Effect of processing conditions on the growth of strained $Si_{1-X}Ge_X$ layers on Si

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We investigate several factors that determine the surface morphology in heteroepitaxial growth of $Si_{1-X}Ge_X$ films on Si, which include composition, temperature, and pressure. Phase boundary lines are derived that define the regions for planar and island growth in terms of composition–temperature and composition–pressure. Also derived is the roughening characteristic length as a function of temperature, pressure, and characteristic time. Our results can explain the literature data satisfactorily. © *1998 American Institute of Physics.* [S0021-8979(98)05716-8]

Surface morphology and roughness evolution during heteroepitaxy, in particular $Si_{1-X}Ge_X$ heteroepitaxy, have drawn considerable interest because of its applicability to fabricating nanostructures.[1,2] The degree of roughening, which is of prime interest in these applications, is enhanced when the lattice mismatch is relatively large or when the growth temperature is relatively high. Otherwise, the grown films tend to relax through plastic deformation, leading to misfit dislocations.[3]

Perhaps because of this reason, most of the reported experiments on the surface morphological evolution during $Si_{1-X}Ge_X$ heteroepitaxy have been limited to relatively high growth temperature (400–750 °C) and compositions.[4,5] In this region, the surface morphology is determined primarily by energetics rather than kinetics. On the other hand, low temperature growth has generally been found to lead to planar surfaces.[6,7]

While a number of experimental results are available, it is not yet clearly delineated as to how the processing conditions determine the surface morphology, i.e., planar [two-dimensional (2D)] versus island [three-dimensional (3D)] growth. Of particular interest in the roughening is the manner in which the characteristic length is determined by processing conditions.

In this communication, we investigate the effect of processing conditions on the growth of $Si_{1-X}Ge_X$ layers on Si in terms of composition, temperature, pressure, and deposition time.

We begin with the net energy change during roughening that has been derived earlier based on ''ripple structure,''[8,9] which is

$$\Delta E=\Delta F_v+\Delta G_s=-2\sqrt{2}\pi\frac{(1+\nu)^2}{(1-\nu)}\mu\epsilon_0^2\lambda t_1^2+\pi^2 t_1^2\gamma, \tag{1}$$

where ΔF_v is the excess volume strain energy, ΔG_s is the increase in surface energy due to the undulations. Here, ν is the Poisson's ratio, μ is the shear modulus for the epilayer material, γ is the surface free energy per unit area, t_1 is the half amplitude of the ripple, and ϵ_0 is the bulk strain induced by the lattice mismatch between film and substrate, which is related to the Ge fraction X through $\epsilon_0=0.042X$.[6] In order for the roughening to take place, the characteristic length λ (period in the ripple) should be larger than a certain critical value or $\Delta E<0$. Then Eq. (1), upon rearrangement, gives

$$\lambda>\frac{\pi\gamma(1-\nu)}{2\sqrt{2}(1+\nu)^2\mu\epsilon_0^2}. \tag{2}$$

The characteristic length can be understood on a more quantitative basis by considering the surface diffusion coefficient and the corresponding characteristic time.

We propose that the characteristic length be treated as a characteristic diffusion length. If we let the incubation time be τ_i and the corresponding initial perturbation length be λ_i, then the characteristic length is

$$\lambda=\lambda_i+\sqrt{D_s(\tau-\tau_i)}, \tag{3}$$

where D_s is the surface diffusivity and τ is the characteristic time scale. In general, λ_i should be dependent on the composition, its value decreasing with increasing composition. For the time scale of practical interest, τ_i may be neglected. Then Eq. (3) reduces to

$$\lambda=(D_s\tau)^{1/2}. \tag{4}$$

There still remains the question of the characteristic time, i.e., the manner in which deposition rate, deposition time, and annealing time are incorporated into the characteristic time. When only annealing is involved, τ is simply the annealing time. On the other hand, both the deposition rate and the deposition time should be considered in determining the characteristic time when deposition is involved. In this case, the deposition rate and the inverse of the deposition time may be considered resistances in parallel, making up the total resistance, $1/\tau$:

$$\frac{1}{\tau}=\frac{1}{\tau_1}+\frac{1}{\tau_2}, \tag{5}$$

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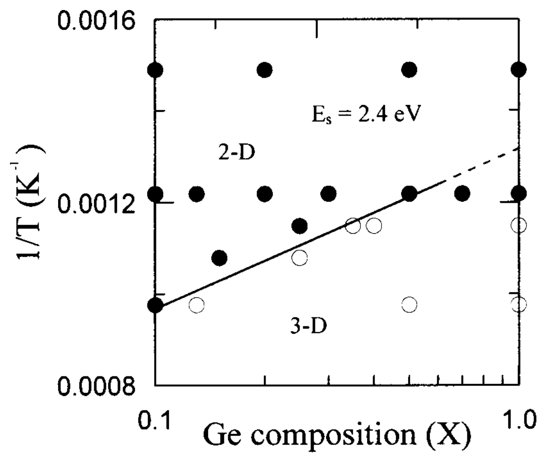

FIG. 1. Phase boundary between planar (2D, closed circles) and island (3D, open circles) structures in terms of composition–temperature. Data points are from Bean *et al.* (Ref. 10) $E_s = 2.4$ eV from the slope.

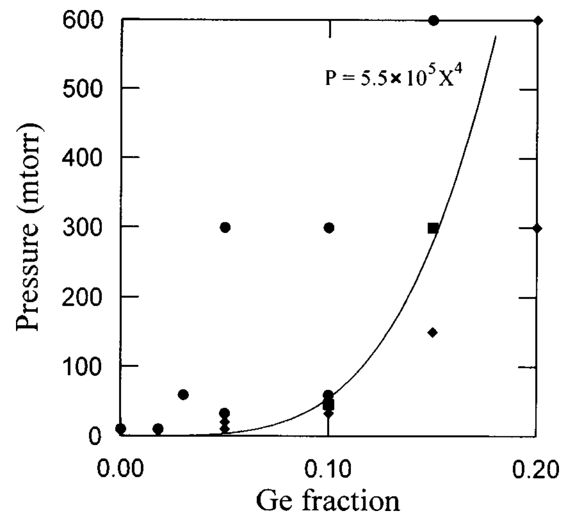

FIG. 2. Phase boundary between planar and island structures in terms of composition–pressure. Data points are from Caymax *et al.* (see Ref. 12). Symbols indicate the island (◆), intermediate (■), and planar (●) structures.

where τ_1 is the characteristic time for the deposition rate, which is inversely proportional to the deposition rate and τ_2 is the characteristic deposition time.

The regions of 2D and 3D growth can now be determined in terms of composition and temperature on the basis of Eqs. (2) and (3). Noting that $\epsilon_0 = 0.042X$, substitution of Eq. (3) into Eq. (2) after rearrangements yields

$$\frac{1}{T} < \frac{4k_B}{E_s} \ln X + \frac{k_B}{E_s} \ln \frac{AD_0 \tau (1+\nu)^4 \mu^2}{\gamma^2 (1-\nu)^2} \tag{6}$$

for 3D or island growth. Here, A is a constant that is 2.52×10^{-6} for $Si_{1-X}Ge_X$. The condition of Eq. (6) states that given the composition X, the temperature should be higher than that specified by the equation for the island growth. Therefore, it defines the regions for 2D and 3D growth in terms of composition and temperature. The data by Bean *et al.*[10] are used in Fig. 1 to test the condition. As can be seen from Eq. (6), the slope of the line separating the two regions should yield E_s, which is the activation energy of adatom surface diffusion. The value obtained from the figure is 2.4 eV, which is a reasonable value in view of the widespread data reported in the literature, ranging from 0.7 to 3.6 eV.[11] The intercept, in general, would vary depending on the process conditions. For example, the line is lowered and the island structure is more suppressed if the deposition rate is increased or the deposition time is decreased.

As apparent from Fig. 1, the line of Eq. (6) representing the phase boundary does not extend all the way to the composition X of unity. Rather, it is independent of the composition and is a parallel line corresponding to approximately 570 °C. This is an indication that the roughening process is dominated by energetics rather than kinetics for large X.

The surface morphology and roughening are also dependent on pressure (or deposition rate). To examine this dependence, Eq. (2) is rearranged to give

$$p < \frac{AD_s \alpha (1+\nu)^4 \mu^2}{\gamma^2 (1-\nu)^2} X^4 \tag{7}$$

for the island growth. Here α is a constant relating the deposition rate, $1/\tau_1$, to the pressure, i.e., $p = \alpha/\tau_1$. For relatively long deposition time, τ_2 may be taken as infinity, which has been used in Eq. (7). This fourth power dependence of the composition on the pressure for the phase boundary between 2D and 3D growth is tested in Fig. 2 using the data by Caymax *et al.*[12] It is seen that the fourth power dependence adequately represents the phase boundary.

Equation (4) can be used to determine the characteristic length λ. When Eq. (5) is substituted into Eq. (4),

$$\lambda = \left(\frac{D_s \tau_2}{1 + \tau_2/\tau_1} \right)^{1/2}. \tag{8}$$

For the purpose of data regression, Eq. (8) can be rearranged in the following, noting that $\tau_2 \propto t$ (deposition time):

$$\frac{1}{t} = \frac{a}{\lambda^2} - b, \tag{9}$$

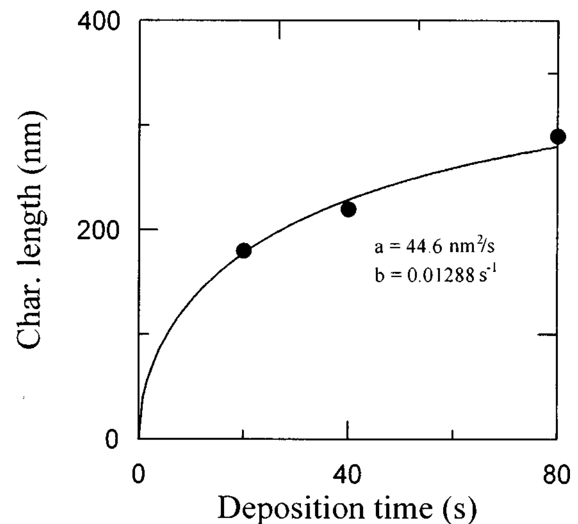

FIG. 3. Comparison of Eq. (9) with the experimental data from Dutartre *et al.* (see Ref. 13).

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where

$$a = D_s\beta, \quad b = \beta/\tau_1 \tag{10}$$

and β is the constant proportionality factor between τ_2 and t. It is seen that for a given deposition rate, the inverse of the deposition time is related to the inverse of the characteristic length squared. Figure 3 shows the regression based on the data by Dutartre *et al.*[13] The regression gives for the two constants a and b: $a = 44.6\ \mathrm{nm}^2/\mathrm{s}$ and $b = 0.01288\ \mathrm{s}^{-1}$.

In summary, the surface morphology and characteristic length for the heteroepitaxial layers of $Si_{1-X}Ge_X$ on Si have been characterized in terms of temperature, pressure, composition, and deposition time. Comparisons with the literature data have been found to be satisfactory. For more accurate modeling, better atomistic consideration accompanied by the appropriate data will be needed, but our analysis can be used for elementary prediction of the surface morphology of SiGe films.

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