kouvetakis *et al.*[12] have reported a composition of 15% Sn to be the point where a direct band gap semiconductor is obtained. The direct and indirect band gaps of Ge and Sn are listed in Table II.[7]

Using pseudopotential calculations, Jenkins and Dow[15] obtained a linear dependence of the gap of the Ge-Sn alloy system with composition. Assuming this holds in Ge-Sn alloys, one expects an indirect to direct band gap crossover point to occur at

$$x = 0.2, \quad \text{with} \quad E(\Gamma^c) = 0.64(\text{eV}), \tag{10}$$

where x is the fraction of Sn and $E(\Gamma^c)$ is the band gap at that composition.

In order to get a better understanding of why the percent-age of Sn required for a crossover to a direct band gap ma-terial is higher in the Sn alloy case than in the pure strain case, we perform an EPM calculation with spin-orbit cou-pling taken into account.

These calculations suggest an estimate of 25% Sn with a direct gap of 0.6 V at the indirect to direct gap crossover in agreement with the calculations of Baldereschi.[16] However, if we remove the Sn pseudopotential contribution to the po-tential and use the Ge pseudopotential entirely, then we re-cover our original estimate of 5% Sn and a gap of 0.66 V.

The difference in spin-orbit coupling does not affect the results significantly. To see why this is reasonable we note that the spin-orbit parameters of Ge and Sn are 0.00097 and 0.00225 (Ref. 7) in atomic units. So, an addition of 5% Sn into Ge changes the Ge parameter by about 6.59%. Since the orginal spin-orbit splitting in Ge was about 0.29 eV, it is reasonable to assume that the change in spin-orbit splitting does not qualitatively alter our conclusions since it is less than a 20 meV effect.
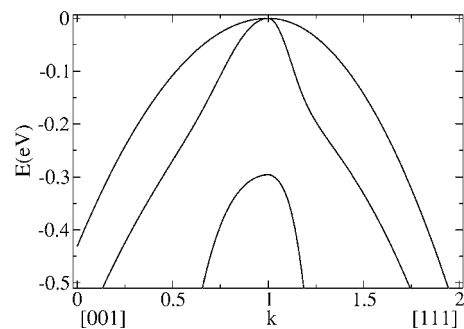

FIG. 1. Unstrained valence band structure of Ge from the [001] to Γ to [111].

Therefore, contrary to expectations, alloying Sn requires about 20% Sn to form a direct band gap semiconductor, which is a larger amount than pure biaxial lattice constant straining would require, which is about 5%.

VI. HOLE MOBILITY IN Ge

The valence band maxima of strained diamond semicon-ductors have a rather complicated structure due to the inter-action of spin-orbit coupling and strain. It comprises a dou-blet of heavy hole band and light hole band which are degenerate at Γ and a split-off band. Since we are interested in room temperature properties we can ignore the split-off band and focus on the heavy-hole and light-hole band. In the unstrained case, the former forms most of the upper valence band edge. The hole mobility in this case is determined not only by the warped valence bands, but it is also limited by interband scattering. In order to estimate the mobilities we calculate the thermally averaged density of states and curva-ture effective masses since the warped band structure does not allow for a simple definition of an effective mass. How-ever, interband scattering cannot be completely neglected even after the bands have been split by strain.

As previously remarked, the degeneracy at the top of the valence band is related to the symmetry group of the dia-mond cubic lattice. Also, $k \cdot p$ calculations show that the den-sity of states effective mass of the heavy hole states is $0.38m_e$, which is much heavier than the light hole state, which has an effective mass of $0.045m_e$, as is apparent from Fig. 1. The curvature or transport effective masses show a similar trend with the heavy-hole band having an effective mass of $0.29m_e$ and the light-hole band having an effective mass of $0.043m_e$. This is a result of the degeneracy at the top of the valence band.

Calculating an accurate value for the heavy-hole mass is difficult when using local EPM, since the inverse of the heavy-hole mass is small due to a cancellation between rela-tively large matrix elements. The pseudopotential method can reproduce the matrix elements and the band gaps to within 10%. Since the inverse effective mass is down by a factor of 5 from the typical values of the matrix element, a direct pseudopotential calculation leads to the effective mass being in error by about 50%. Therefore we use the empirical $k \cdot p$ method for the effective masses.
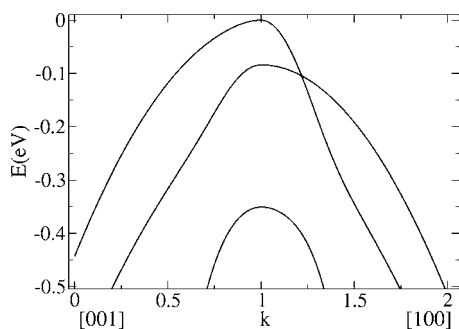
FIG. 2. [100] strained valence band maximum structure of Ge zoomed in around Γ.

However, the symmetry induced degeneracy at the top of the valence band can be lifted by applying a strain on the crystal to break the symmetry. Moreover, an application of strain in certain directions can allow the top of the valence band to be lighter in mass or have the character of the light hole in certain directions. In what follows we study the band structure of the top of the valence band for Ge biaxially strained in three directions. Since the two bands at the top of the valence band cannot be characterized by their masses after the application of strain but are split in energy, we refer to them as the upper and lower valence band edge states, respectively. Even though the splitting of the upper and lower valence band states appears similar in the three cases, straining along the [100] direction appears to lead to the highest mobility.

A. Strain in the [100] direction

To determine the effect of a biaxial strain on the electronic structure perpendicular to the [100] direction we calculated the band structure near the valence band maximum at Γ for Ge using the EPM technique with spin-orbit coupling included. From the band structure shown in Fig. 2, it is clear that in certain directions the top of the valence band has light-hole character. But in other directions the band has heavy-hole character.

The in-plane transport effective mass of the higher valence band edge state is $0.27m_e$, while the out-of-plane mass is $0.17m_e$. The density of states effective mass is $0.20m_e$ for the upper band which is the one that dominates the transport, the other band is lighter with an effective mass of $0.08m_e$ but participates only weakly in transport. Therefore, we find that even though the strain does not reduce the in-plane transport effective mass significantly, it can increase the mobility by reducing the density of states for phonon scattering. Assuming an $m^{3/2}$ scaling in the DOS effective mass [Eq. (3)] for the mobility, we expect the hole mobility to increase to about 5100 cm^2/Vs.

For a biaxial tensile strain of 1.0%, we find the splitting between the upper and lower bands to be 83 meV in both the EPM and the $k \cdot p$ methods which is somewhat higher than room temperature. This is in reasonable agreement with measurements.[10] Therefore, there should be a significant reduction in interband scattering which together with the lower in-plane effective mass is expected to enhance the mobility

significantly. If we can completely neglect interband scattering we may imagine that the scattering phase space and hence the scattering rate is reduced by a factor of 2. Therefore, the mobility enhancement is expected to be stronger than we predict by approximately a factor of 2 due to the suppression of interband scattering.

This expectation is supported by previous theoretical calculations[6] which have found the in-plane hole mobility to be 10000 cm^2/Vs for a biaxial tensile strain of 1.0%, which is more than a factor of 4 higher than the unstrained case.

B. Strain in the [111] and [110] directions

We perform a calculation similar to the [100] case presented above for the [111] case. In this case, as has been pointed out by Martin *et al.*,[17] it is necessary to account for the distortion of the relative displacement of the basis atom. Taking the experimental value for the lattice displacement parameter ζ, we find from our EPM calculations that a 1% biaxial expansive strain splits the heavy- and light-hole bands by 83 meV, which is in quantitative agreement with experimental measurement.[10] This splitting being somewhat higher than room temperature allows a single band to dominate the conductance. The effective masses are similar to the [100] strain case. The in-plane effective mass of the higher valence band edge state is $0.44m_e$, while the out of plane mass is $0.090m_e$. The average density of states effective mass is $0.23m_e$ for the upper band and $0.08m_e$ for the other. The [111] strain reduces the density of states effective mass in a way similar to the [100] strain but appears to increase the in-plane transport effective mass.

Biaxially straining the crystal in the [110] direction reduces the DOS effective mass in a way similar to the other two cases, however, in one in-plane direction it increases the transport effective mass similar to the [111] case and leaves the other transport effective mass relatively unchanged, as in the [100] case. The in-plane effective masses for the higher valence band edge state are $0.64m_e$ and $0.26m_e$, while the out of plane mass is $0.10m_e$. The density of states effective mass is $0.22m_e$ for the upper band and $0.08m_e$ for the other band.

Unlike the situation involving the conduction band, alloying a small amount of Sn does not change the structure of the valence band in any qualitative way. This may be understood in terms of the effective masses being determined by $k \cdot p$ perturbation theory from the various gaps. As has been noted earlier the addition of about 5% Sn does not alter the spin-orbit coupling qualitatively, at least on the scale that strain itself alters the band structure. Therefore, the hole mobility is not altered significantly by the addition of Sn except for the possibility of reduced mobility due to alloy scattering.

VII. ALLOY SCATTERING

In the previous sections we considered the phonon limited mobility of Ge-Sn alloys and found that it was possible to increase both the electron and hole mobilities of Ge by alloying with Sn and straining. However, it is known in Si-Ge alloys that alloy scattering can lead to reductions in mobility, which often offsets any advantage gained from alloying Ge.[6]

Moreover, calculations of alloy scattering in semiconductors until recently[18] were based on an alloy scattering parameter[6] and were therefore not suitable for a first-principles calculation where experimental mobility data is not available.

Therefore, we calculate the alloy scattering contribution to mobilities in Ge-Sn alloys following the first-principles approach of Murphy-Armando *et al.*[18] and calculate the scattering rate given by

$$\frac{1}{\tau_\alpha} = \frac{2\pi}{\hbar} x(1-x) \frac{a_0^3}{8} \sum_\beta |\langle V_{\alpha\beta} \rangle|^2 \rho^\beta(E), \qquad (11)$$

where x is the Sn content, a_0 is the cubic lattice constant, β labels states and ρ^β is the density of states per spin, and the scattering matrix is defined by

$$\langle V_{\alpha\beta} \rangle = \langle V_{\alpha\beta}^{\text{Ge}} \rangle - \langle V_{\alpha\beta}^{\text{Sn}} \rangle = N \langle \psi_\alpha | (V^{\text{Ge}} - V^{\text{Sn}}) | \phi_\beta \rangle, \quad (12)$$

where ψ are the eigenstates of the system with the Sn impurity and ϕ are the wave functions of the pure Ge system.

We average the above scattering rate over a Boltzmann distribution of energies for the electrons[21] and get

$$\frac{1}{\tau_\alpha} = \frac{a_0^3}{32\pi\hbar} x(1-x) \sqrt{\pi k T} \sum_\beta |\langle V_{\alpha\beta} \rangle|^2 \left(\frac{2m_\beta^*}{\hbar^2} \right)^{3/2}. \quad (13)$$

The matrix elements are calculated using a 128 atom supercell with one impurity atom. The calculations are performed in a plane-wave pseudopotential formalism using the PARATEC[19,20] code. We relax the atoms around the impurity up to second nearest neighbors and calculate the matrix elements indirectly from the eigenvalues using two approaches. In the first approach we calculate the difference in the eigenvalues at Γ between the calculations with and without an impurity atom, and in the other we consider the splitting of degeneracies at the edge of the folded-back supercell Brillouin zone. From perturbative treatments of bandstructures in the nearly free electron model it is known that both these quantities are related to the scattering matrix element of the potential. The splitting at the edge of the Brillouin zone from degenerate perturbation theory is twice the matrix element while the eigenvalue shift is equal to the matrix element. For a finite supercell, the splitting approach calculates the matrix elements for states different from Γ since these states are at the edge of the supercell Brillouin zone. For the 128 atom supercell, used, this can lead to significant errors for the extremely light conduction band state at Γ, so we use the eigenvalue splitting as a rough check for the hole calculations. However, the determination of the eigenvalue splitting is independent of the total potential shift which has to be accounted for in the eigenvalue shift approach. Finally, we account for GW (Ref. 8) and spin-orbit corrections to the matrix elements by calculating shifts in the band edges due to these effects. The spin-orbit shift is calculated within the EPM. The total matrix elements V, obtained from the eigenvalue shift and eigenvalue splitting approach and the corresponding mobilities with 8% Sn are shown in Table IV. In Table IV we have given the scattering matrix element used in Eq. (13) from the two methods used to calculate them, i.e., from the eigenvalue shift at Γ and the splitting at the edge of the supercell Brillouin zone. In the next two columns we

TABLE IV. Impurity scattering matrix elements in eV and mobilities in [cm^2/(Vs)].

State	V (shift)	V (split)	μ (shift)	μ (split)
SiGe holes	1.564	1.144	380.088	701.4
strained GeSn holes	0.89	1.58	135694.5	4455.2
GeSn electrons	0.788	0.1	10^6	very large

give the impurity scattering contribution to the mobility calculated from the two matrix elements.

In the above calculation we have ignored the effect of biaxial strain on the matrix elements and other effects such as the use of finite unit cells. We expect that these introduce small errors into the calculation. However, we find that the results in SiGe are in reasonable agreement with experimental data, and so we expect to be able to predict basic trends in mobility. Therefore, based on these calculations we can reasonably expect that a concentration of 8% Sn does not significantly affect the electron mobility, while the effect of alloy scattering on the hole mobility still allows an increase in the total mobility to about 4500 [cm^2/(Vs)] or more, which is more than a factor of 2 from the unstrained mobility.

VIII. CONCLUSION

In summary, we have examined the effect of strain and alloying Sn on electron and hole mobilities in Ge-Sn group IV semiconductor alloys. Consistent with previous work we find that the electron mobility can be increased by at least a factor of 4 by applying about 2.5% tensile uniform volume strain to lower the bottom of the conduction band at Γ below the bottom of the conduction band at L. We have examined two ways of achieving this. One of them is to strain the lattice biaxially through epitaxial strain. For this we estimate that Ge would have to be grown on a Ge-Sn alloy with 12.4% Sn. The other possibility was to alloy Ge and Sn to increase the lattice constant of Ge. In agreement with experiment we find that one would need to alloy 15% Sn.

For the hole mobility we found that the application of about 1% of biaxial strain would split the light-hole and heavy-hole bands, increasing the phonon-limited mobility by a factor of 4. The proposed epitaxial strain technique strains the in-plane lattice constant biaxially by 1.8%, which would presumably increase the hole mobility further.

Therefore, from our study it appears that Ge biaxially strained by growing Ge on a Ge-Sn alloy with 12.4% Sn would increase both electrons and hole mobility. However, a Ge thin film with a large in-plane lattice constant strain of 1.8% might be unstable to the formation of various defects making this scheme impractical.

So we propose a combination of the two methods where we grow a Ge-Sn alloy conduction layer on another Ge-Sn alloy buffer layer, which has a larger concentration of Sn, so that it can create a biaxial strain of 1% in the conduction layer. As previously noted, 1% biaxial tensile strain increases the volume by 1.3%. This decreases the difference between the Γ_7^- and L conduction states to 0.06 V. Therefore, to trans-

form the conducting layer into a direct gap semiconductor one needs to alloy 7.5% Sn into the conduction layer Ge-Sn alloy. In order for the buffer layer to have a sufficiently large lattice constant so that it can apply a 1% tensile biaxial strain to the conduction layer, it should contain 3.7% Sn in excess of the conduction layer. This requires a composition of 11.2% Sn for the buffer layer. Apart from the reduction of mobility due to alloy scattering, the above proposed Ge-Sn system can be expected to be stable and have an increased electron and hole mobility by a factor of 4. We also note that to avoid interband electron scattering between the Γ and L valleys in the Ge-Sn alloy, we may need to raise the calculated Sn content in the above by about 10%. We find that alloy scattering for the electrons is weak while it may reduce the hole mobility to about 4500 $[\text{cm}^2/(\text{V s})]$ which is lower than the phonon-limited value by about a factor of 2, but still continues to be higher than the unstrained case by more than a factor of 2. However, it might also be possible to use the Ge-Sn alloy only for electron transport and use a pure germanium layer with 1% biaxial strain for hole transport. In this case, one can obtain an enhancement of a factor of 4 in both carrier mobilities. Factors other than phonon and alloy scattering such as segregation and misfit dislocations can also limit the mobilities of Ge-Sn alloy layers.[22,23] However, recently Kouvetakis *et al.*[12] have shown that it is possible to grow high quality Ge-Sn alloys with relatively low levels of segregation of Sn and misfit dislocations. Moreover, we are restricting ourselves to a region of 1% tensile strain where for Si-Ge alloys surface roughness is not very large.[22]

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