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**Abstract**  
This "Comment" addresses a recent paper of Cowern et al. concerning the diffusion of boron in GeSi alloys. The discussion indicates that the main factor leading to the retarded diffusion of boron in GeSi, (relative to Si) is the band-gap change. In his original paper, Cowern attributes the diffusion primarily to a change in defect formation energy. Copies of the relevant papers and the "Comment" are included for the convenience of the reader.

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TECHNICAL MEMORANDUM

Recently Cowern *et al.* have suggested a reduction in the point-defect formation energy in strained SiGe (relative to pure Si) to explain enhanced Ge diffusion and intermixing [1]. The same concept is used to explain previously reported results of the retarded boron diffusion observed in SiGe [2].

This interpretation of the retarded boron diffusion is different from the view reported in reference 2. In that letter we attributed the retardation to band-gap lowering rather than a modification of the defect formation energy. This comment clarifies the application of these two different views.

First we note that the boron diffusion experiments, were carried out under extrinsic conditions, with doping concentrations of  $1-8 \cdot 10^{19} \text{ cm}^{-3}$ , whereas intrinsic concentrations at diffusion temperature are lower than  $7 \cdot 10^{18} \text{ cm}^{-3}$  [2]. The density of charged point-defects plays an important role in boron diffusion both in the intrinsic and extrinsic regimes. However under extrinsic conditions, the band-gap reduction has an additional effect on the charged point defect density and must have a pronounced effect on the diffusion process.

The flux for dopant diffusion mediated by charged point defects, can be written as (assuming only neutral and positively charged point-defect contributions):

$$J_{A^-} = -h \left[ d_{A^-X^0}^i \frac{C_{A^-X^0}^i}{C_{A^-}} + d_{A^-X^+}^i \frac{C_{A^-X^+}^i}{C_{A^-}} \left[ \frac{p}{n_i} \right] \right] \frac{\partial C_{A^-}}{\partial x} \quad (1)$$

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where  $h$  is the electric field enhancement,  $p$  and  $n_i$  are the hole and intrinsic carrier concentrations and  $d$  and  $C$  represent intrinsic pair diffusivities and concentration respectively [3]. In a strained layer, all quantities may be modified except for the acceptor concentration  $C_{A^-}$ . In particular, changes in all Fermi-level related quantities, such as the free carrier concentrations and charged point-defect concentrations, should be considered as well as intrinsic parameters such as changes in point-defect forming enthalpies due to strain fields. We use the arguments given by Fair to include a band-gap change [4]. Modification to eq. 1 for the strained system must also allow for possible changes in the pair binding energies (neglected both in [1] and [2]) and the modified dopant/point-defect pair-formation energy, denoted by  $\epsilon$  (proportional to  $\exp(\Delta Q)$  in [1] with  $\Delta Q$  the change in the defect formation energy). The flux in the strained system  $J_{A^-}^*$  is (neglecting small changes in the electric field enhancement factor)

$$J_{A^-}^* = -h \left[ d_{A^-X^0}^i \frac{\epsilon C_{A^-X^0}^i}{C_{A^-}} + d_{A^-X^+}^i \frac{\epsilon C_{A^-X^+}^i}{C_{A^-}} \left[ \frac{p}{n_i} \right] e^R \right] \frac{\partial C_{A^-}}{\partial x} \quad (2)$$

with  $R = -\frac{\Delta E_f^i - \Delta E_{X^+}^i}{kT} - \frac{\Delta E_f}{kT} + \frac{\Delta E_g}{2kT}$  and  $\Delta E_{X^+}^i$  the modified defect energy level. Fair shows that under extrinsic acceptor concentration,  $R = \Delta E_g / 2kT$  with  $\Delta E_g$  the modified bandgap of the strained material (relative to pure Si). Note that the terms in  $R$  include all the bandgap related quantities associated with the change in the concentration of charged point defects and the change in the free carrier concentrations.

For the conditions of the boron diffusion experiment, the second term in eq. (2) dominates the diffusion [2, 5]. The analysis of the boron diffusion treats  $R$  as a fitting parameter, takes  $\epsilon = 1$  and shows that  $\exp(R) = e^{-0.3/2kT}$  in agreement with the expected bandgap change in the strained SiGe alloy [2]. The analysis in ref. 1 ascribed the retarded diffusion to the term  $\epsilon$  only, and noted that the fitted value,  $\exp(-0.17/kT)$ , was in reasonable agreement with the theoretical value for the modified (neutral) defect formation energy under strain [5]. The experimental data for the boron diffusion is clearly in the extrinsic regime, therefore both mechanisms may play a role and a measurement at a single boron concentration cannot distinguish these two factors. However, the boron concentration dependence of the diffusion has been reported [6]. This is a distinguishing experiment since the formation energy term,  $\epsilon$ , modifies both terms in eq. 2 while the bandgap factor,  $\exp(R)$ , modifies only the second term containing the dopant concentration. Kuo *et al.* report a significantly reduced boron concentration dependence for the diffusion in strained SiGe than in Si. This is consistent with the second term of eq. 2 being reduced (relative to the first term) and can be explained only by a bandgap modified mechanism. A change in formation energy only, would not change the relative weight of the two terms.

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## Diffusion in Strained Si(Ge)

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Experiments on Si-rich SiGe layers show an exponential increase in Ge diffusion and an exponential decrease in B diffusion as a function of compressive strain, indicating a linear dependence of activation energy on strain. The effect arises from the structural relaxation of the lattice around the defect mediating diffusion (inward for a vacancy, outward for an interstitial). We infer the mechanisms of Ge and B diffusion in strain-free and compressively strained Si(Ge) at  $T < 1030^\circ\text{C}$ , and draw some general conclusions on strain-modified diffusion in crystalline solids.

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Strained SiGe/Si heterostructures and superlattices are an essential component of many advanced Si-based devices, but the kinetic mechanisms of SiGe layer relaxation during thermal annealing are still poorly understood. Most previous work on strained-layer relaxation has focused on the nucleation, growth, and multiplication of dislocation loops during growth and subsequent thermal annealing. However, some workers have reported an alternative, diffusive relaxation process [1,2]. In particular, Iyer and LeGoues have reported enhanced Si-Ge interdiffusion which is quenched on formation of a high density of dislocations [2]. This observation was attributed to strain-assisted diffusion, based on the thermodynamic analysis of spinodal decomposition by Cahn and Hilliard [3], but no specific physical mechanism for the enhanced Si-Ge interdiffusion has so far been proposed. This remains a significant challenge for our understanding of diffusion in Si and related materials.

Recently, enhanced As diffusion [4] and retarded B diffusion [5,6] have been reported in compressively strained Si-rich SiGe layers. In particular, Moriya *et al.* presented extensive data showing a large reduction (up to a factor of 10) in the intrinsic diffusivity of B in Si(Ge) under compressive strain. By making the critical assumption that B diffusion is mediated by positively charged point defects, Moriya *et al.* were able to explain their result in terms of band-gap narrowing [6]. Although this assumption is consistent with early diffusion data [7], it appears to be incorrect. More extensive diffusion studies, using isoconcentration *p*-type and *n*-type backgrounds, have shown that the contributions of charged and neutral point defects to intrinsic B diffusion are of similar magnitude [8,9]. This conclusion rules out a strong reduction in intrinsic B diffusion due to band-gap narrowing, and points to a more drastic strain-related phenomenon.

A hint as to the nature of this phenomenon can be found in recent total-energy calculations [10,11]. Antonelli and Bernholc computed the formation energies for self-interstitials ( $\Delta E_{II}$ ) and vacancies ( $\Delta E_{IV}$ ) in Si as a function of hydrostatic pressure. A linear increase in  $\Delta E_{II}$  and decrease in  $\Delta E_{IV}$  were found with increasing pressure, corresponding to an outward relaxation of the

lattice around the interstitial, and an inward relaxation of the vacancy. More recently, the same authors computed the effect of tensile strain in a Si layer coherently grown on a  $\text{Si}_{1-x}\text{Ge}_x$  substrate. Again, the calculations suggested linear changes in point defect formation energies. Despite the potential implications for diffusion in strained Si and SiGe, these computational findings have never been tested experimentally.

This paper describes an experimental study of the diffusive relaxation of highly strained SiGe layers. We determine the local diffusion behavior by fitting numerical diffusion simulations to high-resolution depth-profile data obtained by secondary-ion mass spectrometry (SIMS). Strain is measured by high-resolution x-ray diffraction (XRD). Our observations show a clear influence of strain on the local equilibrium properties of point defects in Si. We determine the mechanism of interdiffusion in the Si:Ge system under compressive strain, and find a consistent explanation for anomalies in As and B diffusion in strained SiGe. Our conclusions will be of general relevance to diffusion in a wide range of crystalline solids.

Samples were grown on (100) Si wafers by atmospheric-pressure chemical vapor deposition (APCVD) or molecular-beam epitaxy (MBE). After deposition of a Si buffer layer, SiGe layers with thicknesses in the range 20–120 nm and Ge compositions in the range 0.1–0.3 were deposited, and capped with a second intrinsic Si layer. Samples were subsequently annealed in dry  $\text{N}_2$  at temperatures from 900 to 1050  $^\circ\text{C}$ , for times in the range 4 min to 4 h, using furnace or rapid thermal annealing.

In thin samples, relaxation by interdiffusion is kinetically favored compared with relaxation by growth of dislocations. In this regime, for the samples used in this study, we find that the diffusivity and its dependence on Ge composition are independent of the growth method and choice of layer thickness. Figure 1 shows a typical example. Ge concentration profiles for a MBE-grown sample with an initial Ge composition of 0.3, measured before and after rapid thermal annealing for 4 min and 15 min at 1030  $^\circ\text{C}$ , are plotted. The profiles in this sample are much "flatter" and steep sided than the Gaussian curves that would be produced by a constant diffusion coeffi-

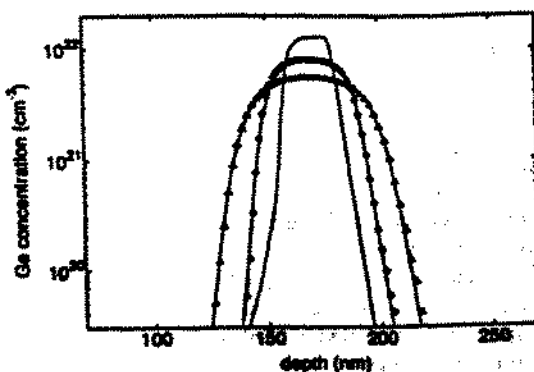


FIG. 1. Concentration-depth profiles of Ge in a MBE-grown Si/SiGe/Si structure, before and after annealing for 4 min and 15 min at 1030 °C. Symbols represent SIMS measurement data and curves represent simulations of strain-assisted diffusion with the dependence  $\hat{D} = D \exp(-Q's/kT)$ .

cient, indicating a strong enhancement of interdiffusion as a function of Ge composition. Because the diffusion at high concentration is so fast, the Ge composition,  $x$ , of a thin layer decreases rapidly in the initial stages of diffusion. For example, in Fig. 1,  $x$  decreases from 0.3 to 0.18 during a 4-min anneal at 1030 °C. In thick samples that relax by dislocation growth, the diffusivity enhancement in the compressively strained SiGe layer is much weaker, correlating with the low level of residual strain measured by high-resolution XRD. Our results confirm the conclusion of Iyer and LeGoues that enhanced Si-Ge interdiffusion in Si-rich SiGe is driven by strain [2].

Quantitative insight into the influence of strain on interdiffusion can be obtained by fitting the measured diffusion profiles for dislocation-free samples, using a numerical solver for nonlinear impurity diffusion. In the absence of evidence for chemical driving forces, thermodynamic considerations indicate a diffusivity enhancement of the form  $\hat{D}/D = f(s)$ , where  $\hat{D}$  is the diffusivity in the strained material,  $D$  is the corresponding diffusivity in unstrained material,  $s(y)$  is the strain in the plane of the SiGe layer at depth  $y$ , and  $f(s)$  is an unspecified function. Although a specific form for  $f(s)$  can be predicted from theory, we avoid consideration of this until the data analysis is complete. According to Vegard's law, in the absence of relaxation via dislocations,  $s$  is related to the Ge composition  $x$  by  $s = (1 - c_{Ge}/c_{Si})x = -0.042x$ . The minus sign indicates that the strain is compressive.

The simulations use the initial as-grown profile as a starting point. Since the diffusion is strongly nonlinear, we deconvolute the SIMS instrumental resolution function,  $I(y)$ , from the measured as-grown profile, prior to the diffusion simulation. The resolution function for our SIMS system, for the conditions of interest here, can be accurately represented by a triangular profile with full width at half maximum  $\Delta$ , convoluted with a function of the form  $\exp(y/\lambda_r)$  ( $x < 0$ ),  $\exp(-y/\lambda_d)$  ( $x > 0$ ). Under the present conditions the parameters of  $I(y)$  are given by  $\Delta = 2.3$  nm,  $\lambda_r = 0.4$  nm, and  $\lambda_d = 2.3$  nm.

The deconvolution is achieved by convoluting a trial function for the true as-grown Ge distribution,  $C_{Ge}(y, t = 0)$ , with the previously determined SIMS instrumental resolution function  $I(y)$ , and fitting the result to the measured as-grown profile. This procedure gives excellent fits to the as-grown profiles for both APCVD and MBE-grown layers. The profile  $C_{Ge}(y, t = 0)$  is then used as the initial condition for computing the nonlinear diffusion solution,  $C_{Ge}(y, t)$ , using the diffusion equation  $\partial C_{Ge}/\partial t = \nabla(D\nabla C_{Ge})$ . Finally, we convolute  $I(y)$  with  $C_{Ge}(y, t)$  to obtain an accurate comparison with SIMS measurements for the diffused profile.

The diffusion simulations are carried out using two forms for the diffusivity  $\hat{D}(s)$ . In the first case, we assume an empirical relation  $\hat{D}/D = 1 + As^n$  where  $n$  is an integer. A crude match to the diffusion profiles can be obtained with  $n = 2$ , but the simulated concentration dependence in the flanks of the profiles is too weak, leading to an exponentially decaying (shocklike) diffusion front that does not appear in the data. In the second case, we assume the form  $\hat{D}/D = \exp(As)$ . This gives a smooth increase of diffusivity with concentration, matching the positive curvature of the diffusion profile that is present down to Ge concentrations of a few times  $10^{20}/\text{cm}^3$  ( $x \sim 0.01$ ).

Using the form  $\hat{D}/D = \exp(As)$ , we have separately fitted all the diffusion profiles obtained in the present study, using  $A$  as an adjustable parameter. The extracted values of  $A$  are found to vary inversely with the annealing temperature, implying a diffusivity of the form  $\hat{D} = D \exp(-Q's/kT)$ , where  $Q'$  has dimensions of energy per unit strain. The diffusion enhancement factor,  $\hat{D}/D$ , plotted as a function of  $s/kT$ , is shown in the upper part of Fig. 2. Each data point represents, in compact form, a complete curve fit to one diffusion profile. For each fit the diffusivity at the peak of the profile is plotted against the corresponding value of  $s/kT$ . The data are within errors consistent with a straight line, yielding  $Q' = 40 \pm 5$  eV per unit strain. Thus, for example, a 1% strain is expected to produce a 0.4 eV change in  $Q$ .

This is the first time, to our knowledge, that an exponential increase of diffusion with strain has been directly determined from experiment. The effect implies a linear dependence of the activation energy of diffusion,  $Q$ , on strain,  $s$ , of the form  $Q(s) = Q(0) + Q's$  where  $Q' = dQ/ds$ .

The present data show no evidence of chemical driving forces that would make  $\hat{D}$  dependent on the Ge concentration gradient. The absence of gradient effects in samples with very high composition gradients can be attributed to the very similar diffusivities of Si and Ge in the Si lattice [12].

Since the measured migration barriers for point-defect diffusion in Si are small [13], the change in activation energy must have arisen from a decrease in the formation energy of the defect mediating interdiffusion. This implies a substantial inward-breathing relaxation, a key

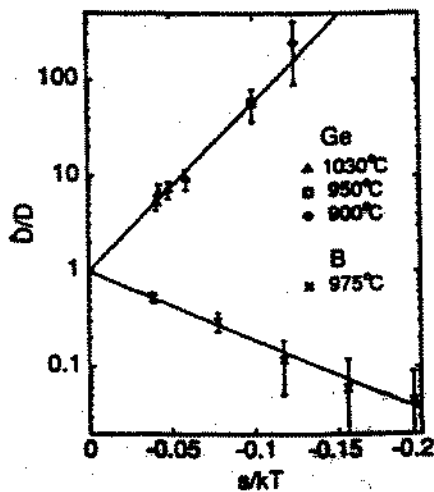


FIG. 2. Diffusion of Ge and B in compressively strained Si(Ge), as a function of  $s/kT$ . Data for Ge are from the present work, and data for B are from Ref. [6]. The positive slope for Ge reflects a decrease in the activation energy of Ge diffusion under compression. The negative slope for B reflects an increase in the activation energy of B diffusion.

piece of evidence as to the identity of the defect. Interstitial defects cause an outward displacement of the surrounding lattice and thus an increase in the defect formation energy in compressively strained Si. This rules out an interstitial mechanism for the enhanced interdiffusion. On the other hand, total-energy calculations predict an inward-breathing relaxation of the bulk vacancy defect in Si [11]. We conclude that the mediating defect is a vacancy.

In the absence of chemical driving forces, the diffusion coefficient in a strain-free crystal is given by  $D = D_{(i)} + D_{(v)}$ , where  $D_{(i)}$  and  $D_{(v)}$  are the interstitial and vacancy-mediated components of diffusion under strain-free conditions. In a strained layer, the diffusivity generalizes to

$$\hat{D} = D_{(i)} \exp(-Q'_{(i)}s/kT) + D_{(v)} \exp(-Q'_{(v)}s/kT). \quad (1)$$

As already mentioned, this formulation assumes that  $Q$  varies linearly with strain. This assumption appears to be reasonable for the values of strain encountered in SiGe films on Si, and is supported by the total-energy calculations in Ref. [11]. Equation (1), with appropriate physical constants, is applicable to both self-diffusion and impurity diffusion. Because of the opposite relaxation behavior of interstitial and vacancy defects, we expect  $Q'_{(i)} < 0$  and  $Q'_{(v)} > 0$ .

In the case of Ge diffusion, we see no evidence of a significant contribution from the first exponential term in Eq. (1). Such a contribution would have displaced the straight-line fit for Ge in Fig. 2 from its intercept of  $\hat{D}/D = 1$  at  $s/kT = 0$ . We infer that  $D_{Ge(v)} > D_{Ge(i)}$  in the temperature range of our experiment. This conclusion is consistent with existing data

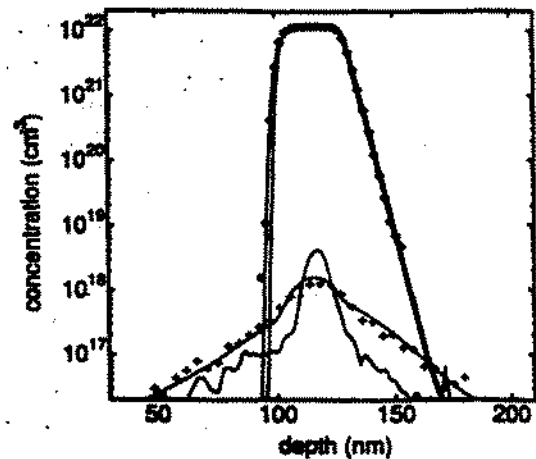


FIG. 3. Diffusion of a Si/Si<sub>0.75</sub>Ge<sub>0.25</sub>/Si structure containing a B dopant spike, annealed for 30 min at 910 °C. Curves represent a simulation of the Ge and B profiles before and after annealing, and symbols represent SIMS measurement data after annealing.

on Ge diffusion in strain-free Si which suggest a transition from vacancy-mediated diffusion at temperatures below 1050 °C, to interstitial-mediated diffusion at temperatures above 1100 °C [12].

In the case of impurity diffusion, the response to strain depends on the relative values of  $D_{(i)}$  and  $D_{(v)}$  for the impurity. Existing data for As and B in Si suggest that  $D_{As(v)} > D_{As(i)}$  [12], but that  $D_{B(v)} \ll D_{B(i)}$  [14]. This suggests an increase in the diffusivity of As as the lattice is compressed, and a corresponding decrease in the diffusivity of B. This accounts perfectly for the trends in As and B diffusion observed in recent experiments [4,6].

The decrease in intrinsic B diffusivity as a function of compressive strain, determined in Ref. [6], is plotted as a function of  $s/kT$  in Fig. 2. The straight-line fit to the data gives a value of  $Q'_{B(i)} = -17 \pm 3$  eV per unit strain, consistent with an outward relaxation of the Si lattice around the migrating B interstitial (or B-interstitial pair) defect. As commented earlier, this effect is much larger than can be explained in terms of band-gap narrowing. The absence of an exponentially increasing component of B diffusion shows that  $D_{B(v)}$  is much smaller than  $D_{B(i)}$ .

We now briefly consider the use of our model in computer-aided design of technology (TCAD) for SiGe strained-layer devices. Figure 3 shows SIMS measurements and simulations of the codiffusion of Ge and B, for a Si/Si<sub>0.75</sub>Ge<sub>0.25</sub>/Si structure grown with a narrow B doping spike, and annealed for 30 min at 910 °C in dry N<sub>2</sub>. The starting point for the simulation consists of the as-grown profiles of Ge and B, extracted from SIMS measurements as described above. In addition to the previously discussed parameters for Ge, we use the standard intrinsic diffusivity of B from Ref. [7], and the value of  $Q'_{B(i)} = -17$  eV per unit strain determined from Fig. 2. Solid curves indicate Ge and B profiles before and after annealing, and symbols represent SIMS measure-



ments. To improve the clarity of Fig. 3, measurement data below about 3 times background ( $\sim 10^{15}/\text{cm}^2$  for Ge and  $\sim 10^{16}/\text{cm}^2$  for B) have been omitted from the figure. The simulation predicts the correct magnitude of the retardation of B diffusion within the SiGe layer. Simulations like this will give engineers a clearer picture of events taking place within a device structure during processing.

In summary, we have been able to reach a consistent picture of the response of interdiffusion and impurity diffusion to strain in the Si lattice. We find a convincing degree of consistency between experimental results on Ge and B diffusion in SiGe, and qualitative insights from computational physics [10,11,15].

Finally, we note some unresolved issues. We have shown that composition dependent effects on interdiffusion are relatively weak in Si-rich SiGe in the range  $x < 0.3$ , but this does not rule out the possibility of substantially different interdiffusion behavior in Ge-rich SiGe. Interdiffusion in Si-rich SiGe is predominantly determined by the diffusivity of Ge in Si, whereas interdiffusion in Ge-rich SiGe will be determined by the diffusivity of Si in Ge, which is currently unknown. The behavior of B diffusion in Ge-rich SiGe is also unclear. Most group-III and group-V impurities diffuse faster in Ge than in Si, but B has a very large volume mismatch in Ge and its diffusion behavior in Ge-rich SiGe might be different from that of other group-III impurities.

Diffusion in Si under tensile strain ( $\epsilon > 0$ ) has yet to be investigated experimentally. Equation (1) predicts an enhancement of interstitial-mediated components of interdiffusion and impurity diffusion, and a retardation of vacancy-mediated components. A comparison of diffusion under compressive and tensile strain will provide a sensitive measure of the  $D_{(i)}$  and  $D_{(v)}$  components of diffusion. This promises a conclusion to the debate over diffusion mechanisms in Si which has persisted for more than a decade.

The discussion in this paper is of general relevance to solid-state diffusion. Even in systems where chemical driving forces are important, Eq. (1) continues to describe the diffusivity under local equilibrium conditions. We therefore expect similar effects to be found in other

coherent systems. By constructing different strained-layer structures it will be possible to manipulate the relative strength of vacancy- and interstitial-mediated components of diffusion and gain deeper insights into point defects and diffusion in a range of materials.

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