Appl. Phys. A 68, 19–24 (1999)

Applied Physics A
Materials
Science & Processing

Dopant diffusion and segregation in semiconductor heterostructures: Part 2. B in $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ structures

C.-H. Chen, U.M. Gösele, T.Y. Tan[*]

Department of Mechanical Engineering and Materials Science, Duke University, Durham, NC 27708-0300, USA

Received: 20 August 1998/Accepted: 23 September 1998

Abstract. This is the second of a series of papers treating the shallow dopant diffusion and segregation problems in semiconductor heterostructures. Employing a segregation mechanism model, which incorporates the chemical effect, the Fermi-level effect, and the effect of the junction carrier concentrations, satisfactory fits of available boron distribution profiles in $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ heterostructures have been obtained. Here the chemical effects seem to be of less importance. The Fermi-level effect determines the ionized boron solubilities in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ and in Si, as well as the thermal equilibrium concentration of the singly-positively-charged crystal self-interstitials I^+ which governs the boron diffusion process. The junction carrier concentration affects the concentration of I^+ and solubility of B in the region and hence controls B diffusion across the heterojunction.

PACS: 61.72.Tt; 61.72.Ss; 61.72.Yx

Boron diffusion in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ epitaxial layers grown on Si substrates has recently drawn a wide interest [1–4]. Because of the higher electron mobilities, p-type $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layers are envisaged to constitute excellent base regions in high-performance Si-based heterojunction bipolar transistors [5, 6]. In these studies [1–4], the epitaxial layers were doped in situ by B during growth, and subsequently annealed to investigate the B diffusion behavior. In the studies of Kuo et al. [1, 2] and Fang et al. [3], distribution of B is primarily confined inside the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layers. The shapes of these B profiles are somewhat different from those expected for B in Si, indicating the existence of a difference in mechanisms governing the distribution of B in the two different cases. In the study of Lever et al. [4], B was introduced to an epitaxial Si layer confined between two $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layers and the diffused B profiles showed two concentration peaks in these confining $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layers. These authors have obtained satisfactory fits to their B diffusion profiles [1–4]. In modeling, however, formation of BGe pairs is assumed, which seems to be highly speculative. This assumption and the assumed B diffusion mechanism and diffusivity values used for obtaining the fits raise questions about the validity of the model employed in the analyses.

We have satisfactorily modeled the p-type dopant distribution problem in III-V compound superlattice (SL) structures (see the accompanying article [7]), for which the most outstanding feature is that the p-type dopants Zn and Be in III-V SL exhibit a prominent segregation behavior among the SL layers. In this model, the dopant segregation behavior is attributed to the solubility difference of the ionized shallow acceptor species in the different layer materials, which is determined by a chemical effect, a Fermi-level effect, and an effect of the junction carrier concentrations. The latter influences the junction-region concentration of the acceptors, and of the triply-positively-charged group III self-interstitials I_{III}^{3+}, which governs the diffusion processes of the acceptor species, and hence also the detailed dopant distribution process.

We expect that a similar model is also applicable to the case of B distribution in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ heterostructures. In the present paper, we report that indeed the available experimental B diffusion profiles [1–4] have been satisfactorily fitted employing just such a model. In the present analysis there is basically no case-to-case adjustable parameter for B distribution involving Si and $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layers with x in the range of 0–0.22. For all cases studied presently, basically the same B diffusivity value, that given in the literature for Si [8, 9], has been used.

1 Formulation of the problem

The B^- diffusivity in Si as suggested by Fair and Pappas [8] and by Fair [9] is

$$D_{\mathrm{s}}^{\mathrm{eff}} = D^+(n_{\mathrm{i}})\left(\frac{p}{n_{\mathrm{i}}}\right), \tag{1}$$

---

[*] E-mail: ttan@acpub.duke.edu

with

$$D^+(n_\mathrm{i}) = 13.1 \exp\left(-\frac{3.7\,\mathrm{eV}}{k_\mathrm{B}T}\right) \mathrm{cm}^2\mathrm{s}^{-1}\,, \tag{2}$$

where $D_\mathrm{s}^\mathrm{eff}$ is the substitutional B$^-$ atom diffusivity, $D^+(n_\mathrm{i})$ is $D_\mathrm{s}^\mathrm{eff}$ under intrinsic conditions, n_i is the Si intrinsic carrier concentration, p is the hole concentration, k_B is Boltzmann's constant, and T is the absolute temperature. In (1) the B$^-$ atom diffusivity is designated as an effective diffusivity $D_\mathrm{s}^\mathrm{eff}$ by reason of the B diffusion mechanism which we now discuss. The form of (1) indicates that a positively-charged point defect species governs B diffusion. This positively-charged point defect species should be the Si self-interstitial I^+ [10], and B diffuses via the interstitialcy mechanism according to

$$\mathrm{B_i^o} \Leftrightarrow \mathrm{B_s^-} + I^+\,, \tag{3}$$

where $\mathrm{B_s^-}$ is an ionized boron acceptor atom occupying a substitutional Si lattice position, and $\mathrm{B_i^o}$ is a neutral boron atom occupying the bond-centered interstitial position [11]. In this interstitialcy mechanism, diffusion of the $\mathrm{B_s^-}$ atoms, which are themselves immobile, is accomplished by the migration of $\mathrm{B_i^o}$ atoms, for which the rate is high, and the subsequent change-over of a $\mathrm{B_i^o}$ to become a $\mathrm{B_s^-}$ and produce an I^+ simultaneously. The thermal equilibrium concentration of $\mathrm{B_s^-}$ is large whereas that of $\mathrm{B_i^o}$ is small, and hence the measured B concentration is simply that of $\mathrm{B_s^-}$. The Si vacancy species also make a small contribution to $\mathrm{B_s^-}$ diffusion [10], which we ignore in the present analysis.

Details of the Fermi-level effect on the thermal equilibrium concentrations of ionized shallow acceptor and on other charged species have been discussed in the accompanying paper [7]. Accordingly, we have

$$C_\mathrm{s}^\mathrm{eq} = \frac{1}{g} C_\mathrm{s^o}^\mathrm{eq} \left(\frac{n_\mathrm{i}}{p}\right) \exp\left(\frac{E_\mathrm{i} - E_\mathrm{v}}{k_\mathrm{B}T}\right)\,, \tag{4}$$

where g is the hole degeneracy factor ≈ 4, C_s^eq is the thermal equilibrium concentration of $\mathrm{B_s^-}$, $C_\mathrm{s^o}^\mathrm{eq}$ is the thermal equilibrium concentration of the neutral boron atoms, $\mathrm{B_s^o}$, which is a constant, n_i is the crystal intrinsic carrier concentration, p is the hole concentration, E_i is the intrinsic Fermi level, E_v is the valence band edge energy, k_B is Boltzmann's constant, and T is the absolute temperature. Here we adopt the convention that the values of E_i and E_v are referenced to the vacuum level at 0 eV. We also have

$$C_\mathrm{I}^\mathrm{eq} = C_\mathrm{I}^\mathrm{eq}(n_\mathrm{i}) \left(\frac{p}{n_\mathrm{i}}\right)\,, \tag{5}$$

where C_I^eq is the thermal equilibrium concentration of I^+, and $C_\mathrm{I}^\mathrm{eq}(n_\mathrm{i})$ is the same quantity under intrinsic conditions. The concentration of $\mathrm{B_i^o}$ is a constant in a single material since it is a neutral species.

Our starting equations describing the diffusion processes of the three species $\mathrm{B_s^-}$, I^+ and $\mathrm{B_i^o}$ are

$$\frac{C_\mathrm{i}}{C_\mathrm{s} C_\mathrm{I}} = \frac{C_\mathrm{i}^\mathrm{eq}}{C_\mathrm{s}^\mathrm{eq} C_\mathrm{I}^\mathrm{eq}} = K\,, \tag{6}$$

$$C_\mathrm{I} = C_\mathrm{I}^\mathrm{eq}\,, \tag{7}$$

$$\frac{\partial C_\mathrm{i}}{\partial t} = \frac{\partial}{\partial x}\left(D_\mathrm{i} \frac{\partial C_\mathrm{i}}{\partial x} - \frac{C_\mathrm{i}}{C_\mathrm{i}^\mathrm{eq}} \frac{\partial C_\mathrm{i}^\mathrm{eq}}{\partial x}\right) - \frac{\partial C_\mathrm{s}}{\partial t}\,, \tag{8}$$

where C_i, C_s, and C_I are respectively the actual concentrations of $\mathrm{B_i^o}$, $\mathrm{B_s^-}$, and I^+, and D_i is the diffusivity of $\mathrm{B_i^o}$. Equation (6) is obtained according to reaction (3) by assuming dynamic equilibrium holding among $\mathrm{B_i^o}$, $\mathrm{B_s^-}$, and I^+. Equation (7) is obtained because B diffusion is slow and hence the I^+ concentration should not have been perturbed substantially from that under thermal equilibrium conditions. Equation (8) is obtained in accordance with reaction (3) using the diffusion–segregation formulation method [12], with the term $(C_\mathrm{i}/C_\mathrm{i}^\mathrm{eq})(\partial C_\mathrm{i}^\mathrm{eq}/\partial x)$ on its right-hand side accounting for the solubility difference of $\mathrm{B_i^o}$ in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ and in Si. In either material, C_i^eq is a constant independent of p since $\mathrm{B_i^o}$ is uncharged. Using (4) and (5), and noting that $C_\mathrm{s} + C_\mathrm{i} \approx C_\mathrm{s}$ holds and hence $\partial(C_\mathrm{s} + C_\mathrm{i})/\partial t \approx \partial C_\mathrm{s}/\partial t$ also holds, (6)–(8) yield

$$\frac{\partial C_\mathrm{s}}{\partial t} = \frac{\partial}{\partial x}\left[D_\mathrm{s}^\mathrm{eff}\left(\frac{\partial C_\mathrm{s}}{\partial x} + \frac{C_\mathrm{s}}{p}\frac{\partial p}{\partial x} - \frac{C_\mathrm{s}}{n_\mathrm{i}}\frac{\partial n_\mathrm{i}}{\partial x} - \frac{1}{k_\mathrm{B}T}\left(\frac{\partial E_\mathrm{i}}{\partial x} - \frac{\partial E_\mathrm{V}}{\partial x}\right) - \frac{C_\mathrm{s}}{C_\mathrm{s^o}^\mathrm{eq}}\frac{\partial C_\mathrm{s^o}^\mathrm{eq}}{\partial x}\right)\right]\,, \tag{9}$$

where $D_\mathrm{s}^\mathrm{eff}$ is the $\mathrm{B_s^-}$ effective diffusivity given by

$$D_\mathrm{s}^\mathrm{eff}(n_\mathrm{i}) = K C_\mathrm{I}^\mathrm{eq}(n_\mathrm{i}) D_\mathrm{i} \left(\frac{p}{n_\mathrm{i}}\right)\,. \tag{10}$$

Comparing this with (1), we see that

$$D^+(n_\mathrm{i}) = K C_\mathrm{I}^\mathrm{eq}(n_\mathrm{i}) D_\mathrm{i}\,. \tag{11}$$

A generalized hole-transport equation has been derived for application in III-V compound SL layers, see the accompanying article [7]. The treated effects include the hole segregation property in the layers and the junction electric field on the hole concentrations in the junction regions. This equation is applicable also to the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$/Si type heterostructures. Accordingly, we have

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x}\left[D_\mathrm{p}\frac{\partial p}{\partial x} - \frac{pD_\mathrm{p}}{N_\mathrm{V}}\frac{\partial N_\mathrm{V}}{\partial x} - \frac{pD_\mathrm{p}}{k_\mathrm{B}T}\frac{\partial E_\mathrm{V}}{\partial x} + \frac{pqD_\mathrm{p}}{k_\mathrm{B}T}\frac{\partial \phi}{\partial x}\right]\,, \tag{12}$$

where D_p is the hole diffusivity, N_V is the valence band effective density of states, q is the magnitude of the electron charge (taken to be positive), and ϕ is the electrostatic potential at the junctions. The potential ϕ satisfies Poisson's equation

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{q}{\varepsilon}\left[n - p + C_\mathrm{a^-} - C_\mathrm{d^+} - C_\mathrm{I}\right]\,, \tag{13}$$

where ε is the layer material dielectric constant, $C_\mathrm{a^-}$ is the ionized shallow acceptor density of all species that may be present, for example, B$^-$ and Al$^-$, $C_\mathrm{d^+}$ is the ionized donor density, and C_I is the I^+ concentration. The quantity $C_\mathrm{d^+}$ is included in (13) to account for also the possible presence of donors in the material layers. In the absence of the electric field, (13) is just the charge neutrality condition. Details of arriving at (12) have been discussed in the accompanying paper [7]. Because of the presence of the electrostatic potential ϕ, the carrier concentration at the junctions differ from those in the bulk of the involved material layers. The junction carrier concentrations influence the dopant distribution rate via their influences on the B_s^- solubility and on the concentration of I^+.

2 Analyses of experimental results

To analyze the experimental results of B_s^- diffusion in Ge_xSi_{1-x}/Si structures [1–4], (9), (10), (12), and (13) are solved numerically using the general-purpose partial different equation solver ZOMBIE [13]. Among the reported experimental results [1–4], Fang et al. [3] and Lever et al. [4] have given B_s^- diffusion profiles that are suitable for analyses. We have fitted these available B_s^- diffusion profiles. Kuo et al. [1, 2] reported extracted B_s^- diffusivity information but did not give useful B_s^- diffusion profiles.

Figure 1 shows the fits of the B_s^- experimental profiles of Lever et al. [4] obtained at 850 °C for $x = 0.03$ and 0.1, from which it is seen that the fits are satisfactory. The materials constants used in obtaining the fits, including the diffusivity value of B_s^-, are listed in Table 1. The other constants

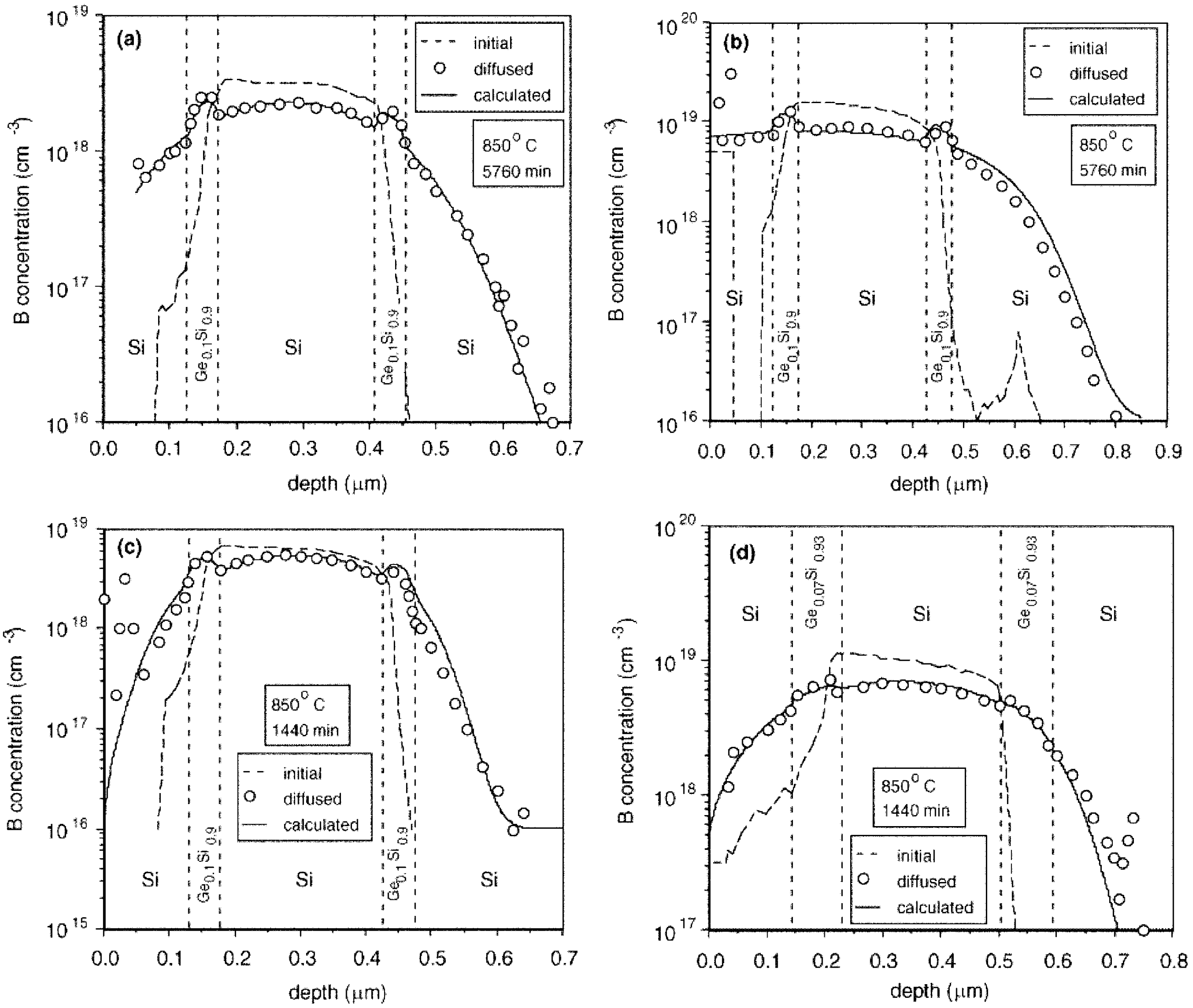

Fig. 1. Experimental B_s^- distribution data of Lever et al. [4] at 850 °C, fitted by the Fermi-level effect model with the effect of the junction carrier concentration also considered. The sample structural conditions and other experimental conditions are included in the drawing for each case

Table 1. Values of materials constants used for obtaining fits to the experimental results of Lever et al. [4]. The values of E_i and E_V are referenced to the vacuum level at 0 eV

Material	n_i /cm^{-3}	E_i /eV	E_V /eV	N_V /cm^{-3}	Structure	$D_S^{eff}(n_i)$ /cm^{2}s^{-1}
a: Si	3.4×10^{18}	−4.62	−5.15	8.2×10^{20}		
b: $Ge_{0.03}Si_{0.97}$	3.86×10^{18}	−4.606	−5.1278	8.2×10^{20}		
c: $Ge_{0.1}Si_{0.9}$	5.2×10^{18}	−4.574	−5.076	5.72×10^{20}		
					a/b/a/b/a	2.8×10^{-16}
					a/c/a/c/a	1.5×10^{-16}

include N_V, E_V, and n_i. For Si and Ge, the listed values are those available from the literature. For Ge_xSi_{1-x}, either available literature values of the appropriate quantity, or values weighted linearly by x from the Si and Ge values, have been used. These used values are room-temperature values, because high-temperature ones are not available, and there is also some needed basic information lacking for extrapolating them from the room-temperature ones to high temperature ones.

Figure 2 shows the fits of the B_s^- experimental profiles of Fang et al. [3] obtained at 850 °C for $x = 0.095$ and 0.225, from which it is seen that the fits are also satisfactory. The materials constants used in obtaining the fits are listed in Table 2.

We specifically note that, in obtaining these fits, the thermal equilibrium concentrations of the neutral B atoms in the Ge_xSi_{1-x} and Si materials, $C_{s^0}^{eq}$, are taken to be of the same value.

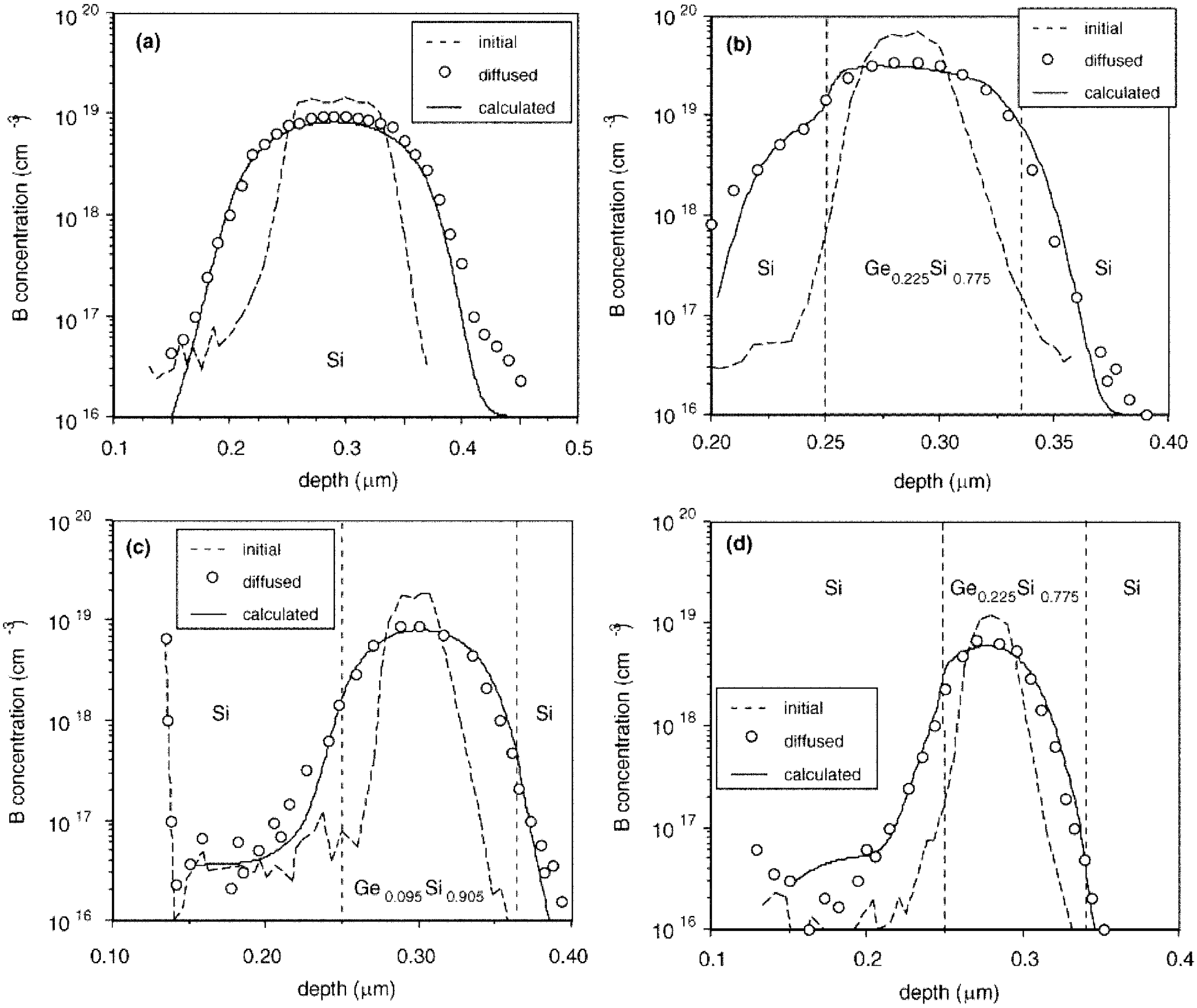

Fig. 2. Experimental B_s^- distribution data of Fang et al. [3] at 850 °C, fitted by the Fermi-level effect model with the effect of the junction carrier concentration also considered. The sample structural conditions and other experimental conditions are included in the drawing for each case

Table 2. Values of materials constants used for obtaining fits to the experimental results of Fang et al. [3]. The values of E_i and E_V are referenced to the vacuum level at 0 eV

Material	n_i /cm^{-3}	E_i /eV	E_V /eV	N_V /cm^{-3}	Structure	$D_S^{eff}(n_i)$ /cm^{2}s^{-1}
a: Si	3.4×10^{18}	−4.62	−5.15	8.2×10^{20}		
b: $Ge_{0.095}Si_{0.905}$	5.16×10^{18}	−4.577	−5.069	5.91×10^{20}		
c: $Ge_{0.229}Si_{0.901}$	8×10^{18}	−4.5	−4.99	4.98×10^{20}		
					a	3×10^{-16}
					a/b/a/b/a	1.9×10^{-16}
					a/c/a/c/a	$1.9–3 \times 10^{-16}$

3 Discussions

In III-V compound superlattices, the segregation process of Zn and Be are determined by: (i) a chemical effect on the thermal equilibrium concentrations of the acceptor species in the neutral state; (ii) in addition to the chemical effect, a Fermi-level effect on the thermal equilibrium concentrations of the acceptor species in ionized state; and (iii) the effect of the junction carrier concentrations, which influences also the diffusion process of the acceptor atoms [7]. Because of the use of the condition that $C_{\mathrm{so}}^{\mathrm{eq}}$ are taken to be of the same value in Si and in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ alloys, we see that here the chemical effect is of no importance. Thus, B segregation between the Si and $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ materials is due to the two other effects, particularly that of the Fermi-level dependence of the B_s^- solubility.

Our present fits to the experimental B_s^- diffusion profiles in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ structure are satisfactory. Based on a fairly different model, these B diffusion profiles have also been satisfactorily fitted by the original authors themselves [3, 4]. Therefore, distinguishing features between the present and previous models do not include the degree of satisfaction of the fits. Rather, the distinguishing features are the involved physical factors. In the present model the role of the B solubility difference in the materials and the carrier concentration at the heterojunctions are emphasized, while these factors have been ignored in the previously employed model [1–4]. Since B_s^- is an ionized shallow acceptor, and its diffusion is governed by a charged point defect species, these factors play an essential roles in B_s^- distribution, and hence must be included in an analytical model. This is a point in favor of the validity of the present model, since it means that these effects should also have been included in the model of the previous authors [1–4]. In contrast, in the previous model, the B diffusion anomalies were attributed to the formation of BGe pairs via the reaction [1–4]

$$\mathrm{B} + \mathrm{Ge} \overset{\mathrm{K}}{\longleftrightarrow} \mathrm{BGe}\,. \tag{14}$$

The BGe pair formation process seems to be just a postulate. We are not aware that the existence of the BGe pairs has been detected in experiments.

Irrespective of being a daily used p-type dopant in Si, the exact nature of the physical mechanism of B diffusion is still not clear even just in Si and in Ge. There is a substantial difference in the assumed B diffusing mechanisms between the present and previous model. In contrast to the present model, B_s^- diffusivity is assumed to be given by

$$D = D^{\mathrm{o}} + D^-(n_\mathrm{i})\frac{p}{n_\mathrm{i}} \tag{15}$$

in the previous model [1–4]. According to (15), B_s^- diffusion is governed by two point defect species, a neutral one leading to the term D^{o}, and a singly-positively-charged one leading to the term $D^-(p/n_\mathrm{i})$. This is clearly in contrast to our presently assumed B_s^- diffusion mechanism as expressed by (1), for which the governing point defect species is assumed to be just the singly-positively charged self-interstitial I^+. The two different mechanisms, as represented by (1) and (15), are both arrived at for B_s^- diffusion in Si based on fits to experimental results. It is still not clear which is superior. That is, either one would offer better fits to some profiles, but usually not by much. Therefore, in principle, the use of either mechanism should be regarded as valid at the present time. We have chosen the I^+ only model to start with because then (1) is obtained via a derivation in accordance with the chosen mechanism, which allows the treatment to be self-consistent. Presently, (15) is still of an empirical form, i.e., it has not yet been consistently derived from the chosen mechanism of involving the contributions of both I^{o} and I^+.

We believe that the strongest factor supporting the validity of the present model is the situation in III-V compounds, see the accompanying article [7]. In a number of III-V compound SL structures, the shallow acceptor species Zn and Be exhibit a similar distribution anomaly, but with the phenomenon so much more pronounced that it is readily apparent that the dopants are strongly segregated among the SL layers. In these layers, the acceptor-atom concentration difference can be a couple orders of magnitude, but in each layer Zn or Be atoms are nearly totally ionized. Therefore, the Zn or Be segregation behavior cannot be due to clustering or pairing of the acceptor atoms with the matrix material atoms in some layers, but rather due to a solubility difference [7]. Since B distribution in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ heterostructures and Zn or Be distribution in III-V compound SLs are analogous cases, we expect the same mechanism to play a role in all these cases.

The B_s^- diffusivity values used in the previous analyses raise some concerns. The used values of D^{o} in (15) by Lever et al. [4] vary as x is changed, which is in principle acceptable. But, the used values also vary with the initial B concentration and annealing times, which is unwarranted. Furthermore, according to Kuo et al. [1, 2], the used values of the quantity $D' = D^{\mathrm{o}} + D^-(n_\mathrm{i})$, for obtaining the fits in the range of x values from 0 to 0.22 at 850 °C [2] and from 0 to 0.53 at 800 °C [1], decreases as the x value in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ layer is increased, see Fig. 3. There is no data available for still larger x values except for pure Ge at 800 °C [14], also see Fig. 3.

The situation shown in Fig. 3 has led to the suggestion [15] that, as x increases from 0 to 1, the B_s^- diffusion

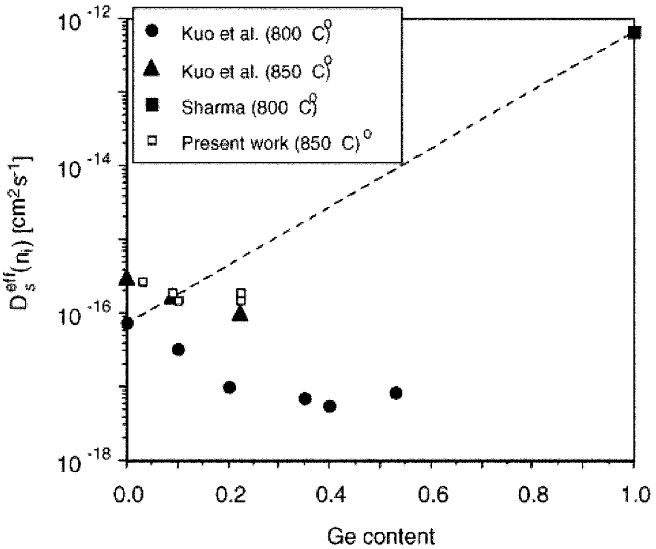

Fig. 3. Effective B_s^- diffusivity values needed to fit the experimental data. Those of Kuo et al. are the $D' = D^0 + D^-(n_\mathrm{i})$ values, and those for the present work are that given by (10). The dashed line indicates the value expected from a first order effect of averaging the B_s^- diffusivity values in Si and in Ge in proportion to Ge content in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ material

mechanism in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ changes from that governed by self-interstitials I to that governed by vacancies V, with V assumed to be the point defect species governing B_s^- diffusion in Ge. While B_s^- diffusion in Si is known to be governed primarily by I^+, it is actually not known which point defect species governs B^- diffusion in Ge. However, judged by this suggestion, the B diffusivity D' dependence on x [1,2] would seem to be unsettling on a quantitative basis. Consider that both I and V make contributions, B_s^- diffusivity in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ may be written as

$$D_\mathrm{GeSi} = D^\mathrm{I}_\mathrm{GeSi} + D^\mathrm{V}_\mathrm{GeSi}\,. \tag{16}$$

On the basis of a first-order effect, let us assume that the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ alloy constitutes an ideal solution. Then, we expect that $D^\mathrm{I}_\mathrm{GeSi}$ and $D^\mathrm{V}_\mathrm{GeSi}$ are linear combinations of the appropriate I and V contributions to B_s^- diffusion in Ge and in Si, in proportion to composition x of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ material. Hence,

$$D^\mathrm{I}_\mathrm{GeSi} = xD^\mathrm{I}_\mathrm{Ge} + (1-x)D^\mathrm{I}_\mathrm{Si}\,, \tag{17a}$$
$$D^\mathrm{V}_\mathrm{GeSi} = xD^\mathrm{V}_\mathrm{Ge} + (1-x)D^\mathrm{V}_\mathrm{Si}\,. \tag{17b}$$

However, the B diffusivity in Ge and in Si are

$$D_\mathrm{Ge} = D^\mathrm{I}_\mathrm{Ge} + D^\mathrm{V}_\mathrm{Ge}\,, \tag{18a}$$
$$D_\mathrm{Si} = D^\mathrm{I}_\mathrm{Si} + D^\mathrm{V}_\mathrm{Si}\,. \tag{18b}$$

Using (17) and (18), (16) becomes

$$D_\mathrm{GeSi} = xD_\mathrm{Ge} + (1-x)D_\mathrm{Si}\,. \tag{19}$$

Equation (19) means that, on the basis of a first order effect, the B diffusivity in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ is simply the average of the B_s^- diffusivities in Ge and in Si weighted by x. With B_s^- diffusivities in Ge and in Si known, the value of (19) is the straight line indicated in Fig. 3. It is seen that the D' values of Kuo et al. [1,2] deviated prominently from that predicted by (19). While this first-order analysis is not expected to be accurate, we would nevertheless also expect that the deviation from that predicted by (19) should not have been so large. This point, however, cannot be used to judge whether our present model or the previous model should be favored, since, at 850 °C, the $D_\mathrm{s}^\mathrm{eff}(n_\mathrm{i})$ values used in the present model are very close to the D' values used in the previous model. The B_s^- profiles of Kuo et al. [1,2] at 800 °C are not available for analysis.

4 Concluding Remarks

The most important physical factors leading to the B_s^- diffusion anomalies in $\mathrm{Ge}_x\mathrm{Si}_{1-x}/\mathrm{Si}$ structures are the Fermi-level effect on the solubilities of B_s^- in the materials and the carrier concentration effect at the heterojunctions. Diffusion of B_s^- in Si and in $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ for small x values is most likely governed by the singly-positively-charged self-interstitial I^+.

References

1. P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, R.J. Jacowitz, T.I. Kamins: Appl. Phys. Lett. **62**, 612 (1993)
2. P. Kuo, J.L. Hoyt, J.F. Gibbons, J.E. Turner, R.J. Jacowitz, D. Lefforge: Mater. Res. Soc. Sym. Proc. **379**, 373 (1995)
3. W.T. Fang, P.B. Griffin, J.D. Plummer: Mater. Res. Soc. Sym. Proc. **379**, 379 (1995)
4. R.F. Lever, J.M. Bonar, A.F.W. Willoughby: J. Appl. Phys. **83**, 1988 (1998)
5. G.L. Patton, J.H. Comfort, B.S. Meyerson, E.F. Grabbe, G.J. Scilla, E. de Fresart, J.M.C. Stork, J.Y.C. Sun, D.L. Harrame, J.N. Burghartz: IEEE Electron Device Lett. **EDL-11**, 171 (1990)
6. E.J. Prinz, J.C. Sturm: IEEE Electron Device Lett. **EDL-12**, 42 (1991)
7. C.-H. Chen, U.M. Gösele, T.Y. Tan: Appl. Phys. A, **68**, 9 (1999)
8. R.B. Fair, P.N. Pappas: J. Electrochem. Soc. **122**, 1241 (1975)
9. R.B. Fair: In *Impurity and Doping Processes in Silicon*, ed. by F.F.Y. Wang (North Holland, NY 1981) Chap. 7
10. T.Y. Tan, U. Gösele: Appl. Phys. A **37**, 1 (1985)
11. G.D. Watkins: Phys. Rev. B **12**, 5824 (1975)
12. H.-M. You, U.M. Gösele, T.Y. Tan: J. Appl. Phys. **74**, 2461 (1993)
13. W. Jüngling, P. Pichler, S. Selberherr, E. Guerrero, H.W. Pötzl: IEEE Trans. Electron. Devices **ED-32**, 156 (1985)
14. B.L. Sharma: Defect Diffusion Forum **70–71**, 102 (1990)
15. N. Moriya, L.C. Feldman, H.S. Luftman, C.A. King, J. Bevk, B. Freer: Phys. Rev. Lett. **71**, 883 (1993)