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The intrinsic As diffusion properties have been determined in relaxed $\text{Si}_{1-x}\text{Ge}_x$ epilayers. The properties were studied as a function of composition x for the full range of materials with $x=0, 0.20, 0.35, 0.50, 0.65, 0.8,$ and 1 . The activation enthalpy E_a was found to drop systematically from 3.8 eV ($x=0$) to 2.4 eV ($x=1$). Comparisons with other impurity atom- and self-diffusion results in Si, Ge, and SiGe show that both interstitials and vacancies contribute as diffusion vehicles in the composition range $0 \leq x \leq 0.35$ and that vacancy mechanism dominates diffusion in the composition range $0.35 < x \leq 1$.

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I. INTRODUCTION

Silicon-germanium (SiGe) alloy has been under intensive study during the last years, since it has turned out to be a promising candidate for the electronic industry as a substituting and accompanying material for Si in integrated circuits (see, for example, Refs. 1,2). In case of SiGe the major advantage over other novel compound semiconductors is that the processing techniques are highly compatible with the conventional Si technology. The knowledge on the diffusion properties of relaxed and strained SiGe has a great importance not only for device processing, but also from the scientific point of view.

For silicon and germanium it is generally accepted that self-diffusion occurs via point defects.³ Since all common impurities used for Si and Ge doping dissolve almost exclusively into substitutional sites, this also holds for dopant atoms. Therefore the nature and concentration of point defects determine the diffusion properties in these semiconductors.

On the other hand, there is a clear difference in the self-diffusion and dopant atom diffusion properties of Si and Ge. Silicon self-diffusion is known to proceed via both interstitial mediated and vacancy mechanisms.⁴ The vacancy fraction for Ge diffusion in silicon has been found to be slightly higher than in case of self-diffusion.⁵ Of typical dopant atoms, antimony atoms have been found to diffuse fully via vacancies whereas phosphorus and boron are interstitial mediated diffusers. In the case of As the diffusion is found to proceed, similar to self-diffusion, by both mechanisms.⁶ Self-diffusion as well as As diffusion in germanium has been found to proceed via vacancies.^{3,7} Also silicon diffusion in germanium has been found to proceed via vacancies, but the diffusion is in this case slightly slower than germanium self-diffusion.⁸

It can be noted that the diffusion properties of the components of SiGe have been well studied, but diffusion in SiGe alloys has received surprisingly modest attention in the literature. The first self-diffusion study for Ge in SiGe was carried out already in 1974 by McVay and DuCharme with polycrystalline samples.⁹ These results and the recently published^{8,10} studies with single-crystal relaxed $\text{Si}_{1-x}\text{Ge}_x$ reveal a change from interstitial contributed to vacancy dominated diffusion in the composition range $x=0.2-0.35$. As in

pure germanium, Si is found to diffuse slightly slower than Ge also in relaxed $\text{Si}_{0.20}\text{Ge}_{0.80}$.¹¹ Systematic impurity diffusion studies in relaxed $\text{Si}_{1-x}\text{Ge}_x$ have been done for Sn (Ref. 12) and Sb (Ref. 13) up to composition $x=0.5$.

In addition to the studies mentioned above, there are also dopant atom diffusion studies in strained SiGe (Refs. 14–18) and studies carried out under extrinsic conditions.^{19–21} However, strain introduces pressure as an additional thermodynamic parameter, which further complicates the interpretation of the diffusion results.¹⁷ By definition intrinsic conditions prevail when the charge carrier concentration is controlled by thermally excited electrons whereas under extrinsic conditions the charge carrier concentration is dominated by electron transitions due to impurities. Changes in Fermi level due to the doping may alter the defect concentration and charge state distribution, which influences impurity-defect interactions. Thus under extrinsic conditions the diffusion is affected both by type and concentration of the dopant atoms. Very high impurity atom concentrations can even introduce impurity-impurity interactions.^{22,23} Strain and extrinsic conditions are important from the SiGe applications point of view, but deep understanding of the processes involved require first knowledge on the diffusion properties in the simplest case. Therefore the present diffusion experiments were carried out in relaxed SiGe and under intrinsic conditions.

In this paper we present the first diffusion results for As in relaxed and intrinsic $\text{Si}_{1-x}\text{Ge}_x$. This is also the first time the full range of compositions from $x=0$ to $x=1$ has been covered for dopant atom diffusion in relaxed $\text{Si}_{1-x}\text{Ge}_x$. The present results are compared with As behavior in intrinsic Si and Ge as well as with relevant previous experimental diffusion results obtained for relaxed, intrinsic SiGe.

II. DIFFUSION VIA VACANCIES AND INTERSTITIALS

Under intrinsic conditions we can assume that the diffusing element forms an ideal dilute solution with the lattice where it diffuses. Excluding also all other free energy gradients, the temperature dependence of the tracer diffusion in a solid via defect of type x can be expressed by the Arrhenius law²⁴

$$D_x^T = f_x C_x^{\text{eq}} D_x = D_{x,0} \exp\left(-\frac{E_{a,x}}{kT}\right), \quad (1)$$

where f_x , C_x^{eq} , and D_x are the correlation factor, atomic fraction in thermal equilibrium, and diffusivity of defects x . $D_{x,0}$ is the preexponential factor, k Boltzmann's constant, and E_a the activation enthalpy. If several defect types are involved, the total diffusion coefficient is just the sum of the individual diffusion coefficients for different defect types.

Since diffusion depends both on concentration and diffusivity of the defect, the pre-exponential factor $D_{x,0}$ and activation enthalpy $E_{a,x}$ can be written as

$$D_{x,0} = f_x g_x a^2 \nu_{x,0} \exp(S_x^f + S_x^m) \quad (2)$$

and

$$E_{a,x} = E_x^f + E_x^m, \quad (3)$$

where f_x , g_x , a , $\nu_{x,0}$ are the correlation factor, numerical factor, lattice parameter, and the attempt frequency of defects x , respectively. S_x^f and S_x^m are the formation and migration entropies and E_x^f and E_x^m are the formation and migration enthalpies.

The preexponential factor values for semiconductors (for Si $D_0 = 2 \times 10^{-1}$ m²/s and for Ge $D_0 = 10^{-2}$ m²/s) are generally much larger than for metals (typically $D_0 = 10^{-4}$ m²/s),^{3,24} which is considered to result from the large entropy of formation of the defects needed for diffusion [see Eq. (2)]. For Si and Ge the large entropy has been explained by the formation of extended defects. In case of Si this means liquidlike self-interstitials and in case of Ge smeared out amorphouslike vacancies.^{3,25,26} Calculations for silicon self-diffusion, however, show that the large entropy may result also from native point defects.²⁷

Impurity atom diffusion involves, in addition to self-diffusion, interactions with impurity atoms and native point defects. The impurities may have different charge state and size than the host atoms in the crystal. Defect-impurity interactions are assumed to result from Coulomb and so-called elastic effects. Electrically charged vacancies interact with the impurities since the impurity atoms are ionized at the diffusion temperatures. Elastic effects are a result of the local strain caused by the host and impurity atom size difference. An oversized impurity atom induces stress to the lattice, which can be relieved by the presence of a vacancy close to it. The extra space in the lattice left by an undersized impurity atom is compensated by a self-interstitial.

The first model to describe impurity atom diffusion via vacancies was introduced by Hu.²⁸ According to this model for one complete diffusion step, the vacancy must diffuse far enough from the impurity atom so that it can return to a different lattice site adjacent to the impurity atom via a different path. In diamond lattice, as in case of silicon and germanium, the vacancy must diffuse at least to a third-nearest neighbor site in order to complete one diffusion step.

The activation enthalpy in this case can be expressed accordingly as²⁹

$$E_a^{\text{AV}} = E_a^{\text{SD}} - 1/2(E_b^2 + E_b^3), \quad (4)$$

where E_a^{SD} is the activation enthalpy of self-diffusion and E_b^2 and E_b^3 are the impurity-vacancy binding energies for a vacancy at the second and third closest neighbor lattice site to the impurity, respectively. According to Eq. (4) if no attraction exists between the impurity and the vacancy, activation enthalpy of diffusion is equal to that of self-diffusion. Otherwise the activation enthalpy is lower than for self-diffusion, as has been experimentally observed to be the case for most impurities.^{3,24}

It can be also noted from Eq. (4) that if the vacancy-impurity atom interaction extends further than the third nearest neighbor site, the vacancy does not need to overcome the full binding energy induced potential barrier in order to diffuse. This can lead to a so-called E -center or correlated diffusion where the vacancy and the impurity can diffuse as a pair. Both the strength and nature of the vacancy-impurity interaction determine the atomic details of vacancy diffusion. Similar to the vacancy mechanism, in interstitial mediated diffusion the defect-impurity binding is suggested to be the reason for the lower impurity atom activation enthalpy when compared to self-diffusion.²²

III. EXPERIMENTAL TECHNIQUES

Several $\text{Si}_{1-x}\text{Ge}_x$ materials with differing compositions were studied. The 1- μm -thick relaxed $\text{Si}_{1-x}\text{Ge}_x$ (with $x = 0.35, 0.50, 0.65,$ and 0.80) epilayers were grown by low energy plasma enhanced chemical vapor deposition (LEPECVD)³⁰ on graded buffer layers with thicknesses 3.5, 5, 6.5, and 8.0 μm , respectively. The density of the threading dislocations was estimated to be about 10^6 cm⁻².³¹ The 1- μm -thick $\text{Si}_{80}\text{Ge}_{20}$ material was grown by chemical vapor deposition (CVD) on a graded buffer layer provided by Okmetic, Ltd., Vantaa, Finland. The Ge specimens were 1-mm thick, p -type, Czochralski (CZ) grown with high purity and dislocation free³² The studied 300- μm -thick p -type CZ-grown Si was pure and dislocation free (Okmetic).

The diffusion studies of As were performed by means of a modified radiotracer technique employing ⁷³As (half-life $T_{1/2} = 80.3$ d and decay by electron capture to ⁷³Ge) and ⁷²As ($T_{1/2} = 26.0$ h and decay by β^+ to ⁷²Ge) tracers. The ⁷³As implantation was carried out at the on-line isotope separator (ISOLDE) of the European Organization for Nuclear Research (CERN) in Geneva, Switzerland. The implantation energy was 60 keV, total fluence 4×10^{11} ions/cm² and implanted area 7 mm². The ⁷²As tracers were implanted at the ion guide isotope separator on-line (IGISOL) of the University of Jyväskylä, Finland. The implantation energy was 40 keV, total fluence 3×10^9 ions/cm² and implanted area 13 mm². The ⁷²As tracers were produced via reaction ⁷²Ge(p,n)⁷²As using 15 MeV proton bombardment on enriched 2-mg/cm²-thick ⁷²Ge layer evaporated on a thin Havar backing. In the implantations the As beam direction was at an angle 7° off to the (100) face in order to minimize the channeling effects. After implantation, part of the samples were cleaned in a similar manner as described in Ref. 8 and the rest were simply

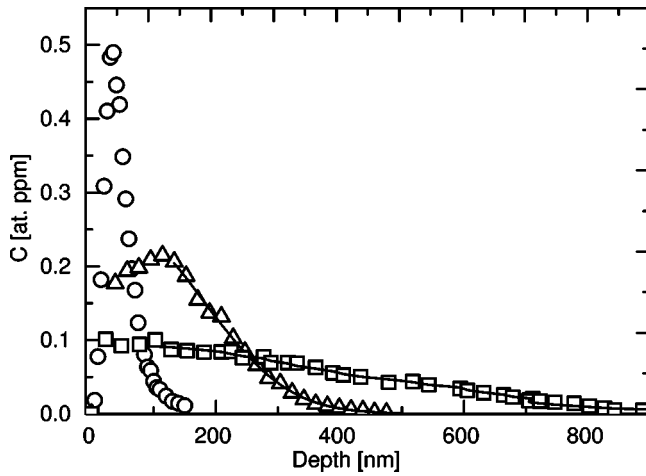


FIG. 1. ^{73}As profiles in $\text{Si}_{0.80}\text{Ge}_{0.20}$ epilayers produced by 60 keV implantation (\circ) and subsequent diffusion annealing at 882°C for 261 h (\square) and at 1060°C for 15 min (\triangle). The solid lines represent a fit of an appropriate solution of the diffusion equation to the diffusion profile.

cleaned with acetone, ethanol and distilled water.

Isothermal annealings were performed in a vacuum furnace under a pressure of 1×10^{-6} mbar and for part of the samples in an argon atmosphere. The studied temperature range was 490 – 1120°C and the annealing times varied from 10 min to 230 h.

The subsequent sample serial sectioning was done by 1.2 keV ion beam sputtering with a mixture of O^+ and N^+ . The removed material was collected on a foil that was wound up segment by segment as film in camera. The concentration profiles were constructed by determining the radioactivity of the individual foil segments proportional to the radiotracer concentration at corresponding depth. The results were corrected for the nuclide decay. A cooled Ge detector with a thin Be window was used for measuring the γ rays emitted due to the deexcitation of the daughter nuclei ^{72}Ge and ^{73}Ge .

IV. RESULTS

A typical as-implanted profile representing the initial conditions and subsequent diffusion profiles are shown in Fig. 1. The solid lines represent solutions of the diffusion equation, which fulfill appropriate boundary conditions. From such fits the diffusion coefficients D were extracted and are presented in Fig. 2 together with the literature data for As diffusion in Si (Ref. 33) and Ge.^{34–36} As can be noted from Fig. 2, for all compositions the As diffusion follows the Arrhenius law [Eq. (1)]. No clear difference in the results obtained for the two used isotopes (i.e., isotope effect) and for different implantation fluences were observed. As was shown earlier,¹¹ the used fluences are so low that the effect of radiation damage due to implantation is negligible. The results were also independent of the sample cleaning procedures prior annealing as well as of the applied annealing conditions. The obtained activation enthalpies (E_a) and preexponential factors (D_0) of As diffusion in SiGe are compiled in Table. I.

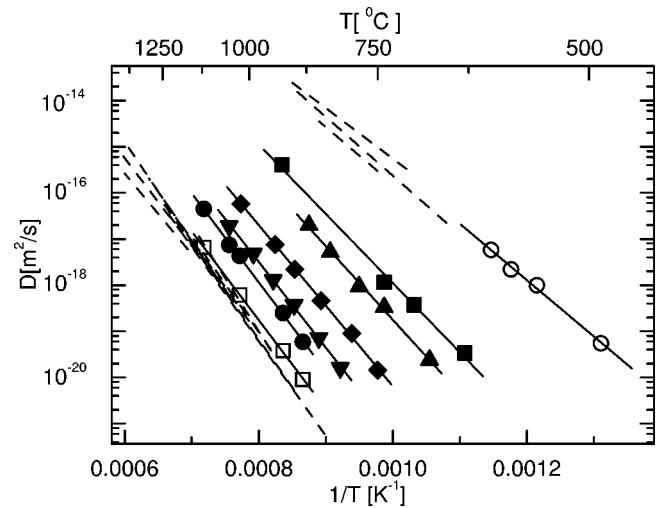


FIG. 2. Arrhenius plots of diffusion coefficients for As in Si (\square), $\text{Si}_{1-x}\text{Ge}_x$ (\bullet : $x=0.20$, \blacktriangledown : $x=0.35$, \blacklozenge : $x=0.50$, \blacktriangle : $x=0.65$, \blacksquare : $x=0.80$) and in Ge (\circ). The literature values for As diffusion in Si (Ref. 33) and Ge (Refs. 34–36) are presented as dashed lines.

V. DISCUSSION

The present results obtained in pure Si and Ge show fairly good agreement with the literature data taking into account the wide range scatter in available literature data. The scatter is probably due to the different experimental methods and conditions employed in these studies.

The results obtained from diffusion studies carried out in thermal equilibrium do not yield direct information on microscopic diffusion mechanisms. However, we can draw some conclusions of them by comparing the present results with recent self-diffusion^{8,10} and Sb (Ref. 13) data for relaxed SiGe. The results for Sn (Ref. 12) are omitted since they differ qualitatively from the present results and from those of Ref. 13 (having much higher D_0 values). Furthermore, the diffusion of Sn in Si has been found to be anomalous.³⁷

All self-diffusion studies suggest that above $x=0.35$ diffusion in $\text{Si}_{1-x}\text{Ge}_x$ is vacancy dominated.^{8–10} Diffusion of As in Ge is also considered to proceed via vacancies.³ When

TABLE I. Activation enthalpies (E_a) and pre-exponential factors (D_0) of the As tracer diffusion coefficients as a function of $\text{Si}_{1-x}\text{Ge}_x$ composition x . The stated uncertainties are from line fittings to points presented in Fig. 2.

$\text{Si}_{1-x}\text{Ge}_x$ composition x	Temperature range [$^\circ\text{C}$]	E_a [eV]	D_0 [$10^{-4} \text{ m}^2 \text{ s}^{-1}$]
0	882–1120	3.81 ± 0.05	4.3 ± 2.5
0.20	882–1120	3.83 ± 0.06	30 ± 20
0.35	812–1050	3.68 ± 0.06	23 ± 16
0.50	750–1020	3.47 ± 0.06	18 ± 13
0.65	675–870	3.16 ± 0.11	16 ± 54
0.80	696–925	2.97 ± 0.15	11 ± 64
1.00	490–600	2.42 ± 0.11	5.8 ± 3.2

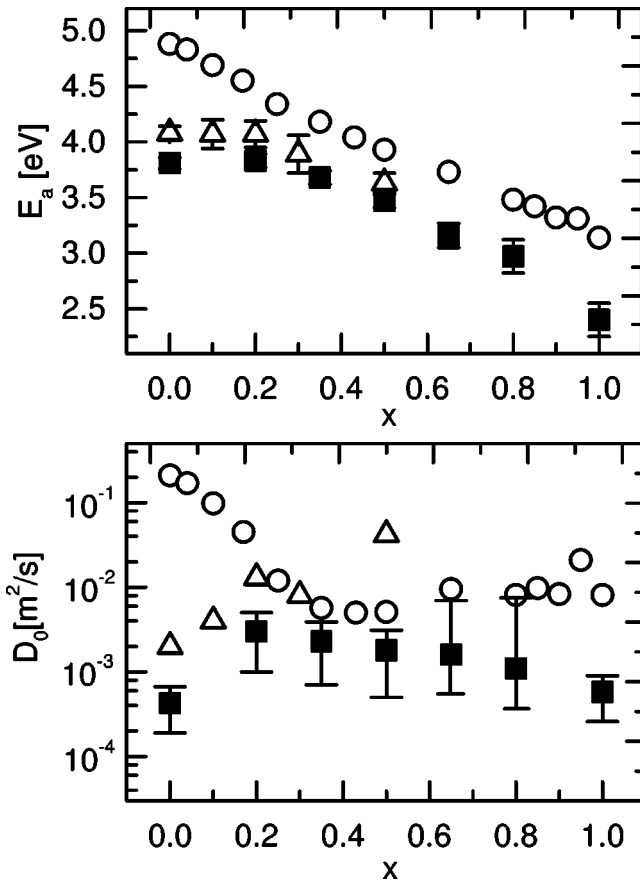


FIG. 3. Activation enthalpies E_a (upper) and preexponential factors D_0 (lower) as a function of $\text{Si}_{1-x}\text{Ge}_x$ composition for As (■), Sb (△) (Ref. 13), and self-diffusion (○) (Ref. 8). The error bars given represent statistical uncertainties.

the present As activation enthalpies are compared with Ge self-diffusion values for SiGe at the composition region $0.35 < x \leq 1$, it can be noted that first, their dependence of the SiGe composition is very similar and second, the values for As are constantly about 0.5 eV lower (Fig. 3). On the basis of the first observation, we suggest the vacancy mechanism also dominates for As diffusion in SiGe within composition region $0.35 < x \leq 1$. The decrease in activation enthalpy as a function of x results from the decrease in vacancy formation energy. This has also been confirmed by calculations.³⁸ The second observation can be interpreted by comparisons with calculations. In the absence of well established calculations for vacancy diffusion in Ge, the present results are compared with calculations for As-vacancy interactions and diffusion in Si. Recent results show that vacancy-As diffuse as a pair in Si.³⁹ When As-vacancy binding energies at different lattice sites are taken into account, according to Eq. (4) the difference in the activation enthalpies is 0.4–0.5 eV for self-diffusion and As diffusion via vacancies in Si.^{39,40} As the present results are in excellent accordance with the calculations, we suggest that the vacancy mediated As diffusion in SiGe also proceeds as As-vacancy pairs.

The situation is less clear within the composition range $0 \leq x \leq 0.35$. In Fig. 3 the results for Sb are also shown which is known to diffuse only via vacancies throughout the

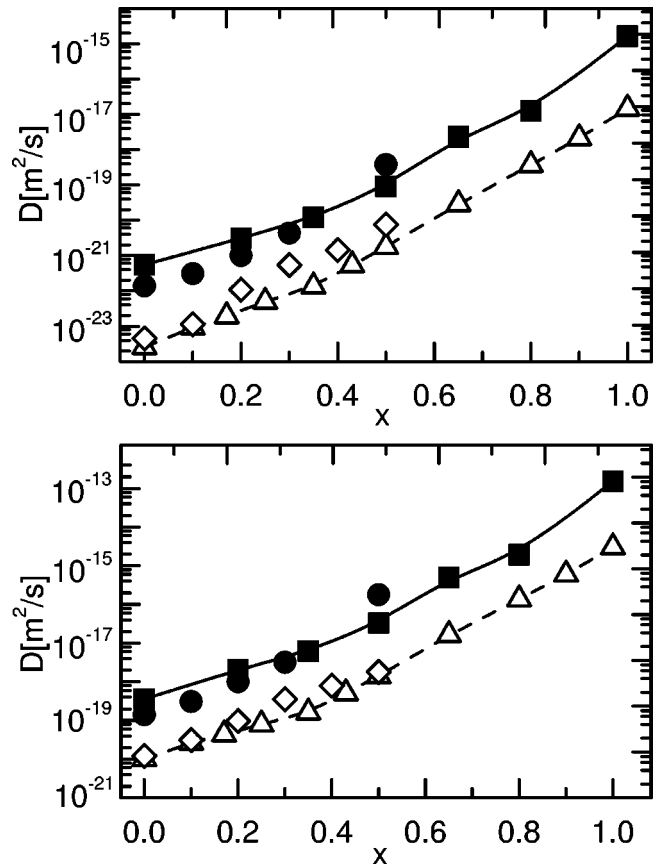


FIG. 4. Comparison of diffusion rates as a function of composition for As (■) and Sb (●) (Ref. 13) at $T = 1000^\circ\text{C}$ (upper figure) and $T = 800^\circ\text{C}$ (lower figure). The corresponding values for self-diffusion are also given \triangle from Ref. 8 and \diamond from Ref. 10.

composition range. The similarity in E_a compositional dependency suggests that vacancy mechanism prevails also for As diffusion in this composition range. This is, however, in contradiction with the finding that As diffuses both via vacancies and interstitials in Si.⁶ To study the situation in more detail the compositional dependency of As and Sb diffusion rates at constant temperatures $T = 1000$ and 800°C are plotted in Fig. 4. According to literature at these temperatures As is found to diffuse in Si slightly faster than Sb.^{3,24} On the other hand, the vacancy mechanism diffusion model predicts that Sb should diffuse faster than As in Si since vacancy-impurity binding energies for Sb (> 1.44 eV) are higher than for As (> 1.23 eV)⁴¹ [see Eq. (4)].

From Fig. 4 it can be noted that the D values for Sb are systematically lower than for As in $\text{Si}_{1-x}\text{Ge}_x$ with $0 \leq x \leq 0.35$. It should be, however, taken into account that the results of Fig. 4 for Sb and As have been obtained by different techniques. Therefore, also the self-diffusion results obtained with these experimental methods are shown. The self-diffusion studies reveal that MBE-grown heterostructures combined with depth profiling by secondary ion mass spectrometry (SIMS)^{10,13} yield consistently slightly higher D values than those obtained by the modified radiotracer technique applied in this work and in Ref. 8. The reason for this discrepancy is at the moment unclear. Taking into account

this possible difference induced by the experimental methods, As diffusion seems to be enhanced relative to Sb diffusion as x approaches zero. This enhancement is most probably due to the contribution of the interstitial mediated mechanism as the diffusivity composition dependencies for As and self-diffusion⁸ are similar. The relative enhancement seems to be more or less the same at both temperatures $T = 800$ and 1000°C shown in Fig. 4. This indicates that interstitial contribution on diffusion is not (at least strongly) temperature dependent at temperatures $T < 1000^\circ\text{C}$. This is in accordance with findings for different diffusion mechanism contributions in Si.⁶

The phenomenological model presented by Pakfar⁴² for diffusion in SiGe supports also the contribution of interstitials in As diffusion in the composition range $0 \leq x \leq 0.35$. On the basis of the diffusion results of Ref. 13 for Sb and P in strained SiGe (Refs. 17,43) the model predicts the compositional dependence of the ratio $D(\text{SiGe})/D(\text{Si})$ up to $x = 0.4$ for interstitial and vacancy mediated mechanisms. The diffusion enhancement as a function of increasing x for relaxed SiGe is assigned as a chemical effect. This effect results essentially from the increase in the number of weaker and less stiff Si-Ge and Ge-Ge bonds compared with the number of more stiff and strong Si-Si bonds.⁴⁴ Present As results for the compositional dependence of $D(\text{SiGe})/D(\text{Si})$ values settle between the values for vacancy and interstitial mediated mechanisms. This indicates the contribution of both interstitials and vacancies to As diffusion.

The D_0 values for As diffusion (Fig. 3) seem to be lower than for self-diffusion⁸ throughout the composition range. The large experimental uncertainties assigned to the D_0 values hinder to draw definite conclusions, but this might result

from defect-As atom binding. The binding may diminish the smearing of extended defects or possible vibrational states of point defects and this in turn decreases the entropy [see Eq. (2)].

VI. CONCLUSIONS

We have measured the diffusion coefficients of implanted ^{72}As and ^{73}As in relaxed $\text{Si}_{1-x}\text{Ge}_x$ within the full composition range of $0 \leq x \leq 1$. The diffusion of As is seen to enhance as a function of x . This is mostly due to the decrease in the activation enthalpy values since the preexponential factor values are nearly independent of x . By comparing the present results with previous experimental data for relaxed SiGe, we conclude that in the composition range $0 \leq x \leq 0.35$ As diffuses both via interstitials and vacancies. In the range $0.35 < x \leq 1$ the diffusion is dominated by the vacancy mechanism. On the basis of the diffusion model for vacancies and theoretical calculations, we further conclude that the vacancy mechanism diffusion proceeds via vacancy-As pairs.

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