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Strain-induced diffusion in a strained $Si_{1-x}Ge_x$/Si heterostructure

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Diffusivity of a strained heterostructure was theoretically investigated, and general diffusion equations with strain potential were deduced. There was an additional diffusivity by the strain potential gradient as well as by the concentration gradient. The strain-induced diffusivity was a function of concentration, and its temperature dependence was formulated. The activation energy of the strain-induced diffusivity was measured by high-resolution transmission electron microscopy. This result can be generally applied for the investigation of the diffusion in strained heterostructures. © 2000 American Institute of Physics. [S0003-6951(00)02247-6]

Strained $Si_{1-x}Ge_x$/Si heterostructures have been investigated extensively by many research groups in recent years. In these structures, a $Si_{1-x}Ge_x$ layer is grown under compressive stress between Si substrates. The strain-induced band offset at the heterointerface leads to the formation of a two-dimensional hole gas in the strained $Si_{1-x}Ge_x$ layer, and a substantial enhancement of the hole mobility over that in bulk silicon was observed.[1] However, the prerequisite for a high carrier mobility is atomically abrupt heterointerfaces.[2] Therefore, the interdiffusion under thermal stress is of great concern.

In a $Si_{1-x}Ge_x$/Si heterostructure, the strain due to the lattice mismatch in the epilayer plays an important role in interdiffusion. In the literature, much evidence of the enhanced diffusion by strain in strained epilayers has been shown.[3–6] Moreover, the surface migration by strain gradient in $Si_{1-x}Ge_x$ islands was also reported.[7] However, although many authors have reported the strain effects on the diffusion in strained heterostructures, the qualitative relation between the strain and the diffusivity has not yet been proposed.

In this letter, the theoretical model of the interdiffusion of a strained $Si_{1-x}Ge_x$/Si heterostructure is proposed and a strain-induced diffusivity is formulated by defining a strain potential gradient. The activation energy of the strain-induced diffusivity is measured by a high-resolution transmission electron microscopy, and the experiments are consistent with the theoretically expected results. This model can give general information on the enhanced diffusion, and can be generally applied for various strained heterostructures.

A $Si_{0.83}Ge_{0.17}$ thin layer was grown on a Si (001) wafer by reduced pressure chemical vapor deposition. The thickness of the layer was 56.6 nm. The composition of the sample was measured by a high-resolution x-ray diffracto-

meter and by Rutherford backscattering spectroscopy. After deposition, the sample was annealed in dry N_2 at temperatures from 700 to 1000 °C, for times in the range of 30 min to 6 h, using vacuum furnace. The transmission electron microscopy (TEM) observations were performed in a JEM 2000 EX TEM operating at 200 kV along a [110] zone axis.

The strained $Si_{0.83}Ge_{0.17}$/Si (001) heterostructure has a self-strain energy, and the energy induces an elastic deformation of the heteroepitaxial layer. The areal strain energy of the strained layer is given by[8]

$$E_{str} = 2G\left(\frac{1+\nu}{1-\nu}\right)\varepsilon_0^2 z_0, \tag{1}$$

where G is a shear modulus, ν is a Poisson's ratio, ε_0 is an in-plain strain, and z_0 is a film thickness. However, because the strain energy is the extrinsic property depending on the depth, it cannot be used as the driving force of the flux. Therefore, a strain potential, μ_{str}, is defined in order to find the effect of strain on the diffusion. Strain potential means the strain energy per unit volume at an arbitrary depth of the film, and it is an intrinsic property. The strain potential is given by

$$\mu_{str}(z) = 2G\left(\frac{1+\nu}{1-\nu}\right)\varepsilon^2(z), \tag{2}$$

where $\varepsilon(z)$ is an in-plain strain at an arbitrary depth.

From Fick's first law, the flux will be linearly proportional to the derivative of Eq. (2).[9] Therefore, there are two kinds of origins for the diffusion. One is the diffusion by concentration gradient, the other is by the strain potential gradient. Because the strain in the annealed heterostructure is mainly relaxed by interdiffusion rather than by defects, the relaxation by defects can be negligible.[10] Therefore, $\varepsilon(z) = \varepsilon_0 C(z)/C_0$, and the flux with the strain potential gradient in the heterostructure can be described as.
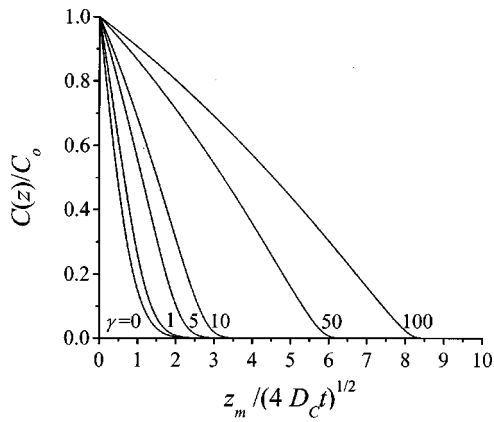
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FIG. 1. The calculated concentration profiles with concentration-dependent diffusity.

FIG. 2. The relation between γ and η_C at a constant concentration.

$$J = -D_C \frac{dC(z)}{dz} - D_\mu \frac{d\mu_{str}(z)}{dz}$$

$$= -\left[D_C + 4G\left(\frac{1+\nu}{1-\nu}\right)\left(\frac{\varepsilon_0}{C_0}\right)^2 D_\mu C(z) \right] \frac{dC(z)}{dz}$$

$$= -(D_C + D_{str})\frac{dC(z)}{dz} = -D_{app}\frac{dC(z)}{dz}, \qquad (3)$$

where J is the flux, $C(z)$ is the concentration at a depth, C_0 is the concentration of the as-deposited layer, D_μ is the coefficient of the strain potential gradient, and D_C, D_{str}, and D_{app} are the concentration gradient diffusivity, the strain-induced diffusivity, and the apparent diffusivity in the heterostructure, respectively.

From Eq. (3), we can find that there is an additional diffusivity due to the strain potential gradient. The strain-induced diffusivity is linearly proportional to the concentration, and the result shows that the diffusivity in a strained layer is not a constant. Therefore, the diffusion will be enhanced and we can define a diffusion enhancement factor, γ,

$$D_{app} = (D_C + D_{str}) = D_C\left[1 + 4G\left(\frac{1+\nu}{1-\nu}\right)\frac{\varepsilon_0^2}{C_0}\frac{D_\mu}{D_C}\frac{C(z)}{C_0} \right]$$

$$= D_C\left(1 + \gamma\frac{C(z)}{C_0} \right). \qquad (4)$$

Although the diffusivity in strained heterostructures has been investigated by many authors, it has been treated as a constant in a strained layer.[3–7] However, our model shows that the diffusivity in a strained layer is not a constant, and the error function solution for Fick's second law is not invalid in this case. We calculated the concentration profiles by a numerical iterative method,[11] and the calculated concentration profiles are shown in Fig. 1. The concentration profiles can be plotted as a function of $\eta_C = z/\sqrt{4D_C t}$, and they are strongly dependent on the diffusion enhancement factor.

Figure 2 shows the relation between γ and η_C at a constant concentration obtained from Fig. 1. In Fig. 2, η_C^2 is linearly proportional to the diffusion enhancement factor at a constant concentration. Because the apparent diffusivity has two terms, the activation energy of the apparent diffusivity may not be the same as that of concentration diffusivity
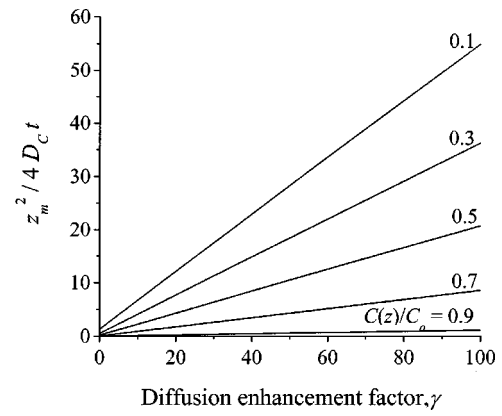
and/or that of the strain-induced diffusivity. From Eq. (4), the temperature dependency of the apparent diffusivity can be described as

$$D_{app} = D_C^0 \exp\left(\frac{-E_A^C}{kT}\right) + D_{str}^0 \exp\left(-E_A^{str}/kT\right)$$

$$= D_C^0 \exp\left(\frac{-E_A^C}{kT}\right)\left[1 + \frac{D_{str}^0}{D_C^0}\exp\left(\frac{-(E_A^{str}-E_A^C)}{kT}\right) \right],$$

$$(5)$$

where E_A^{str} and E_A^C are the activation energy of strain-induced diffusivity and that of concentration gradient diffusivity, respectively. Therefore, the temperature dependency of diffusion enhancement factor can be achieved from Eqs. (4) and (5),

$$\gamma \propto \exp\left(\frac{-(E_A^{str}-E_A^C)}{kT}\right). \qquad (6)$$

However, because $\gamma/\eta_C^2 = $ constant at a certain concentration, the activation energy of the strain-induced diffusivity can be evaluated by

$$\frac{z^2}{t} \propto D_C \exp[-(E_A^{str}-E_A^C)/kT] \propto \exp[-E_A^{str}/kT]. \qquad (7)$$

To measure the activation energy of strain-induced diffusivity, the annealed $Si_{0.83}Ge_{0.17}/Si$ heterostructures are examined by highresolution transmission electron microscopy (HRTEM). Figure 3(a) is a cross-sectional HRTEM image of the as-deposited sample. There is an abrupt $Si_{0.83}Ge_{0.17}/Si$ interface (I_O) 56.6 nm from the film surface. Therefore, intermixing of Si and Ge during growth can be negligible. However, the cross-sectional HRTEM image of a sample [Fig. 3(b)] annealed at 750 °C for 2 h shows that migrated interface (I_M) is produced below the original interface. This interface migration was also observed in other annealed samples, and originated from the interdiffusion of Si and Ge atoms by thermal annealing. Because of the interdiffusion by thermal annealing, the abrupt concentration profile at the original interface in the as-deposited sample was modified and the Ge concentration in the annealed samples decreased slowly from I_O to I_M. The annealing conditions and the corresponding migration distances are summarized in Table I.
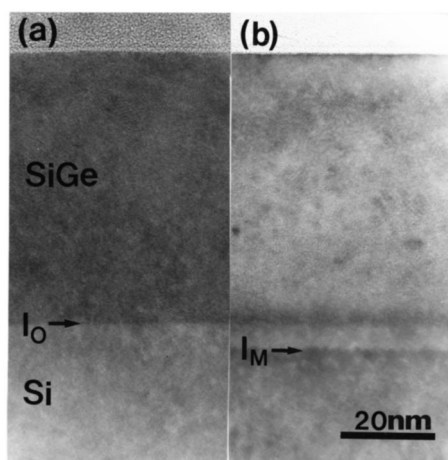
FIG. 3. (a) Cross-sectional HRTEM micrograph of the as-deposited $Si_{0.83}Ge_{0.17}$/Si and (b) cross-sectional HRTEM micrograph of the $Si_{0.83}Ge_{0.17}$/Si annealed at 750 °C in a dry N_2 ambient for 2 h. I_O and I_M are the original interface and migrated interface, respectively.
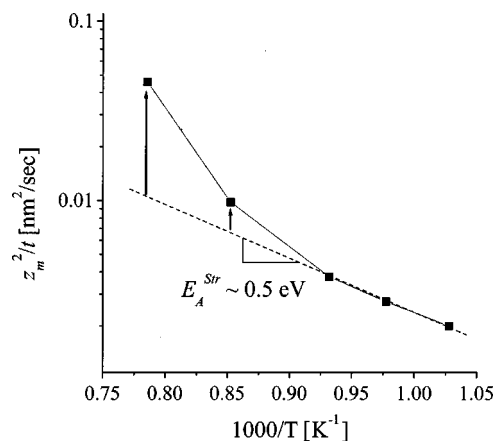

FIG. 4. The Arrhenius plot of z_m^2/t. The slope is the activation energy of the strain-induced diffusivity.

The interface migration is the result of the interdiffusion of Si and Ge. Although we cannot know the exact concentration at the migrated interface, because the formation mechanisms of the migrated interface were all the same, and because the interfaces were examined by a identical method, it can be assumed that the concentrations at the migrated interfaces (C_I) are all the same in this experiment. Therefore, because $C(z_m)=C_I$ in all annealing conditions shown in Table I, the activation energy of the strain-induced diffusivity can be evaluated from Eq. (7).

The Arrhenius plot of z_m^2/t is shown in Fig. 4. The slope shows good linearity up to 800 °C, and is very consistent with the expected result from Eq. (7). In our experiments, the activation energy of the strain-induced diffusivity was about 0.5 eV below 800 °C. However, above 800 °C, the increase of the activation energy was observed. During the annealing process, an initial interdiffusion is enhanced by the presence of the strain in the SiGe layer, leading to a relaxation of the strain, which precedes a slower interdiffusion stage.[5] Therefore, the increase of the activation energy originated from the decrease of the driving force for the strain-induced diffusion by strain relaxation.

The activation energy of the concentration gradient diffusivity is about 3.0–4.7 eV, and that of the strain-induced diffusivity is much lower than that value.[12] Because the apparent diffusivity in the heterostructure is the sum of the strain-induced diffusivity and the concentration gradient diffusivity, the apparent diffusivity will follow the strain-

induced diffusivity at a low temperature range, and it will be the same for the concentration gradient diffusivity at a high temperature range. Therefore, the effect of the strain on the diffusion phenomena in strained heterostructures is especially important at low temperature annealing. Furthermore, the low activation energy of the strain-induced diffusivity measured in this experiment is the main origin of the low activation energy of the apparent diffusivity in the strained SiGe/Si heterostructures reported in Refs. 5, 6, and 10.

In conclusion, a theoretical model of the diffusion in a strained SiGe/Si heterostructure was proposed and a strain-induced diffusivity was formulated by defining a strain potential gradient. A method for measuring the activation energy of the strain-induced diffusivity was proposed, and it was examined by high-resolution transmission electron microscopy. Interface migration by diffusion was observed in annealed $Si_{0.83}Ge_{0.17}$/Si heterostructures, and the activation energy of the strain-induced diffusivity was calculated from the measured interface migration distances. The experiments were consistent with the theoretically expected results. This model can explain the enhanced diffusion by strain effect very well, and can generally be applied to the investigation of the diffusion in various strained heterostructures.

TABLE I. Annealing conditions and the measured interface migration distances.

Annealing temperature (°C)	Annealing time, t (sec)	Interface migration distance, z_m (nm)	z_m^2/t (nm²/s)
700	7200	3.8	2.00×10^{-3}
750	7200	4.4	2.74×10^{-3}
800	1800	2.6	3.76×10^{-3}
900	1800	4.2	9.80×10^{-3}
1000	6300	17	4.59×10^{-2}

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