Critical thickness of heavily boron-doped silicon-germanium alloys

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In this work, the effect of boron concentration on the critical thickness of heavily boron doped $Si_{1-x}Ge_x$ alloys ($Si_{1-x-y}Ge_xB_y$) has been studied using Raman spectroscopy. The experimental results indicate that while boron decreases the stored strain energy, it can substantially increase the critical thickness for a given Ge concentration. The $Si_{1-x-y}Ge_xB_y$ critical thickness was calculated using two different models based on energy balance and kinetic considerations. The results show that the kinetic model provides a good estimate for the $Si_{1-x-y}Ge_xB_y$ critical thickness. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2374870]

It has been shown that for epitaxial $Si_{1-x-y}Ge_xB_y$ alloys grown on Si substrates one boron atom is able to compensate the strain due to approximately 6.9 Ge atoms.[1] In this letter, we present the impact of boron on strain relaxation in $Si_{1-x-y}Ge_xB_y$ by studying the stored strain energy density in films of varying thicknesses and compositions. The $Si_{1-x-y}Ge_xB_y$ critical thickness has been calculated using two different models based on energy balance and kinetic considerations and the results were compared to experimental data.

$Si_{1-x-y}Ge_xB_y$ epitaxial layers were grown on 150 mm, 5 Ω cm, *n*-type Si wafers of (100) orientation. Windows were defined in an isolation oxide by photolithography and wet etching. *In situ* boron doped $Si_{1-x}Ge_x$ epitaxial layers were selectively grown in these windows by ultrahigh vacuum rapid thermal chemical vapor deposition.[2] Films with 17% and 28% Ge were grown at ~550 °C while films with 50% Ge were grown at ~500 °C in order to obtain two dimensional growth. The growth rates obtained for different layers are summarized in Table I. The film thickness was determined by measuring the step height between the selectively grown layer and the surrounding oxide using atomic force microscopy. The Raman analysis was carried out using a Dilot™ micro-Raman spectrometer (λ=488 nm).

Table I summarizes the results of the strain measurements. The Si–Ge peak positions are given for $Si_{1-x-y}Ge_xB_y$ layers with different germanium and boron concentrations and thicknesses. The relative strain energy in the epitaxial layers was determined by measuring the shifts of these peaks from their original positions in relaxed $Si_{1-x-y}Ge_xB_y$ alloys as demonstrated in an earlier publication from this laboratory.[1] For some of the samples, the peak shifts were below the detection limit of the spectrometer. The strain values for these samples have been left blank in Table I. Analysis of the data shows that addition of boron reduces the strain energy density due to boron strain compensation (25 nm films for all Ge concentrations and 60 nm film for $x=0.17$) if the layers are strained even without boron. For thicknesses and Ge concentrations that lead to partially relaxed films without boron, strain compensation postpones relaxation resulting in higher strain energy densities (e.g., 60 nm, $x=0.5$ and 0.28). For undoped, 105 nm thick films (all Ge concentrations) the measured strain energy is zero suggestive of complete relaxation. Addition of boron to the film with $x=0.28$ yields a finite strain energy, which indicates that the film is not fully relaxed.

A point of interest is the impact of boron on the critical thickness defined as the threshold thickness at which the epitaxial layer begins to relax via formation of dislocations. The experimental data shown in Table I suggest that while boron strain compensation reduces the strain energy density, it results in a larger critical thickness for a given Ge concentration. To study this effect, we have employed two different models to calculate the critical thickness for $Si_{1-x-y}Ge_xB_y$ alloys with different B and Ge concentrations and have compared the resulting values with the experimental data. The first step of these calculations was to define an equilibrium lattice parameter for boron a_B based on the relative covalent radii of Si, Ge, and B, which was determined to be 3.806 Å.[1] The strain in the epitaxial $Si_{1-x-y}Ge_xB_y$ layer was calculated from

$$\varepsilon = \frac{a_{\mathrm{SiGeB}} - a_{\mathrm{Si}}}{a_{\mathrm{Si}}} = \frac{a_{\mathrm{Ge}} - a_{\mathrm{Si}}}{a_{\mathrm{Si}}}x + \frac{a_{\mathrm{B}} - a_{\mathrm{Si}}}{a_{\mathrm{Si}}}y, \tag{1}$$

where a_{SiGeB}, a_{Si}, and a_{Ge} are the lattice parameters of $Si_{1-x-y}Ge_xB_y$, Si, and Ge, respectively. Assuming that there are no dislocations at the $Si_{1-x-y}Ge_xB_y/Si$ interface, the stored strain energy density E_{st} in $Si_{1-x-y}Ge_xB_y$ was then calculated using[3]

$$E_{\mathrm{st}} = 2\mu\varepsilon^2\frac{1+\nu}{1-\nu}h, \tag{2}$$

where h is the layer thickness, μ is the shear modulus, and ν is Poisson's ratio for $Si_{1-x-y}Ge_xB_y$ calculated using the respective constants for Si, Ge, and B by linear interpolation.[4]

In the energy balance model proposed by People and Bean,[5] the critical thickness is calculated as the thickness at which the strain energy density given by Eq. (2) is equal to the energy density associated with an isolated screw dislocation at a distance h from a free surface. This energy is given by

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TABLE I. Si–Ge phonon peaks and corresponding strain energy determined using Raman spectroscopy.

Ge content (x)			0.5			0.28			0.17	
Growth temperature (°C)			500			550			550	
Growth rate (nm/s)			0.20			0.25			0.20	
Film thickness (h in nm)		25	60	105	25	60	105	25	60	105
Undoped	Peak position (cm^{-1})	409.5	405.8	405.3	408.2	⋯	406.7	405.6	405.6	405.1
	Strain energy (J/m^2)	2.3	0.8	⋯	0.8	⋯	⋯	0.3	0.7	⋯
Doped	Peak position (cm^{-1})	407.6	407.6	405.3	407.2	407.2	407.0	405.1	405.1	405.1
	Strain energy (J/m^2)	1.3	3.0	⋯	0.3	0.5	0.7	⋯	⋯	⋯

$$E_{\mathrm{dis}} \simeq \frac{\mu b^2}{8\pi\sqrt{2}a_{\mathrm{SiGe}}} \ln\left(\frac{h}{b}\right), \tag{3}$$

where $b=0.4$ nm and a_{SiGe} is the lattice parameter of the $Si_{1-x}Ge_x$ alloy. The critical thickness for $Si_{1-x-y}Ge_xB_y$ calculated using this model is shown in Fig. 1 (dashed lines) as a function of boron concentration for $x=0.17$, 0.28, and 0.50.

The kinetically limited critical thickness of metastable $Si_{1-x}Ge_x$ layers has been modeled by Houghton.[6] Unlike the energy balance model described above, this model includes the thermal history of the epitaxial layer in calculating the critical thickness. This model has been shown to provide a better fit to the experimental results. According to this model, the effective stress τ_{eff} in a $Si_{1-x}Ge_x$ alloy is given by

$$\tau_{\mathrm{eff}} = \frac{a_{\mathrm{Ge}} - a_{\mathrm{Si}}}{a_{\mathrm{Si}}} \mu \cos\psi \left(\frac{1+\nu}{1-\nu}\right)\left[x - \frac{0.55}{h}\ln\left(\frac{4h}{b}\right)\right], \tag{4}$$

where $\cos\psi=0.816$ is the geometrical factor. The strain lost to relaxation during a given thermal cycle is expressed as

$$\Delta\epsilon(t) = \frac{BV_0N_0t^2b\cos\lambda}{2}\left(\frac{\tau_{\mathrm{eff}}}{\mu}\right)^y \exp\left(-\frac{Q_s}{kT}\right), \tag{5}$$

where B, V_0, and N_0 are material constant and $b\cos\lambda$ is the projected Burgers vector width of the 60° misfit segment in the strained interface. The critical thickness is then extracted by summing the above expression over all thermal cycles and equating the result to the threshold strain of 10^{-5}, which is regarded as the lower bound for the detectable strain using common analytical techniques. To apply Houghton's model to $Si_{1-x-y}Ge_xB_y$ alloys, the Ge fraction x in Eq. (4) was replaced by an effective Ge fraction x_{eff} given by

$$x_{\mathrm{eff}} = x + \frac{a_B - a_{\mathrm{Si}}}{a_{\mathrm{Ge}} - a_{\mathrm{Si}}} y. \tag{6}$$

The resulting critical thickness values are plotted in Fig. 1 (solid lines). It can be observed that the general trend is the same for both models, i.e., for a given Ge fraction, the critical thickness increases with boron concentration due to boron strain compensation.

Figure 2 shows the strain energy density calculated using Eq. (2) as a function of the germanium fraction in the alloy for undoped $Si_{1-x}Ge_x$ films (solid lines). The experimentally determined values from Table I are included for comparison (symbols). Also shown are the critical strain energy density values calculated using the energy balance and kinetic models for $x=0.17$, 0.28, and 0.50.

According to Eq. (3), as the germanium concentration is increased, the energy density associated with a dislocation (screw dislocation assumed) decreases due to increasing a_{SiGe} and decreasing h, which can be observed in Fig. 2. The kinetic model which includes the thermal history of the alloy is expected to predict the critical energy density more accurately. According to this model, as the germanium concentration increases from $x=0.17$ to 0.28 the critical energy density increases due to the higher growth rate obtained for the latter, yielding a shorter growth time as shown in Table I. As the germanium concentration is further increased to $x=0.50$, the

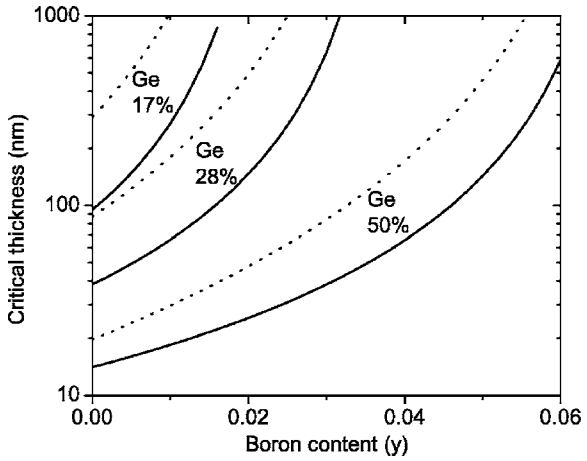

FIG. 1. Critical thickness for $Si_{1-x-y}Ge_xB_y$ alloys calculated using two models. Solid lines show the critical thickness calculated using kinetic theory, while dashed lines using energy balance theory.

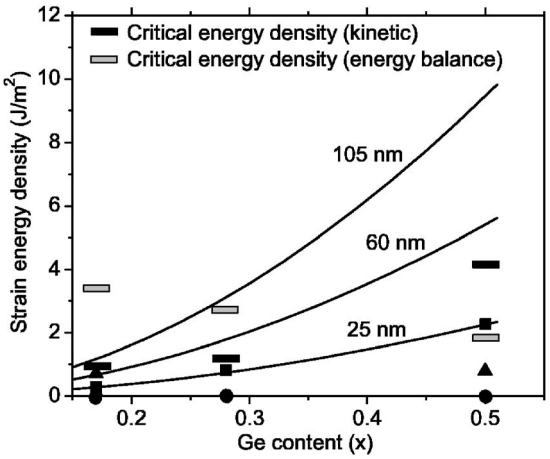

FIG. 2. Strain energy density stored in a $Si_{1-x}Ge_x$ alloy as a function of Ge content (x). The lines represent theoretical calculations for different film thicknesses. The squares, triangles, and circles represent experimental data for films of ~26, 60, and 105 nm thick, respectively. Critical strain energies calculated from kinetic and energy balance models are also shown.

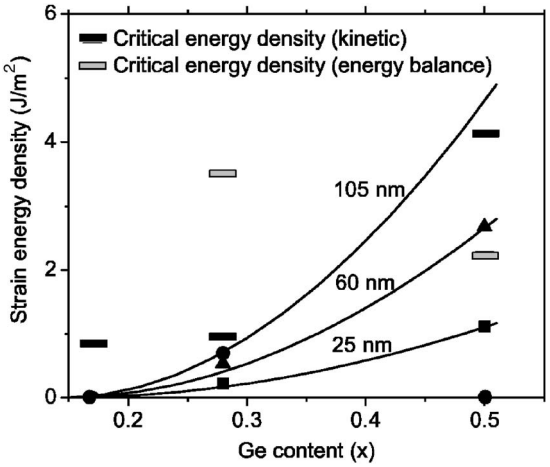

FIG. 3. Strain energy density stored in a $Si_{1-x-y}Ge_xB_y$ alloy as a function of Ge content (x) with B content (y)=0.02. The solid lines represent theoretical calculations for different film thicknesses. The squares, triangles, and circles represent experimental data for films ~26, 60, and 105 nm thick, respectively. Critical strain energies calculated from kinetic and energy balance models are also shown.

critical energy density increases even more due to the lower growth temperature.

Based on the calculated strain energy densities, samples that fall below the critical value are expected to be strained while others should relax. In Fig. 2, it is observed that the experimentally determined strain energy density for h =25 nm (squares) coincides with the theoretical curve. This should be expected since the theoretical curve is below the critical strain energy density values predicted by both models. For h=60 and 105 nm, the stored energy density is above the critical energy values predicted by the kinetic model in agreement with the measured strain density values, which are well below the theoretical curve indicative of relaxation. The only exception is the 60 nm thick film with x =0.17, which falls below the critical energy density and hence, it coincides with the theoretical value. If the experimental data followed the energy balance model, then the 105 nm film with x=0.17 should be fully strained while the 60 nm film with x=0.50 should be partially or fully relaxed. Hence these data show that the kinetic model can predict the critical thickness more accurately compared to the energy balance model.

Figure 3 shows the equivalent results obtained for $Si_{1-x-y}Ge_xB_y$ with y=0.02. It has been shown that heavy doping levels in $Si_{1-x}Ge_x$ can lead to shifts in the Raman peaks due to Fano-like interactions.[7] This phenomenon is expected to affect the calculations of the strain energy in $Si_{1-x-y}Ge_xB_y$ alloys. Indeed, measurements obtained from undoped and doped relaxed $Si_{1-x}Ge_x$ samples show a small shift associated with the doping density but these shifts are smaller than the shifts due to boron strain compensation observed in strained layers. Nevertheless, in order to alleviate this source of error, the strain energy calculations for strained $Si_{1-x-y}Ge_xB_y$ samples were made by comparing them with relaxed films having the same boron doping. It can be seen that the measured energy density values for h=25 and 60 nm lie below the critical energy values predicted by the kinetic model for all three Ge concentrations and they are in close agreement with the theoretical curves. For h=105 nm, the measured energy density is below the critical energy density when x=0.27 and the measured value again agrees with the kinetic model. On the other hand, for x=0.50 the film is too thick to retain any strain energy and it is fully relaxed. An important difference between Figs. 2 and 3 is that while the sample with h=60 nm and x=0.5 and the sample with h =105 nm and x=0.28 are both relaxed without boron, they are strained when 2% boron is added to the films, which clearly demonstrates the larger critical thickness obtained due to boron strain compensation.

In summary, the results presented in this letter indicate that the kinetic model proposed by Houghton provides a good estimate for the critical thickness of $Si_{1-x-y}Ge_xB_y$ alloys grown on Si substrates. We believe that this result will prove useful in optimizing the process parameters of devices with heavily boron doped $Si_{1-x}Ge_x$ layers including p-channel metal oxide silicon field effect transistors with uniaxial compressive channel stress obtained by using recessed, heavily boron doped $Si_{1-x-y}Ge_xB_y$ junctions.[8]

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