Sb-enhanced diffusion in strained $Si_{1-x}Ge_x$: Dependence on biaxial compression

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Enhanced Sb diffusion in biaxially compressed $Si_{1-x}Ge_x$ layers ($x=0.1$ and 0.2) is investigated. It is shown that the contribution of the biaxial strain to enhance the process of Sb diffusion in $Si_{1-x}Ge_x$ increases with increasing misfit compression from a factor of ~ 3 at 0.73 GPa ($x=0.1$) to ~ 10 at 1.40 GPa ($x=0.2$). Assuming the prefactors to be stress-independent, the Sb diffusion coefficients in biaxially compressed $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ were extracted as $0.4\times 10^2 \exp\{-[3.98\,(\mathrm{eV})\pm 0.12]/kT\}$ and $1.3\times 10^2 \exp\{-[3.85\,(\mathrm{eV})\pm 0.12]/kT\}\ \mathrm{cm^2/s}$, respectively. [S0163-1829(99)02808-8]

Diffusion processes in strained and relaxed $Si/Si_{1-x}Ge_x$ heterostructures are currently a topic of great interest, since they illustrate how a strain field actually affects the diffusion mechanisms in semiconducting materials.[1–5] However, the experimental results reported until now on the ability of the misfit strain to enhance/retard the diffusion in semiconducting heterostructures are contradictory.[1–5] There are several reasons for this disagreement. First, in the early reports[1,2] the diffusion enhancement in strained $Si_{1-x}Ge_x$ was extracted in comparison to that in unstrained Si while in more accurate recent communications[4,5] the comparison was provided between the diffusivities in strained and relaxed $Si_{1-x}Ge_x$ epilayers, and as a result the ''composition'' effect[4,5] was separated from the actual contribution of the strain field. Second, different types of diffusion tracers [e.g., Ge,[3] B,[4] and Sb (Ref. 5)] were used in order to detect the effect of the biaxial compression on the diffusion processes in $Si_{1-x}Ge_x$. For example, the diffusivity of B in $Si_{1-x}Ge_x$ ($x\leqslant 0.2$) was found to be almost stress-independent.[4] In contrast, Kringhøj *et al.*[5] detected a slight increase (by a factor of ~ 2) of the Sb diffusion coefficient in strained $Si_{0.91}Ge_{0.09}$ epilayers; the fact that this effect is so small was attributed to the low value of stress in the $Si_{0.91}Ge_{0.09}/Si$ heterostructure. It is a challenge to extend this measurement to higher compression ranges, i.e., $x\geqslant 0.1$, because of the difficulty to prepare thick enough strained epilayers which do not undergo stress relaxation during diffusion measurements at elevated temperatures.[6] Indeed, the in-plane compression stress in the epilayer is given by[7] $\sigma_\perp = -2\mu(v+1/v-1)f_m(x)$, where μ is the shear modulus of elasticity, v is Poisson's ratio of the epilayer, and $f_m(x)$ is the misfit parameter. In the case of the pseudomorphic $Si/Si_{1-x}Ge_x$ heterostructure $f_m(x) = (a_{Si_{1-x}Ge_x} - a_{Si})/a_{Si} = 0.0418x$, where a_i is the lattice constant of the respective material, and the absolute values of $\sigma_\perp$ are directly proportional to the Ge content.[7] For instance, for $x=0.1$ and 0.2, $\sigma_\perp$ yields 0.73 and 1.40 GPa, respectively.[8]

In the present experiment, the effect of the enhancement of Sb diffusion in biaxially compressed $Si_{1-x}Ge_x$ layers ($x=0.1$ and 0.2) is investigated. Relatively thin ($\leqslant 400$ Å) undoped strained $Si_{1-x}Ge_x$ epilayers ($x=0.1$ and 0.2) were used to accommodate Sb diffusion from a source buried in a Si-buffer layer with an abrupt profile towards the $Si_{1-x}Ge_x$ spacer. The result for the Sb diffusion coefficient in strained $Si_{0.9}Ge_{0.1}$ ($^*D^{Sb}_{Si_{0.9}Ge_{0.1}}$) is compared to those reported in Refs. 5 and 9 and Sb diffusivity values are also extracted in strained $Si_{0.8}Ge_{0.2}$ ($^*D^{Sb}_{Si_{0.8}Ge_{0.2}}$). Further, $^*D^{Sb}_{Si_{0.9}Ge_{0.1}}$ and $^*D^{Sb}_{Si_{0.8}Ge_{0.2}}$ were subsequently compared to Sb diffusion coefficients[10] in the unstrained (relaxed) $Si_{0.9}Ge_{0.1}$ ($D^{Sb}_{Si_{0.9}Ge_{0.1}}$) and $Si_{0.8}Ge_{0.2}$ ($D^{Sb}_{Si_{0.8}Ge_{0.2}}$), respectively.

Heterostructures with strained epitaxial layers of either $Si_{0.9}Ge_{0.1}$ or $Si_{0.8}Ge_{0.2}$ were grown by molecular beam epitaxy (MBE) in a VG-80 system on Si, (100)-oriented n^+ substrates. First, an $\sim$100-nm-thick undoped and, subsequently, an $\sim$300-nm Sb-doped Si-buffer layer were deposited on the substrate. The Sb concentration (N^{Sb}) was kept constant at $\sim 10^{19}\ \mathrm{cm^{-3}}$ throughout the doped layer. Further, undoped $Si_{0.9}Ge_{0.1}$ or $Si_{0.8}Ge_{0.2}$ spacers, 40 and 35 nm thick, were deposited. The use of these diffusion structures (with the source of Sb buried between the $Si_{1-x}Ge_x$ and the undoped part of the Si-buffer layers) made it possible to measure Sb diffusivities in both Si and $Si_{1-x}Ge_x$ within one heterostructure. The strained $Si_{1-x}Ge_x$ layers were deposited at 450 °C in order to suppress the nucleation of dislocations. Finally, the wafers were capped with an $\sim$100-nm silicon layer to increase the thermal stability of the structures.[11] A fraction of each wafer was not subjected to any further annealing and was used to measure the initial dopant and Ge profiles. Subsequently, to study Sb diffusion, the samples were heat treated in a vacuum furnace (10^{-7} Torr range) in the temperature range from 740 to 925 °C with an accuracy of ± 2 °C for a given temperature. Long time anneals were used in order to minimize the error related to the heating/cooling stages of <5 min. The annealing temperatures were different for the structures with different composition of the strained $Si_{1-x}Ge_x$ layers. For the samples with higher Ge content, the lower temperatures were used (in order to avoid stress relaxation and, in fact, rather fast Sb diffusion through the thin $Si_{0.8}Ge_{0.2}$ spacer).

Chemical Sb and Ge profiles were measured by secondary ion mass spectrometry (SIMS) using a Cameca IMS4f instrument with 3.5 keV O_2^+ primary ions. Si, Ge, and Sb isotopes

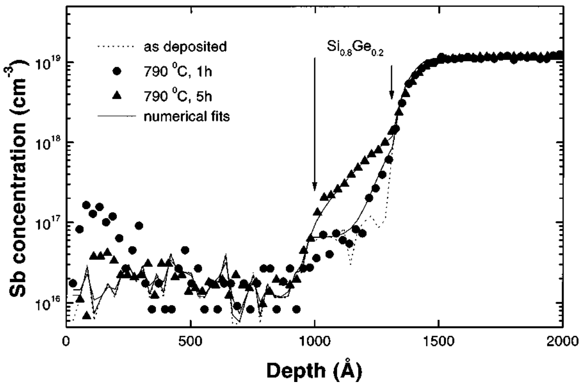

FIG. 1. Sb concentration vs depth profiles of the $Si/Si_{0.8}Ge_{0.2}/Si$ heterostructure before (dashed line) and after 790 °C anneals for 1 h (filled circles) and 5 h (filled triangles). The solid lines represent numerical solutions of the corresponding diffusion equations with $^*D^{Sb}_{Si_{0.8}Ge_{0.2}} = 6\times10^{-16}\,cm^2/s$.

were monitored in the form of positive secondary ions. The concentration calibration was provided by the measurement of an ion-implanted ($^{123}Sb^+$) reference sample. Under the assumption of a constant erosion rate, the depth calibration was obtained by measuring the total crater depth using an Alphastep 200 surface stylus profilometer.

Extensive structural characterization of both virgin and annealed $Si/Si_{1-x}Ge_x/Si$ samples was undertaken as well. It is important to emphasize that structural transformations which could potentially affect the Sb diffusion were accurately controlled, as presented elsewhere.[12] For instance, the structural quality of the samples and any possible strain relaxation in the $Si/Si_{1-x}Ge_x/Si$ heterostructures during the heat treatment for diffusion were checked by x-ray diffraction (XRD) using a $K\alpha_1$ Cu irradiation source. In particular, the diffusion data were collected only for those treatments which did not show any measurable strain relaxation. The actual Ge content in the as-deposited samples was measured by XRD and confirmed by Rutherford backscattering spectrometry (RBS).

The diffusion of Sb through the $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ layers is well described by a parabolic equation using the Sb distribution measured in as-deposited samples as the initial one together with appropriate boundary conditions. No segregation of Sb into the $Si_{1-x}Ge_x$ layer or away from it is detected in our samples.[13] The intrinsic carrier concentrations (n_i) in strained $Si_{1-x}Ge_x$ spacers, as calculated for the corresponding annealing temperatures and actual band offsets,[14] are comparable to the Sb concentration levels in the present experiment, and thus the effect of n_i on the diffusion process is expected to be small.[15] The actual values of $^*D^{Sb}_{Si_{1-x}Ge_x}$ were extracted by fitting of the experimental Sb profiles with the corresponding numerical solutions of the ordinary diffusion equation. For some of the high-temperature anneals, the values of Sb diffusivity in silicon (D^{Sb}_{Si}) were determined as well.

Experimental Sb profiles through the strained $Si/Si_{0.8}Ge_{0.2}/Si$ heterostructure annealed at 790 °C for 1 and 5 h are shown in Fig. 1. The numerical solution of the diffusion equation yields $^*D^{Sb}_{Si_{0.8}Ge_{0.2}} = 6\times10^{-16}\,cm^2/s$, which is considerably higher than D^{Sb}_{Si}, which was estimated to be

TABLE I. Experimentally determined diffusivities of Sb in strained $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ epilayers.

Temperature (°C)	Sb diffusivity (cm^2/s) $Si_{0.9}Ge_{0.1}$	Sb diffusivity (cm^2/s) $Si_{0.8}Ge_{0.2}$
740		1×10^{-17}
790		6×10^{-17}
815	1.8×10^{-17}	1.6×10^{-16}
830		2.5×10^{-16}
840		3.5×10^{-16}
855	8×10^{-17}	
905	4×10^{-16}	
925	8×10^{-16}	

$\sim10^{-17}\,cm^2/s$ at 790 °C. Similar measurements were performed at four other temperatures in strained $Si/Si_{0.8}Ge_{0.2}/Si$ and $Si/Si_{0.9}Ge_{0.1}/Si$ samples and the results for $^*D^{Sb}_{Si_{1-x}Ge_x}$ are listed in Table I. In accordance with previous reports,[5,9] $^*D^{Sb}_{Si_{1-x}Ge_x} \gg D^{Sb}_{Si}$, where the ratios of $^*D^{Sb}_{Si_{1-x}Ge_x}/D^{Sb}_{Si}$ include both ''compositional'' and stress contributions.[4,5] In order to extract the contribution of stress, $^*D^{Sb}_{Si_{1-x}Ge_x}$ is compared to reference data for Sb diffusion through relaxed $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ epilayers at the corresponding temperatures.[10] The difference between $^*D^{Sb}_{Si_{1-x}Ge_x}$ and $D^{Sb}_{Si_{1-x}Ge_x}$ was found to be dependent on x, and, for instance, in $Si_{0.8}Ge_{0.2}$ it is more than one order of magnitude at 740 °C, as illustrated in Fig. 2.

Further, the Sb diffusion coefficients in strained and relaxed $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ are compared in Figs. 3(a) and 3(b), respectively. Figure 3(a) demonstrates that the present experimental results are in accordance with the observations reported recently on the enhancement of Sb diffusion in biaxially compressed $Si_{0.9}Ge_{0.1}$ relative to relaxed $Si_{0.9}Ge_{0.1}$.[5,9] Moreover, the absolute values of $^*D^{Sb}_{Si_{0.9}Ge_{0.1}}$ determined in the present experiment are in agreement with those reported by Kringhøj *et al.*[5] in spite of completely different sample structures. However, the value given by Paine *et al.*[9] is considerably higher than both the present determination and that

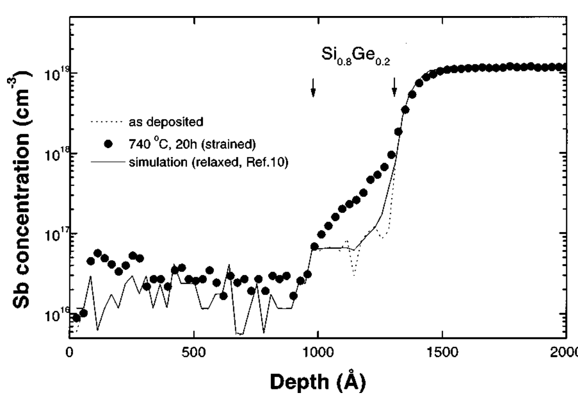

FIG. 2. Sb concentration vs depth profiles in $Si/Si_{0.8}Ge_{0.2}/Si$ heterostructures before (dashed line) and after 740 °C anneals for 20 h (filled circles). The solid lines represent a simulation of Sb diffusion in relaxed $Si_{0.8}Ge_{0.2}$ at the same temperature and for the same time, using $D^{Sb}_{Si_{0.8}Ge_{0.2}} = 7.3\times10^{-19}\,cm^2/s$ (Ref. 10).

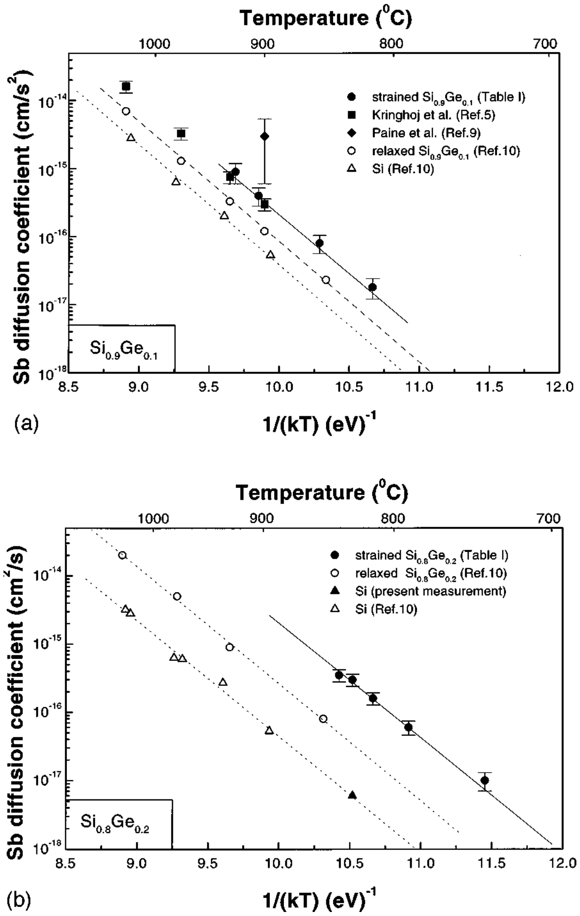

FIG. 3. Arrhenius dependence of Sb diffusion coefficients in $Si_{0.9}Ge_{0.1}$ (a) and $Si_{0.8}Ge_{0.2}$ (b). The present results (filled circles) are compared to the Sb diffusion coefficients determined in relaxed $Si_{1-x}Ge_x$ layers (open circles, after Ref. 10). Filled squares and diamonds refer to the recent measurements of Sb diffusivity in strained $Si_{0.91}Ge_{0.09}$ and $Si_{0.9}Ge_{0.1}$ after Refs. 5 and 9, respectively. Triangles represent the Sb diffusivity in silicon D_{Si}^{Sb} as determined in the present experiment (filled symbol) and as reported in Ref. 10.

in Ref. 5. This difference may be attributed to a considerable experimental uncertainty as shown by the error bars in Fig. 3(a).[9] A comparison of our results with those reported in Ref. 10 (open circles in Fig. 3) shows that the biaxial compression enhances the Sb diffusion in $Si_{1-x}Ge_x$, and, moreover, its contribution increases with increasing misfit compression from a factor of ~3 at 0.73 GPa ($x=0.1$) to ~10 at 1.40 GPa ($x=0.2$). To the best of our knowledge, this is the first experimental demonstration of a gradual increase of the Sb diffusivity upon the application of biaxial compression. In the following these results will be further interpreted.

Generally, temperature (T) and stress are the two parameters that define the change of the Gibbs free energy of a system during diffusion: $\Delta G^{dif}=\Delta E^{dif}-T\Delta S^{dif}+\sigma\Delta V^{dif}$, where ΔE^{dif}, ΔS^{dif}, and ΔV^{dif} are the activation energy, entropy, and volume of the diffusion process, respectively.[16] In accordance with the theory for the thermally activated processes,[16] the diffusion coefficient, for example $^*D^{Sb}_{Si_{0.8}Ge_{0.2}}$, is determined by the Arrhenius equation $A\exp(-\Delta G^{dif}/kT)=D_0\exp(-\Delta H^{dif}/kT)$, where A is a proportionality factor, $D_0=A\exp(\Delta S^{dif}/k)$ is the so-called prefactor, $\Delta H^{dif}=\Delta E^{dif}+\sigma\Delta V^{dif}$ is the activation enthalpy, and k is Boltzmann's constant.[17]

The trade-off between the strain relaxation process and the rate of Sb diffusion implies serious limitations for an independent determination of the activation enthalpies and prefactors for $^*D^{Sb}_{Si_{1-x}Ge_x}$. However, it is generally accepted that stress (in the range of 1–2 GPa) does not significantly affect the prefactor of the diffusion coefficient,[18] and under this condition ΔH^{dif} determines the change of the diffusion coefficient as a function of σ. Thus, using the prefactors given in Ref. 10 for "unstrained" $Si_{1-x}Ge_x$ (also listed in Table II), the Arrhenius expressions for $^*D^{Sb}_{Si_{0.9}Ge_{0.1}}$ and $^*D^{Sb}_{Si_{0.8}Ge_{0.2}}$ become $0.4\times10^2\exp\{-[3.98\,(\mathrm{eV})\pm0.12]/kT\}$ and $1.3\times10^2\exp\{-[3.85\,(\mathrm{eV})\pm0.12]/kT\}\,\mathrm{cm^2/s}$, respectively (Fig. 3, solid lines). In this case ΔV^{dif} can be estimated from $^*D^{Sb}_{Si_{1-x}Ge_x}/D^{Sb}_{Si_{1-x}Ge_x}=\exp(\Delta Q^{dif}/kT)$, where $\Delta Q^{dif}=\Delta E^{dif}-\Delta H^{dif}$ is the difference between the activation values of Sb diffusion in relaxed and strained $Si_{1-x}Ge_x$, respectively. Table II summarizes the Arrhenius parameters of $^*D^{Sb}_{Si_{1-x}Ge_x}$ and $D^{Sb}_{Si_{1-x}Ge_x}$, the values of ΔQ^{dif}_{Sb}, and the ratios of $\Delta Q^{dif}_{Sb}/\sigma_\perp$, which are related to a perpendicular component of the ΔV^{dif} tensor. Interestingly, the mean values obtained for $\Delta Q^{dif}_{Sb}/\sigma_\perp$ are of the order of Ω in both $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$ (where Ω is the volume corresponding to a silicon lattice site).[19] Further, using either the mean values of $\Delta Q^{dif}/\sigma_\perp$ from Table II or $Q'=24\pm5$ eV/unit strain[19] we arrive at a qualitative agreement with recent estimates by Aziz[20,21] (based on the experimental data from Ref. 5), which supports the hypothesis of the operation of a vacancy-mediated mechanism during Sb diffusion in $Si_{1-x}Ge_x$.[22]

In conclusion, a gradual enhancement of Sb diffusion with increasing biaxial compression in $Si_{1-x}Ge_x$ ($x=0.1$ and 0.2) layers has been observed. Relative to that in unstrained layers, the enhancement of Sb diffusion increases with the contribution of the biaxial strain from a factor of ~3 at 0.73 GPa ($x=0.1$) to ~10 at 1.40 GPa ($x=0.2$). Assuming the prefactors to be stress-independent, the Sb diffusion coefficients in biaxially compressed $Si_{0.9}Ge_{0.1}$ and $Si_{0.8}Ge_{0.2}$

TABLE II. Characteristic parameters of Sb diffusion in relaxed and strained $Si_{1-x}Ge_x$ epilayers. The last two columns represent the contribution of biaxial compression.

x	σ (GPa)	$D^{Sb}_{Si_{1-x}Ge_x,0}$ (Ref. 10) ($\mathrm{cm^2/s}$)	ΔE^{dif}_{Sb} (Ref. 10) (eV)	ΔH^{dif}_{Sb} (eV)	$\Delta Q^{dif}_{Sb}=\Delta E^{dif}_{Sb}-\Delta H^{dif}_{Sb}$ (eV)	$\Delta Q^{dif}_{Sb}/\sigma_\perp$ (Ω)
0	0	0.2×10^2	4.08 ± 0.07			
0.1	0.73	0.4×10^2	4.07 ± 0.13	3.98 ± 0.07	0.09 ± 0.20	1.00 ± 2.23
0.2	1.40	1.3×10^2	4.07 ± 0.12	3.87 ± 0.07	0.21 ± 0.19	1.18 ± 1.07

are extracted as $0.4\times 10^2 \exp\{-[3.98\,(\mathrm{eV})\pm 0.12]/kT\}$ and $1.3\times 10^2 \exp\{-[3.85\,(\mathrm{eV})\pm 0.12]/kT\}$ cm^2/s, respectively. Comparison of the present results with reference data on Sb diffusion in unstrained $Si_{1-x}Ge_x$ supports the hypothesis of the operation of a vacancy-mediated mechanism during Sb diffusion in $Si_{1-x}Ge_x$.

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[1] N. Moriya, L. C. Feldman, H. S. Luftman, C. A. King, J. Bevk, and B. Freer, Phys. Rev. Lett. **71**, 883 (1993).

[2] P. Kuo, J. L. Hoyt, J. F. Gibbson, J. E. Turner, R. D. Jacowitz, and T. I. Kamins, Appl. Phys. Lett. **62**, 612 (1993).

[3] N. E. B. Cowern, P. C. Zalm, D. J. Gravesteijn, and W. B. de Boer, Phys. Rev. Lett. **72**, 2585 (1994).

[4] P. Kuo, J. L. Hoyt, J. F. Gibbson, J. E. Turner, and D. Lefforge, Appl. Phys. Lett. **66**, 580 (1995).

[5] P. Kringhøj, A. Nylandsted Larsen, and S. Yu. Shirayev, Phys. Rev. Lett. **76**, 3372 (1996).

[6] J. W. Matthews and A. E. Blakeslee, J. Cryst. Growth **27**, 118 (1974); see also a recent review of R. Hull, in *Properties of Strained and Relaxed Silicon Germanium* (INSPEC, London, 1995).

[7] S. C. Jain, H. E. Maes, K. Pinardi, and I. De Wolf, J. Appl. Phys. **79**, 8145 (1996).

[8] A linear extrapolation of the Si and Ge elastic constants to the actual alloy composition was used in the present estimation of σ. For more details, see S. P. Baker and E. Artz, in *Properties of Strained and Relaxed Silicon Germanium* (INSPEC, London, 1995).

[9] A. D. N. Paine, M. Morooka, A. F. W. Willoughby, J. M. Bonar, P. Phillips, M. J. Dowsett, and G. Cooke, Mater. Sci. Forum **196-201**, 345 (1995).

[10] A. Nylandsted Larsen and P. Kringhøj, Appl. Phys. Lett. **68**, 2684 (1996).

[11] D. B. Noble, J. L. Hoyt, J. F. Gibbons, M. P. Scott, S. S. Laderman, S. J. Rosner, and T. I. Kamins, Appl. Phys. Lett. **55**, 1978 (1989).

[12] A. Yu. Kuznetsov, J. Cardenas, B. G. Svensson, J. Lundsgaard Hansen, and A. Nylandsted Larsen, in *Diffusion Mechanisms in Crystalline Materials*, edited by Yu. Mishin, G. Vogl, N. Cowern, R. Catlow, and D. Farkas, MRS Symposia Proceedings No. 527 (Materials Research Society, Pittsburgh, 1998), p. 435.

[13] S. M. Hu, D. C. Ahlgren, P. A. Ronsheim, and J. O. Chu, Phys. Rev. Lett. **67**, 1450 (1991).

[14] R. People, Phys. Rev. B **32**, 1405 (1985).

[15] P. M. Fahey, P. B. Griffin, and J. D. Plummer, Rev. Mod. Phys. **61**, 289 (1989).

[16] P. G. Shewmon, *Diffusion in Solids* (J. Williams Book Company, Jenks, USA, 1983).

[17] Note that both σ and ΔV^{dif} are, in general, tensors.

[18] R. N. Jeffery and D. Lazarus, J. Appl. Phys. **41**, 3186 (1970).

[19] The interpretation may be also performed in terms of Q' which has the dimension of "eV/unit strain" (Refs. 3 and 5) if one *a priori* assumes that $^*D^{\mathrm{Sb}}_{\mathrm{Si}_{1-x}\mathrm{Ge}_x}/D^{\mathrm{Sb}}_{\mathrm{Si}_{1-x}\mathrm{Ge}_x}=\exp\{-[Q' f_m(x)]/kT\}$. The value of $Q'=24\pm 5$ eV/unit strain has been calculated for both compositions using the data from Table I and Ref. 10. Note, that similar values of Q' can be reached from the mean values of ΔQ^{dif} (Table II) using $Q'=\Delta Q^{\mathrm{dif}}/f_m(x)$. The choice of a Q'—or ΔQ^{dif}—interpretation is, in fact, a compromise between a higher accuracy or a higher generality.

[20] M. J. Aziz, Appl. Phys. Lett. **70**, 2810 (1997).

[21] According to Aziz (Ref. 20) the equality $V^{\mathrm{dif}}+(3/2)\Delta Q^{\mathrm{dif}}/\sigma_\perp =\pm\Omega+(V_\parallel - V_\perp)$ holds for a diffusion process under biaxial compression, where $V_\parallel$ and $V_\perp$ are the dimension changes parallel and perpendicular to the direction of the net transport when the point defect reaches its saddle point. Assuming (i) a vacancy mechanism, using (ii) $\Delta Q^{\mathrm{dif}}/\sigma_\perp \approx 0.65\Omega$ (after 13 ± 3 eV/unit strain from Ref. 5), and (iii) neglecting the $V_\parallel - V_\perp$) term Aziz obtained that the equality holds for $V^{\mathrm{dif}}\approx 0$. Our mean values of $\Delta Q^{\mathrm{dif}}/\sigma_\perp$ (as well as $Q'=24\pm 5$ eV/unit strain) are somewhat higher than the one reported in Ref. 5 which may indicate a positive contribution of the $(V_\parallel - V_\perp)$ term in our samples.

[22] A. Yu. Kuznetsov, J. Grahn, J. Cardenas, B. G. Svensson, J. Lundsgaard Hansen, and A. Nylandsted Larsen, Phys. Rev. B **58**, R13 335 (1998).