Ab-initio Calculations of Shear Stress Effects on Defects and Diffusion in Silicon

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***Abstract*— In recent years a lot of attention has been given to engineering the stress state in ULSI devices to enhance device performance. As a result the stress conditions inside state-of-the-art devices are significantly more complex than simple hydrostatic or biaxial stress situations. In this paper we extend previous work on normal stress effects on point-defect equilibrium concentrations as well as point-defect and dopant diffusion to also include shear. We find there is little effect of shear stress on point-defect equilibrium concentrations. However shear is important for vacancy (V), interstitial (I), and boron (B) migration since it introduces anisotropies and off-diagonal elements in the diffusivity tensor. Diffusivity can no longer be view as a diagonal tensor, but instead a general tensor needs to be used to describe I, V, and B diffusion correctly.**

I. Introduction

Large stresses are present in the most recent ULSI devices due to geometry and material choices. Since it has been shown that stress can be utilized to increase device performance by enhancing carrier mobility [1], during recent years there has been an increasing effort to develop process recipes to incorporate additional stress. One example is the epitaxial growth of SiGe in the source/drain regions to compressively stress the channel [2]. The stress state in such devices is extremely geometry/material dependent and is significantly more complex than in simple hydrostatic or biaxial stress situations. Since experiments are extremely difficult and therefore predominately targeted toward hydrostatic and biaxial stress scenarios for simplicity [3], [4], we utilize *ab-initio* calculations to extend previous work on normal stress effects on formation and migration of point-defects and boron (B) diffusion [5] to investigate the effects of shear stress.

Since the standard MOS device configuration aligns the channel along the <110> direction of a (100) wafer surface, typically significant shear stresses are present for such devices in crystal coordinates. Our analysis extends beyond simple hydrostatic activation volumes [3] in order to predict anisotropies associated with more complex stress states which includes the determination of the general diffusivity tensor for defect and dopant migration.

Of particular interest are interstitial (I) and vacancy (V) equilibrium concentrations C_{I}^{*} and C_{V}^{*} since they are closely linked to dopant diffusion and activation. These quantities are directly related to the formation energies of the defects. Previous work [5] focused on the effect of normal stress on defect and dopant migration and found anisotropic diffusion for interstitial and boron migration. Nevertheless the diffusivity tensor remained diagonal in crystal coordinates. In the presence of shear stress this property of the diffusivity tensor changes. Here we determine the shear stress dependence of the off-diagonal elements.

This paper is organized in three main sections. First, we briefly review the most important parts of the methodology. In the second part we discuss the change in formation energy due to shear stress of interstitial and vacancy structures in different configurations to determine changes in C_{V}^{*} and C_{I}^{*}. The last part of the paper looks into the effects of shear stress on the I, V, and B diffusivity tensor. For all our calculations, we used the density functional theory (DFT) code VASP [7] with ultrasoft Vanderbilt type pseudopotentials [8]. The calculations were performed in generalized gradient approximation (GGA) with a 64/216 atom super-cell and different energy cut-off and Monkhorst-Pack **k**-point sampling to ensure convergence for different defects.

II. Methodology

Following the methodology of Ref. [5], the formation energy E_f of a defect in the presence of an arbitrary stress state σ can be written as a function of the elasticity tensor $C_{\alpha\beta}^{\mathrm{Si}}$ and the induced strain $\Delta\epsilon_\alpha$ of the defect:

$$E_f(\sigma) = E_f(0) - \Omega_0 \Delta\epsilon_\alpha C_{\alpha\beta}^{\mathrm{Si}} \epsilon_\beta + O(\epsilon^2) \approx E_f(0) - \Omega_0 \Delta\epsilon_\alpha \sigma_\alpha. \quad (1)$$

Ω_0 is the atomic volume of crystalline Si. The indices α and β run over the six different strain/stress types. The complexity to determine the induced normal and shear strains is strongly symmetry dependent. In previous work [5] induced normal strains for various defect structures were extracted for various defect structures by fitting the energy dependence to an equation-of-state. For defects with orthotropic symmetry the analysis to determine induced shear strains gets significantly reduced due to the special form of the elasticity tensor. When applying a simple shear stress there is no mixing between different shear/normal strains (see Eqn. 2 and 3) and the induced shear strains as well as shear moduli can be straightforwardly extracted. Equation 1 reduces to

TABLE I

COMPARISON OF EXPERIMENTAL LATTICE CONSTANT b_0 AND ELASTIC CONSTANTS C_{ij} OF SI WITH LDA AND GGA CALCULATIONS.

Method	b_0 [Å]	C_{11} [GPa]	C_{12} [GPa]	C_{44} [GPa]
Experiment [6]	5.4309	168	65	80
LDA	5.3903	158	65	
GGA	5.4566	156	55	75

$$\Delta E_f(\sigma) = -\Omega_0 \Delta\epsilon_n \sigma_n - \Omega_0 \Delta\epsilon_s \sigma_s + O(\epsilon^2), \qquad (2)$$

where the subscripts n and s refer to the normal and shear components of induced strain and stress respectively. Changes in formation energy due to normal and shear stress completely decouple. All defect configurations investigated in this paper have orthotropic symmetry. In previous work [5] the first term involving normal stresses was determined. Here we focus to compute the effects due to the second term:

$$\Delta E_f^s = -\Omega_0 \Delta\epsilon_s \sigma_s = -\Omega_0 (\Delta\epsilon_{xy}\sigma_{xy} + \Delta\epsilon_{xz}\sigma_{xz} + \Delta\epsilon_{yz}\sigma_{yz}). \qquad (3)$$

$\Delta\epsilon_{ij}$ and σ_{ij} $(i,j \in \{x,y,z\})$ denote induced shear strains and present shear stress respectively. All results are reported in crystal coordinates where x, y, and z refer to Si crystal axis along the <100> directions.

To validate this approach we computed the elastic properties of Si. Table I lists the lattice constant and elastic properties of Si extracted using above methodology and its experimental values. Both normal as well as shear moduli are predicted well by LDA and GGA. The slight under/overprediction of the lattic constant is a well-known artifact of the DFT functionals (LDA/GGA).

III. SHEAR STRESS EFFECT ON POINT-DEFECT EQUILIBRIUM CONCENTRATIONS

To predict the shear dependence of C_{V}^* we calculated the induced shear strain for a symmetric vacancy (V_{sym}) as well as for a vacancy structure including Jahn-Teller distortions (V_{JT}). In the absence of stress the Jahn-Teller distorted vacancy has a 0.16 eV lower formation energy. Both vacancy structures show no induced shear strains. This results in no shear strain dependence of C_{V}^*. In the case of C_{I}^* we determined the induced shear strains for a hexagonal (I_{hex}) and a <110> split interstitial (I_{split}). In the absence of stress I_{split} has a 0.09 eV lower formation energy than I_{hex}. Similar to the vacancy behavior I_{hex} does not exhibit any induced shear strains. The shear stress dependence of C_{I}^* is purely determined by I_{split} which exhibits a rather large induced shear strain of $\Delta\epsilon_{xy} = -0.5383$ (see Fig. 1).

When combining all contributions to C_{I}^* (different orientations of <110> I_{split}) we find that any type of shear stress always enhances C_{I}^*, but the actual enhancement is rather small (less than 20% enhancement at 0.5 GPa shear stress). Table II summarizes the induced shear strains for various point-defects and B structures.

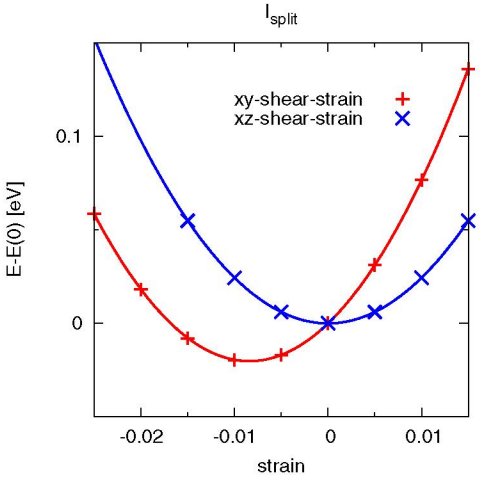

Fig. 1. Energy vs. shear strain for a $[1\bar{1}0]$ split interstitial in a $64\,\Omega_0$ cell. $E(0)$ is the system energy in the absence of any stress.

TABLE II

INDUCED SHEAR STRAINS $\Delta\epsilon$ FOR DIFFERENT DEFECT AND DOPANT CONFIGURATIONS. SYMMETRY RELATIONS ARE INDICATED BY $\Delta\epsilon_{ij}$ ENTRIES. THE INDUCED SHEAR STRAIN IS DETERMINED BY THE LOCATION OF THE MINIMUM ENERGY IN FIGS. 1, 2, AND 6.

Structure	$\Delta\epsilon_{xy}$	$\Delta\epsilon_{xz}$	$\Delta\epsilon_{yz}$
V_{sym}	0.0000	$\Delta\epsilon_{xy}$	$\Delta\epsilon_{xy}$
V_{JT}	0.0000	0.0000	$\Delta\epsilon_{xz}$
I_{hex}	0.0000	$\Delta\epsilon_{xy}$	$\Delta\epsilon_{xy}$
I_{split}	−0.538	0.0000	$\Delta\epsilon_{xz}$
B_s	0.0000	$\Delta\epsilon_{xy}$	$\Delta\epsilon_{xy}$
V_{trans} [111]	−0.368	−0.361	−0.365
I_{trans} $[31\bar{1}]$	−0.472	+0.402	+0.015
B_{trans} $[\bar{1}31]$	+0.340	−0.324	−0.349

IV. SHEAR STRESS EFFECT ON I, V, AND B DIFFUSION

To investigate the shear stress dependence of V, I, and B diffusion we determined the induced shear strains of the associated transition states V_{trans}, I_{trans}, and B_{trans}. As reported in earlier work, in the absence of shear stress V migration gets enhanced under compressive stress [5], but does not show any anisotropy (diagonal diffusivity tensor with single diffusivity). Our analysis shows that since V_{trans} shows induced shear strains (see Fig. 2) this symmetry gets broken in the presence of shear introducing anisotropies and off-diagonal elements in the diffusivity tensor.

We determined the actual shear stress dependence by considering a two-step migration process similar to I migration analysis [5]. Since the induced normal strains are equal in all three directions, all transition states get affected in the same way by normal stress which leads to a uniform diffusivity enhancement/reduction. This degeneracy of the transition states is lost in the presence of shear stress. Figure 3 illustrates the shear stress dependence of the diagonal V diffusivity tensor entries for a range of temperatures. Shear stress can introduce anisotropies in the diffusivity tensor which results in anisotropic diffusion. Nevertheless the anisotropies are only at the 10% level for shear stresses on the order of 0.5 GPa.

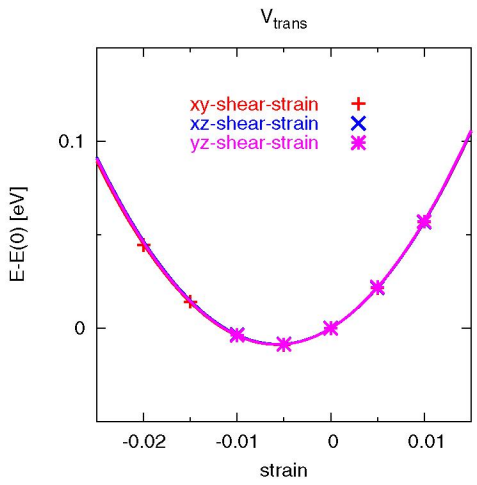

Fig. 2. Energy vs. shear strain for V_{trans} ([111] transition path) in a $64\,\Omega_0$ cell. $E(0)$ is the system energy in the absence of any stress. Due to the symmetry of the transition state the results for the three different shear strain conditions are essentially identical.

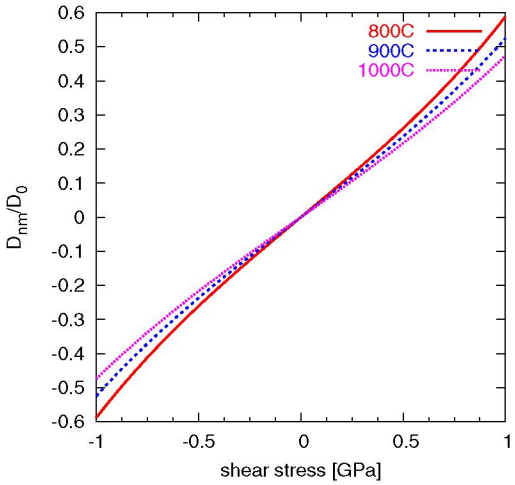

Fig. 4. Shear stress dependence of off-diagonal terms of the V diffusivity tensor for different temperatures. D_{nm} is a function of only the associated shear stress σ_{nm} $(n, m \in \{x, y, z\})$. In the absence of shear stress the off-diagonals vanish.

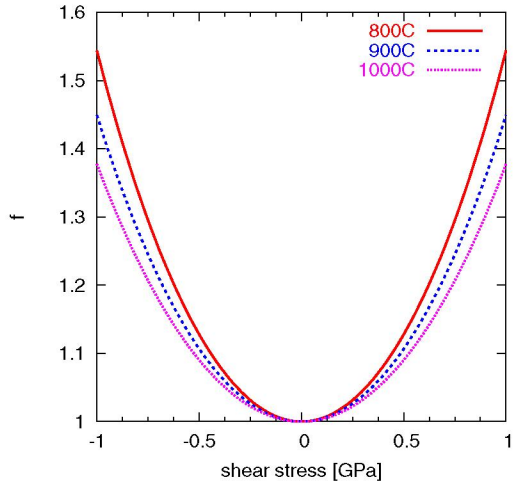

Fig. 3. Shear stress dependence of the diagonal enhancement function $f(\sigma)$ for V migration. The diagonal terms of the V diffusivity tensor get enhanced as $D_{nn}/D(0) = 1/2\,(f(\sigma_{nm}) + f(\sigma_{nl}))$ with $n, m, l \in \{x, y, z\}$ and $n \neq m \neq l$.

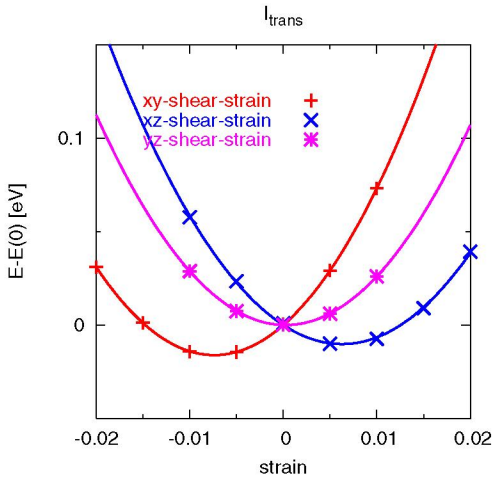

Fig. 5. Energy vs. shear strain for I_{trans} ([$31\bar{1}$] transition path) in a $64\,\Omega_0$ cell. $E(0)$ is the system energy in the absence of any stress.

Figure 4 shows the shear stress dependence of the off-diagonal terms of the V diffusivity tensor. In the presence of shear the diffusivity tensor is no longer diagonal which has important implications to V diffusion modeling. For instance a device under 1 GPA uniaxial compressive stress along the <110> channel direction exhibits -350 MPa shear stress in crystal coordinates which leads to a 20% off-diagonal term in the V diffusivity tensor (see Fig. 4).

Similar to the analysis for determining the induced shear strains for the V_{trans} we also computed the shear stress response for the interstitial I_{trans} and boron B_{trans} transition state. Figure 5 and 6 show the results. Both transition states exhibit rather large induced shear strains which suggest anisotropies and off-diagonal elements in the diffusivity tensor. Interstitial and boron diffusion share a very similar migration mechanism [5] which is significantly more complicated that V migration. In both cases the migration happens via two consecutive hops along <311> directions. Following the analysis to determine the normal stress dependence of I and B diffusion in Ref. [5] the effects of shear stress can be accounted for. Nevertheless the resulting expressions are rather cumbersome. Due to the nature of the special two-hop migration, normal and shear stress terms mix making it difficult to report the two effects individually.

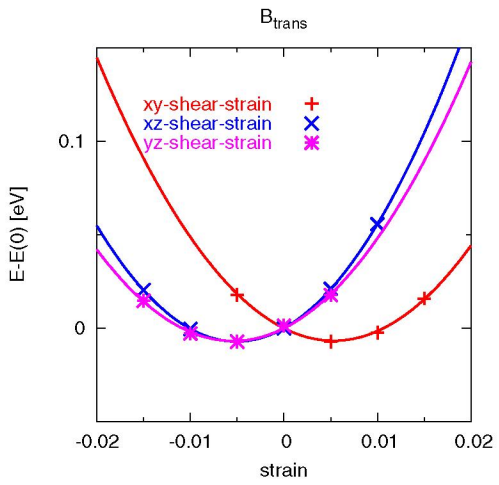

Fig. 6. Energy vs. shear strain for B_{trans} ([131] transition path) in a $64\,\Omega_0$ cell. $E(0)$ is the system energy in the absence of any stress.

V. Conclusion

In conclusion, there is little effect of shear stress on C_{I}^{*} and C_{V}^{*} respectively. However shear is important for V, I, and B migration since it introduces anisotropies and off-diagonal elements in the diffusivity tensor. Diffusivity can no longer be view as a diagonal tensor, but instead a general tensor needs to be used to describe I, V, and B diffusion correctly. This change critically affects the lateral diffusion in the tip region of highly scaled MOSFETs.

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