Multiscale modeling of point defects in strained silicon

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Abstract— A multiscale Green's function method is described for modeling substitutional point defects and vacancies in strained silicon. The model seamlessly links the length scales from atomistic to macro. The model accounts for the discrete lattice effects, elastic anisotropy, nonlinear effects, and the presence of point defects as well as surfaces and interfaces in the solid. An effective force, called the Kanzaki force, is defined, which is a characteristic of the defect configuration. This force can be calculated and stored for later use, which makes the method numerically convenient for subsequent calculations. The Kanzaki force is used to calculate the dipole tensor that is a measure of the strength of the defects and can be directly used to calculate the strains from the familiar continuum Green's function. Numerical results are presented for the lattice distortion in half-space silicon due to a Ge impurity and the dipole tensors for various point defects (vacancy and substitutional germanium and carbon impurities) in two models of strained silicon. Calculated values of elastic constants are reported for strained silicon.

***Index Terms*— elastic constants of strained silicon, multiscale Green's function, point defects in strained silicon, strained silicon.**

I. INTRODUCTION

As characteristic dimensions of CMOS transistors reach 45 nm or even lower, strain engineering of silicon is becoming increasingly more important in the fabrication of high performance devices. Strained silicon (sSi) has significantly improved carrier mobility and reduced power consumption enabling much higher switching speeds. Excellent reviews of sSi have been published by Chidambaram et al. [1] and Lochtefeld [2]. Strained silicon can be made by introducing layers of germanium in silicon lattice or by

Manuscript received ??.

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depositing silicon on $Si_{1-x}Ge_x$, which expands the silicon lattice and hence increases the carrier mobility. It is also possible to make sSi on insulator without the $Si_{1-x}Ge_x$ layer [2].

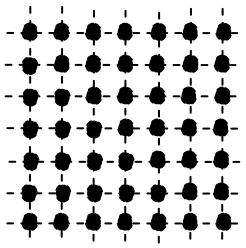
An important problem [1] in the design of sSi based devices is that it has not yet been possible to measure all components of strain in the finished device. It is therefore necessary to have reliable theoretical models for calculating strain distribution in strained silicon.

A mathematical model is also needed to calculate the strains introduced by the point defects such as vacancies, additional Ge, and C (carbon) impurities in sSi. These defects may be inherently present or deliberately introduced in the device. They can affect the mobility of the carriers and the overall performance and reliability of the devices. In particular, a C impurity can act as a strain compensator in silicon containing Ge. A very useful application of the mathematical model is to identify measurable parameters. A comparison between the calculated and the measured values of these parameters would validate the theory and help characterizing the state of the strain in the device.

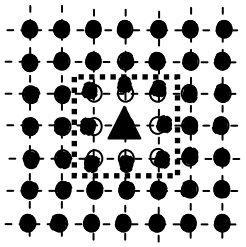
Strain is a macroscopic parameter of the continuum model of a solid that affects the measurable Raman and X-ray spectra of the solid. However, for a detailed quantum mechanical calculation of the electronic wave functions and the mobility of the carriers, knowledge of strain alone is not enough. It is necessary to know the precise location of the host atoms in sSi. Hence a reliable model for sSi must give the local atomistic distortion in the lattice as well as strains in the entire solid. The model must account for the local discrete structure of the lattice including nonlinear effects where necessary. It should also account for the presence of surfaces and interfaces in the solid. It is necessary to relate the characteristics of the discrete lattice model such as lattice distortion and interatomic forces to strains and elastic constants that are parameters of the continuum model. Modeling of sSi is thus a multiscale problem.

We shall give a brief review of our multiscale Green's function (GF) model and its application to half-space silicon and infinite (without free surfaces) sSi. The multiscale GF is calculated numerically by imposing the continuum GF as the boundary condition and not the Born's periodic boundary condition. It accounts for the nonlinear and discrete lattice effects near the defect, and free surface and interfaces if desired to be included. The multiscale GF links the length scales seamlessly from atomistic to macro and relates the discrete lattice distortion to strain in the corresponding continuum model. One useful mathematical result of our theory is that the discrete lattice contributions can be represented in terms of an effective force, called the Kanzaki force, which is a characteristic of the host lattice as well as of the defect configuration. This force can be calculated and stored for later use which makes it numerically very convenient for subsequent calculations on the same system.

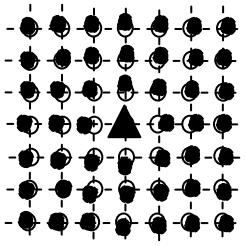
The Kanzaki force is used to define the elastic dipole tensor of a defect, which is a measure of the strength of the defect and can provide a signature of the defect configuration. It is useful [3] for calculating the strain in the whole solid using the standard continuum theory. It is also possible to experimentally measure some components of the dipole tensor.



(a) $\boldsymbol{X}_R$



(b) $\boldsymbol{X}$



(c) $\boldsymbol{X}_F$

Figure 1. (a) Reference lattice XR; (b) partially relaxed defect lattice X; (c) fully relaxed defect lattice XF. The solid circles represent atoms while the open ones represent the reference lattice sites. The solid triangle represents an impurity atom or a vacancy. In (b), the dotted line defines a nominal nonlinear core in which the atomic position is constantly updated in the iterative solution process.

The work described in this paper is a report of our work in progress on a project dealing with the modeling of sSi. We first consider a single substitutional Ge impurity in half-space silicon lattice. This system is of interest because sSi is often made by using SiGe with varying concentrations of Ge. We then consider two models of infinite sSi. One is a trilayer model consisting of a layer of germanium atoms in between two half space silicon lattices. The other is a free standing model of sSi that is laterally stretched to the dimensions of the germanium lattice. However, in these preliminary results, we have neglected the effect of free surfaces in the free standing sSi. The model is based upon the standard adiabatic approximation of the Born von Karman model at zero temperature in which the effect of electrons is included only in a phenomenological

manner through an effective interatomic potential. Our model, therefore, would not account for effects such as Jahn-Teller distortion that is normally significant for a vacancy in silicon.

We will present numerical results on the lattice distortion due to an isolated Ge atom in half-space silicon lattice, the change in the lattice constant of the sSi due to a layer of Ge atoms in the trilayer model, and the dipole tensors for a vacancy and substitutional Ge and C impurities in a free standing model of the sSi. We will also report the calculated values of the elastic constants for the free standing model of the sSi. The change in the lattice constant of the sSi gives the overall strain in the solid. Similarly the dipole tensor is a measure of the state of strain in the material [3]. More detailed results on the actual strain field will be published elsewhere.

II. MULTISCALE GREEN'S FUNCTION

The multiscale GF method has been described in detail in earlier papers [3] – [7]. Here we give only the features that are specifically applicable to sSi. Consider a lattice of N atoms. We first define a reference state X_R as shown in Fig. 1(a). We then introduce defects in the lattice and let the lattice relax to its final state X_F as shown in Fig. 1(c). In some cases, as when the nonlinear effects are included using an iterative procedure, it is convenient to define an intermediate or a partially relaxed state X as shown in Fig. 1 (b).

We assume that the coupling between the atoms in the reference state is given by the force-constant matrix $\mathbf{\Phi}$. We use the Tersoff potential [8] to calculate $\mathbf{\Phi}$. The GF for the reference system is defined by

$$\mathbf{G} = [\mathbf{\Phi}]^{-1}. \tag{1}$$

Both $\mathbf{\Phi}$ and $\mathbf{G}$ are 3Nx3N matrices. We assume that $\mathbf{\Phi}$ and hence $\mathbf{G}$ are known. We introduce additional defects in the lattice and also subject it to an external force field. As the lattice relaxes to its final state, it gets strained. The objective is to calculate the lattice relaxation or distortion given by the displacement field $\mathbf{u}$ in the final state measured with respect to the reference state. Hence $\mathbf{u}$ =0 in the reference state.

The effect of the defects is to change the force constant matrix and also exert forces on the lattice sites. If $\mathbf{\Phi}^*$ denotes the force constant matrix in the final state,

$$\mathbf{\Phi}^* = \mathbf{\Phi} - \Delta\mathbf{\Phi}, \tag{2}$$

where $\Delta\mathbf{\Phi}$ denotes the change in $\mathbf{\Phi}$ caused by the defects. The defect GF, that is, the GF for the final state is defined as follows in analogy with Eq. (1):

$$\mathbf{G}^* = [\mathbf{\Phi}^*]^{-1}. \tag{3}$$

The defect GF is given [3] by the solution of the Dyson equation

$$\mathbf{G^* = G} + \mathrm{G}\Delta\Phi\mathbf{G^*}. \quad (4)$$

The lattice distortion in the final state is given by [3]

$$\mathbf{u = G^*F} \quad (5)$$

where **F** is the Nx1 column matrix of forces on the atomic sites and **u** is the Nx1 column matrix of atomic displacements induced by the defect. For a discrete lattice **u** is a discrete variable defined only at the discrete lattice sites. The force **F** may be exerted by the presence of the defects or by imposing an external strain. The points where **F** is nonvanishing are called the source points and the points where **u** is calculated are called the field points.

For multiscale modeling, we recast Eq. (2) in the following equivalent form by using Eq. (4):

$$\mathbf{u = GF^*(u),} \quad (6)$$

where

$$\mathbf{F^*(u) = F} + \Delta\Phi\,\mathbf{u}, \quad (7)$$

The effective force **F*** is called the Kanzaki force which is equal to the force exerted by the defect at the relaxed lattice sites. It is a function of **u**. It contains all the characteristics of discrete lattice structure in and around the source point [3] – [7] and depends upon the detailed nature of the defect. The Kanzaki force also includes the effect of local anharmonicity, if any. Since **G** is a property of the reference state, it does not depend upon the defect. It can be calculated and stored for later calculations on different defects in the same host lattice.

In the harmonic approximation $\Delta\Phi$ is independent of **u** and Eq. (6) is a linear equation in **u**. The atomic displacements in this case can be directly calculated from Eq. (6) by using the method of matrix partitioning [3], [4]. When the nonlinear effects are significant, as in sSi, $\Delta\Phi$ is a function [6] of **u** and Eq. (6) becomes a nonlinear equation. In this case we solve Eq. (6) by iteration [6] by defining an intermediate state X for each iteration as shown in Fig. 1 (b).

Equation (6) is the master equation of the multiscale GF method. The multiscale linking is achieved through **G**. When the reference state is the perfect lattice and the harmonic approximation is applicable, Eqs. (5) and (6) reduce to those given in [3] and [4]. It can be shown analytically [3] that in the asymptotic limit, when the distance between the source and the field point is large, the lattice GF reduces to the continuum GF. This correspondence provides the basis for the multiscale linkage of the GF over different scales.

The discrete lattice effects are important at the field points that are near the defect. These points form the core structure of the defect where the nonlinear effects may also be significant. For such field points we use the lattice statics GF for **G**. In the asymptotic limit, when the field points are far away from the source points, the solid can be modeled as a continuum. In this case we can use the continuum expression for **G.**

The continuum model GF is also useful for including the effect of surfaces and interfaces that are far enough from the defect that the asymptotic approximation is valid. Standard methods are available in the literature [9] for calculation of the continuum GF. The continuum GF is also useful for boundary element analysis [10] that is applicable to solids of arbitrary shapes. In this paper, however, the free surface is included in the discrete lattice calculation because the defects can be close enough to the surface for the discrete and the nonlinear effects to be significant.

Thus we see that Eq. (6) gives the lattice distortion in and near the core of the defects by using the lattice GF. It also gives the macroscopic strains far away from the defect while still retaining the discrete lattice and nonlinear effects in the core of the defect. Equation (6) thus links seamlessly the atomistic scales near the core of the defect to macroscopic parameters of the continuum model.

The macroscopic strains are obtained by using the continuum GF in Eq. (6) which automatically makes the displacement field a continuous and differentiable function. In a purely discrete calculation, the displacement field is a discrete variable. Its derivatives, and therefore strains, are not uniquely defined. The use of the continuum GF along with the Kanzaki force in Eq. (6) removes this lack of uniqueness.

The strains induced by a defect in a lattice can be characterized in terms of the dipole tensor of the defect. It is a second rank tensor defined in the lattice theory as follows [3],[6]

$$M_{ij} = \sum r_i F^*_j, \tag{8}$$

where **r** is the position vector of an atom and i,j=1,2, and 3 corresponding to the Cartesian coordinates x,y, and z respectively. The dipole tensor, which is a measure of the strength of the defect, is used to model the defect as an inclusion in the continuum theory and directly gives the strain field in a solid [9]. Since we define it in terms of the Kanzaki force, it retains all the information about the discrete structure of the core of the defect and includes the nonlinear effects in the core. It is thus an important multiscale parameter that characterizes the state of strain in the solid.

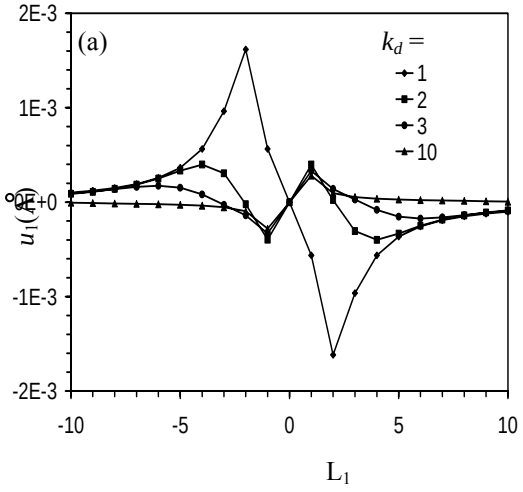
For a perfect lattice, **G** can be calculated by using the Fourier transform technique [3], [4]. In the present more general case, we calculate the multiscale GF directly using a hybrid model [5], [6]. In the reference lattice, we apply a unit force on a reference atom that we assume to be the source point. We draw a super cell of the lattice around the source. The super cell includes the free surface in the half space model of the solid. Atoms that directly interact with any atom outside the super cell are identified as

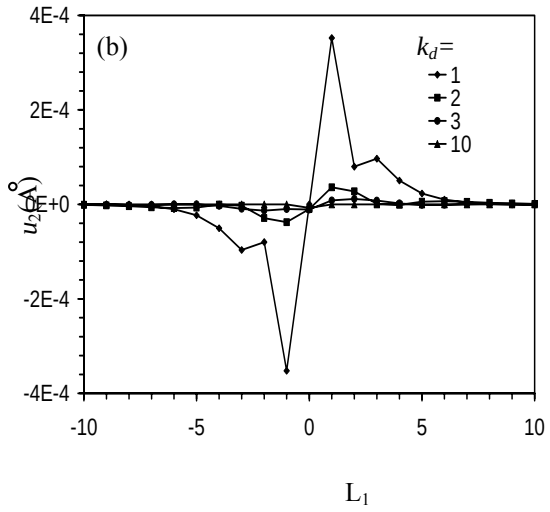
boundary atoms. For a sufficiently large super cell, the displacements of the boundary atoms and all the atoms outside the super cell are specified as those predicted by continuum GF [10] which provides the boundary condition for the hybrid GF. The continuum model GF used is chosen to be the half-space GF or infinite GF according to the model used. The calculated GF is multiscale in the Mott-Littleton sense that it is discrete near the defect and continuum in the far field region. We test the convergence of the model by varying the size of the super cell and ensuring that the results are independent of the size of the super cell.

III. SUBSTITUTIONAL POINT DEFECTS IN SILICON

In this section we present our detailed results for the lattice distortion caused by a single Ge atom in a half-space silicon lattice containing a free surface. The effect of the free surface is significant in the nanostructures and therefore must be included. This system is of interest because SiGe is used in making sSi. We have also calculated the dipole tensors for vacancy and Ge and C impurities in a perfect silicon lattice in order to compare their values with those for sSi which will be discussed in the next section.

We calculate the atomic displacement field in the silicon lattice as a function of the depth of the Ge impurity below the free surface. We include the effect of the free surface in calculating **G** as described earlier. In this method we do not include the effect of the surface reconstruction and direct interaction between the defect and the free surface. This is a limitation of our model.





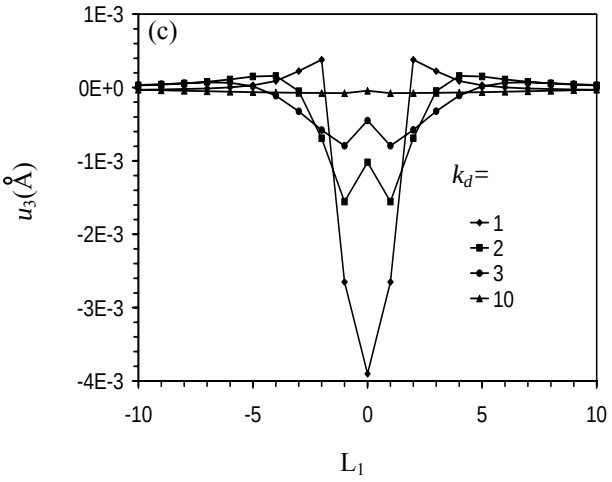


Figure 2. Variation of the x,y, and z components of the atomic displacements in Angstroms for atoms along a horizontal line (L_1, L_2, L_3) where $L_2 = 0$ and $L_3=k_d$ for various values of the depth k_d of the Ge impurity (a) u_1 (b) u_2 (c) u_3. The impurity is located at ($L_1=0$, $L_2 = 0$, $L_3=k_d$).

Hence, we consider only the case when the defect is least one lattice constant away from the surface. To take into account the surface reconstruction, the lattice at the surface should be modified according to experimental observations or by using a more advanced theory. The model must eliminate any net force in the system before introducing a defect.

We assume a frame of reference in which the coordinate axes are parallel to the crystallographic axes with the Z axis pointing into the solid. We assume that the free surface to be the (0,0,1) plane. Silicon lattice structure consists of two interpenetrating fcc lattices. We refer to the lattice sites of these two lattices as type A and type B. The origin of the frame of reference is assumed to be at an atom of type A at the free surface.

The atoms of type B are shifted with respect to type A by the vector (1/4,1/4,1/4). The atomic coordinates are expressed in units of the lattice constant of the host silicon lattice. The coordinates of the type A atoms are given by (L_1,L_2,L_3). We assume that Ge atom is at the lattice site (0,0,k_d) so k_d denotes the depth of the impurity below the free surface.

The displacements of the atoms along the line (L_1,0,k_d) in the silicon lattice containing a substitutional Ge impurity are shown in Figs. 2 (a)-(c) for different values of k_d. We see that the effect of the free surface is significant on the lattice distortion when the defect is close to the surface. However, the effect fades away quickly as the depth increases. When the defect is deep inside the solid (k_d = 10), the atomic displacements are radial as expected intuitively on the basis of the continuum model. This implies u_2 and u_3 are nearly zero for atoms along the line (L_1,0,k_d) parallel to the X axis. Only u_1 remains significant, which is responsible for laterally straining the silicon lattice along the X-axis. Further, the variation of u_1 shows that the Ge impurity pulls the host atoms closer to itself for k_d = 1, but pushes them away when k_d = 10. This result is important for the interpretation of measurements such as those obtained by X-ray scattering, since the effect of the defect depends upon its depth below the free surface.

Figure 2(c) shows that u_3 has an oscillatory behavior, especially when the depth is small. The oscillation extends over a fairly large distance, that is, over a few unit cells, from the defect. The surface attracts the atoms very close to the defect but repels the others.

We see from Fig. 2 (b) that, as mentioned before, u_2 is nearly zero for k_d = 10. This agrees with the continuum solution assuming the cubic anisotropy of the host lattice and spherical dilatational defects [9]. When the defect is close to the surface, u_2 becomes significant due to the effect of the lattice asymmetry caused by the presence of the surface. As we will see in the next section, the local asymmetry near the interface makes the dipole tensor nondiagonal. In contrast, the continuum model predicts a zero value of u_2 independent of k_d.

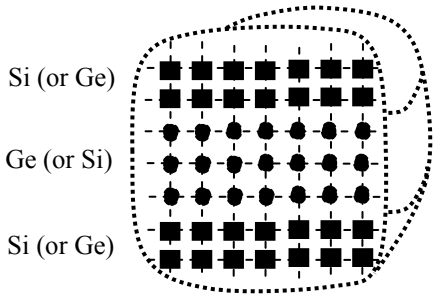


Figure 3. Schematic of a trilayer lattice of Si/Ge/Si or Ge/Si/Ge

IV. SUBSTITUTIONAL IMPURITIES IN STRAINED SILICON

Strained silicon is usually made by depositing silicon on $Si_{1-x}Ge_x$. It is now possible to have x = 1 that corresponds to just a layer of Ge atoms. Here we consider this extreme case. This system can be modeled as a trilayer material system consisting of a layer of Ge atoms sandwiched between two semi-infinite or half-space silicon lattices as shown in Fig. 3. This system can be visualized as a Ge quantum well in silicon, which will have the effect of locally stretching the silicon lattice. This model is symmetric about the germanium layer and amounts to having two layers of sSi separated by a layer of germanium atoms. Although not relevant for the present paper, a corresponding system can also be modeled for silicon quantum well in germanium.

Now it is also possible [2] to stretch the silicon lattice by depositing it on SiGe and removing the SiGe layer. This leads to the sSi on an insulator. If we neglect the effect of the insulator substrate, this system can be modeled as a free standing sSi. In this paper we consider the two limiting cases: the free standing sSi that has been laterally stretched to the lattice constant of germanium and the trilayer system described above.

We are presently in the process of calculating the effect of the $Si_{1-x}Ge_x$ substrate for different values of x and also the insulator substrate on strains in sSi by using the multiscale GF as described in Sec. II.

We first consider the free standing sSi. The lattice constants of normal silicon and germanium lattices as predicted by the Tersoff potential are 5.4320 Å and 5.6567 Å respectively. We stretch the silicon lattice in the (1,0,0) plane so as to match with the lattice constant of the germanium lattice. We then allow the lattice to relax in the perpendicular direction keeping the lateral dimensions fixed. This decreases the lattice constant of silicon (the Poisson effect) in the perpendicular direction from 5.4320 Å to 5.1952 Å . The symmetry of the resulting structure is reduced from cubic to tetragonal. This gives a model of free standing sSi.

An important mechanical parameter for sSi is the fourth rank elastic constant tensor with components C_{ijkl}. We calculate the elastic constants for the sSi as given below. In these calculations we account for the full elastic anisotropy.

The stress in the solid is given by

$$\sigma_{ij} = \frac{\partial V}{\partial \varepsilon_{ij}}, \tag{9}$$

where V is change in the potential energy of the solid on relaxation and ε_{ij} is the infinitesimal strain, defined by

$$\varepsilon_{ij} = \tfrac{1}{2}(u_{i,j} + u_{j,i}). \tag{10}$$

We assume that the lattice is in the final relaxed state and is subjected to no body force. We first calculate the "stress" at an atom called the reference atom. We identify all the neighboring atoms that directly interact with the reference atom. Now we apply a

displacement field on the neighboring atoms according to a specified infinitesimal strain in the finite-difference form of Eq. (9). We then calculate the potential energy of the reference atom in the field of all the neighboring atoms with and without relaxation. The difference between the two gives the relaxation energy.

From Eq. (9) the relaxation energy is equal to the product of the stress and the perturbing strain tensors. Repeating the above process six times with different perturbing strains, we obtain six such equations. We solve this set of six equations for the six components of the symmetric stress tensor. For computational convenience, we can assume that at any one time only one component of the perturbing strain is nonzero.

The elastic constants of a solid are defined by

$$C_{ijkl} = \frac{\partial \sigma_{ij}}{\partial \varepsilon_{kl}}, \tag{11}$$

where the indices i,j,k, and l range over 1 to 3 corresponding to the Cartesian components of the tensor. The fourth rank elastic constant tensor is in general anisotropic and can be represented as a 6x6 matrix using the standard Voigt notation.

We evaluate each component numerically by first drawing a sufficiently large cell of atoms, for instance, a block of 20 x 20 x 20 unit cells. We impose a displacement field on the atoms according to the strain field specified above. The system is then relaxed while the boundary atoms are tightly held. The physical cell boundary consists of two layers of atoms. This is because in the Tersoff potential each atom interacts with up to its second neighbor atoms.

Finally, we calculate the stress at the reference atom as described above. The change of stress is set equal to the product of the elastic constants and perturbing strain according to Eq. (11). This again gives a set of six independent equations. Repeating the above process six times with different perturbing strains, we obtain 6 x 6 such equations that we solve for all 6 x 6 components of the elastic constant tensor in the Voigt contracted notation. The calculated elastic constant tensor exhibits the full symmetry of the solid.

The calculated values of the elastic constants for the free standing sSi that has tetragonal symmetry are given below in units of eV/ Å^3

C_{11} = 0.867, C_{12} = 0.381, C_{13} = 0.404, C_{33} = 0.700,
C_{44} = 0.387, and C_{66} = 0.464.

The values of the elastic constants of silicon in the same units, as predicted by the Tersoff potential, are C_{11}=0.89, C_{12}=0.471, and C_{44}=0.432.

We now calculate the effect of the substitutional defects in the sSi. The substitutional defects that we consider are vacancy, C and Ge impurities. As mentioned earlier, the defect can be fully characterized in terms of **M**, the dipole tensor, defined in Eq. (8). We calculate the values of the dipole tensor **M** in the sSi and compare these values with those obtained for the same defects in ordinary silicon. Ordinary silicon lattice has cubic

symmetry whereas sSi has tetragonal symmetry. Consequently **M** is diagonal and $M_{11}=M_{22}$ in both the cases. In the cubic case M_{33} is equal to M_{11} and M_{22}, but different in the tetragonal case.

For the cubic case of ordinary silicon, using the method described in Sec. III, we obtain the following values in eV for vacancy, Ge and C, respectively: M_{11} = 5.37, 1.45, and -16.2. For the sSi, the corresponding values of M_{11} and M_{33} in the same order and the same units are: M_{11}=8.22, 1.32, and -15.3; M_{33}=5.31, 1.52, and -13.7. We notice that the values of the components of **M** for C are negative which shows that C can act as strain compensator. The values of M are significantly different in the two cases, which shows the effect of large strain in the sSi. These values can also be measured in principle, and used to characterize the defects.

Now we consider the trilayer system described at the beginning of this section. As shown in Fig. 3, we form the reference state by placing a layer of compressed germanium lattice between two half-space silicon lattices. All layers are assumed to be parallel to the (0,0,1) plane of the silicon lattice.

The germanium layer is compressed enough in the lateral direction so that its lattice constant matches with that of the silicon lattice. We then allow the lattice to relax in the perpendicular direction keeping the lateral dimensions fixed. Similar to the previous case, this increases the lattice constant of germanium in the perpendicular direction from 5.6567 Å to 5.8145 Å, which we obtain by minimizing the energy under fixed lateral dimensions. The symmetry of the compressed germanium lattice is also reduced from cubic to tetragonal. We then allow the reference system to relax to its final equilibrium state leading to the sSi. The structure of the relaxed state is calculated by using the hybrid multiscale GF as described in Sec. II.

The relaxation of the lattice changes the interplanar spacings in the final state of the sSi. The interplanar spacings are a measure of strain in the sSi. We have calculated the interplanar spacing for the (0,0,1) planes as a function of the distance of the planes from the Si-Ge interface by minimizing the total energy [5]. The values are: 1.458 at the interface, and 1.3542, 1.3583, and 1.3580 in Å at the first, second, and third planes respectively in sSi. On the germanium side of the interface, the corresponding spacings are 1.4580, 1.4533, and 1.4536 in Å. We see that the spacing at the interface is almost equal to the average of the long distance interplanar spacings in silicon and germanium at large distances. These spacings can be measured and used to characterize the strain in the sSi.

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