Damage and strain in epitaxial Ge_xSi_{1-x} films irradiated with Si

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The damage and strain induced by irradiation of both relaxed and pseudomorphic Ge_xSi_{1-x} films on Si(100) with 100 keV ^{28}Si ions at room temperature have been studied by MeV ^{4}He channeling spectrometry and x-ray double-crystal diffractometry. The ion energy was chosen to confine the major damage to the films. The results are compared with experiments for room temprature Si irradiation of Si(100) and Ge(100). The maximum relative damage created in low-Ge content films studied here ($x=10\%$, 13%, 15%, 20%, and 22%) is considerably higher than the values obtained by interpolating between the results for relative damage in Si-irradiated single crystal Si and Ge. This, together with other facts, indicates that a relatively small fraction of Ge in Si has a significant stabilizing effect on the retained damage generated by room-temperature irradiation with Si ions. The damage induced by irradiation produces positive perpendicular strain in Ge_xSi_{1-x}, which superimposes on the intrinsic positive perpendicular strain of the pseudomorphic or partially relaxed films. In all of the cases studied here, the induced maximum perpendicular strain and the maximum relative damage initially increase slowly with the dose, but start to rise at an accelerated rate above a threshold value of $\sim 0.15\%$ and 15%, respectively, until the samples are amorphized. The pre-existing pseudomorphic strain in the Ge_xSi_{1-x} film does not significantly influence the maximum relative damage created by Si ion irradiation for all doses and x values. The relationship between the induced maximum perpendicular strain and the maximum relative damage differs from that found in bulk Si(100) and Ge(100).

I. INTRODUCTION

Heterostructures of Ge_xSi_{1-x} on Si (Si/Ge_xSi_{1-x}) are of great technological interest today because the carrier mobilities in Ge_xSi_{1-x} are higher than those in Si and such heterostructures are compatible with Si integrated-circuit technology. They have been studied for applications to heterojunction bipolar transistors, modulation-doped field effect transistors, bipolar inversion-channel and field effect transistors, bipolar and complementary metal-oxide-semiconductor circuits, infrared superlattice detectors, and mixed tunneling transistors.[1–5]

Ion implantation is one of the key processing steps in doping and processing semiconductor devices. Recently, several studies have been made on implantation or irradiation of Si/Ge_xSi_{1-x} heterostructures.[6–14] When compared with the data for Si, significant damage enhancement in strained Ge_xSi_{1-x} films has been observed, such as the selective amorphization for ion-bombarded Ge_xSi_{1-x} strained-layer superlattices.[9,10] Haynes *et al.*[11] have also reported a similar damage enhancement for relaxed Ge_xSi_{1-x} layers, and Vos *et al.*[12] have qualitatively compared the damage found in Si, Ge, pseudomorphic and relaxed Ge_xSi_{1-x} layers.

Strain is of primary importance for the stability of practical devices fabricated from lattice-mismatched Si/Ge_xSi_{1-x} heterostructures, and it has been reported that ion irradiation will induce further strain in the pseudomorphically strained Ge_xSi_{1-x} layers.[13,14] The goal of this study is to investigate the strain and damage induced in pseudomorphic and relaxed Ge_xSi_{1-x} films by ion irradiation when the ion range is limited such that the $Si\text{-}Ge_xSi_{1-x}$ interface is not significantly damaged. The results are compared with those observed in Si(100) and Ge(100) single crystals. The relationships of irradiation-induced strain and damage versus the Si ion dose are reported for Si, Ge, and for both pseudomorphic and relaxed Ge_xSi_{1-x} films. We also make quantitative comparisons between the damage produced in fully strained and relaxed Ge_xSi_{1-x} layers for a range of irradiation doses with the same Ge composition.

For the sake of brevity, unless otherwise specified, we will use expressions such as $x=0.10$ to replace pseudomorphic $Si/Ge_{0.10}Si_{0.90}$ while fully relaxed $x=0.10$ will refer to fully relaxed $Si/Ge_{0.10}Si_{0.90}$ films.

II. EXPERIMENTAL PROCEDURES

Pseudomorphic films of Ge_xSi_{1-x} on Si(100) substrates were grown by conventional ultrahigh vacuum molecular-beam epitaxy at the University of California at Los Angeles (UCLA). The sample growth temperatures, minimum yields, pseudomorphic strain values, and thickness for $x=0.10$, 0.13, 0.15, and 0.20 are summarized in Table I. All samples are of excellent crystalline quality, with a minimum channeling yield of $\sim 3\%$ to 4% in both

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TABLE I. Basic information about the pseudomorphic Si/Ge_xSi_{1-x} samples used in this article.

x (Ge content)	T_{growth} (°C)	$\epsilon^{\perp}_{exp}$ (%)	$\epsilon^{\perp}_{theo.}$ (%)	χ_{min} (%)	Thickness (Å)
0.10	~450	0.72	0.74	~4	2450
0.13	~450	0.95	0.95	~3	2350
0.15	~400	1.10	1.08	~4	2400
0.20	~400	1.38	1.45	~4	2000

Si and Ge signals. Film thickness was determined by MeV ^4He backscattering spectrometry. High-resolution double-crystal x-ray rocking curves evidence the pseudomorphic nature of the heterostructures, with a parallel strain equal to zero within the experimental sensitivity ($\sim 10^{-4}$). All of the strain values refer to the difference in lattice constant with respect to those of the substrates. These measured strain values are consistent with the predictions of linear elasticity theory for the pseudomorphic films.

Another $x=0.10$ layer ~ 3 μm thick, also grown by molecular beam epitaxy at UCLA, was shown by x-ray rocking curve analysis to have a lattice constant of 5.454 Å, which is that of a fully relaxed film. A 600-nm-thick layer with $x=0.22$ was grown at the Institute of Thin Film and Ion Technology (ISI) in Jülich, Germany, where strain measurement with MeV ^4He ions channeled parallel to an inclined [110] axis yielded a tetragonal distortion of 4.9×10^{-3} for that sample. We confirmed the thickness by backscattering spectrometry. X-ray rocking curves yielded strain values equivalent to a tetragonal distortion of 5.0×10^{-3}, in agreement with the channeling experiments. This sample is therefore partially relaxed, with residual strain about 17% of that of a pseudomorphic film. Both this partially relaxed $x=0.22$ and the fully relaxed $x=0.10$ films are of rather good crystalline quality, with minimum channeling yields of $\sim$4% and $\sim$5% in the Si and Ge signals, respectively.

All of the $Si(100)/Ge_xSi_{1-x}$ epilayers described above, as well as Si(100) and Ge(100) wafers, were irradiated at room temperature in high vacuum ($\sim 10^{-7}$ Torr) with 100 keV ^{28}Si ions to doses ranging from 10^{13} to 10^{15} Si/cm^2. All samples were chemically cleaned before loading into the implanter (10 min each in ultrasonic baths of trichloroethane, acetone, and methanol, followed by a dip in 0.1% HF solution until a hydrophobic surface was obtained, finally rinsed in de-ionized water, and then blown dry with nitrogen gas). During irradiation, the sample normal was tilted by 7° with respect to the incident beam to minimize channeling. The beam current was limited to <0.1 $\mu A/cm^2$ and kept fairly steady to limit beam heating or dose-rate effects. The ion doses reported here are within ±5% accuracy.

X-ray double crystal diffractometry was used to monitor the strain in the implanted layer. Both symmetrical (400) and asymmetrical (311) rocking curves were taken at room temperature in air as little as 1 h after irradiation, as well as several months later. The strain profiles as a function of depth were extracted by simulating the experimental rocking curves using the dynamical x-ray diffraction theory.[15] MeV ^4He channeling spectrometry was used to measure relative damage in the implanted layers.[16] There was no detectable increase in the channeling yield as a result of the He irradiation. The relative damage profiles were extracted from these channeling spectra using a numerical, iterative fitting model.[17]

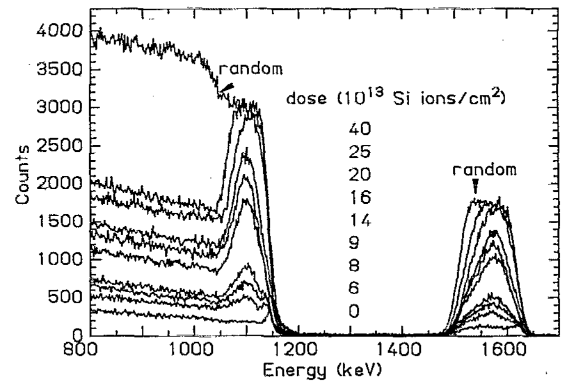

FIG. 1. The ^4He axial channeling spectra along the [100] direction of $x=0.10$ irradiated with 100 keV Si to various doses at room temperature. The detector angle is 170° with respect to the direction of the incidence ^4He beam.

We have utilized an ion energy of 100 keV for irradiation of Ge_xSi_{1-x} films in order to limit the damage at the interface. The change in the ion energy from 100 keV for the case $x=0$ (Si), 0.10, 0.13, 0.15, 0.20 to 300 keV for $x=1$ (Ge) should be noted. This was done to maintain approximately similar values of average energy densities deposited in the collision cascade by the energetic ions.

III. RESULTS AND DISCUSSION

A. Damage and strain

Figure 1 shows the 2 MeV ^4He [100] axial channeling spectra for $x=0.10$ irradiated with various doses of Si, together with the spectrum for random beam incidence. For both Ge and Si signals, the irradiation causes damage peaks that rise with increasing Si ion dose, until they reach the level of the random incidence spectrum. We have used the Si signals in these spectra to extract profiles of damage.

Figure 2 shows a set of selected x-ray rocking curves from symmetrical (400) diffraction for $x=0.10$. The negative angular shift of the epilayer signal with respect to that of the substrate at 0° indicates a positive perpendicular strain of the film, $\epsilon^{\perp}$, which clearly increases with the irradiation dose. The perpendicular strain relaxes very little at room temperature ($<0.01\%$ in strain value in the experimentally accessible time frame of 1 h to many months after irradiation). The parallel strain, $\epsilon^{\parallel}$, of all pseudomorphic samples considered here, irradiated or not, is zero within the experimental sensitivity ($<0.01\%$). Because of the damage created by the ion irradiation, the intensity of the x-ray diffraction peak from the irradiated layer decreases as the dose rises.

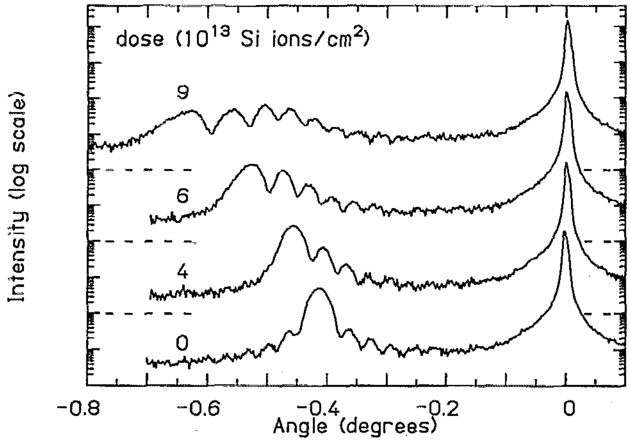

FIG. 2. The x-ray rocking curves from symmetrical (400) diffraction of x=0.10 irradiated with 100 keV Si to various doses at room temperature. The samples for 6 and 9×10^{13} Si ions/cm^2 in Fig. 1 and here are identical. The origin of the abscissa is placed at the Bragg angle θ_B=45.475° of the Si substrate.

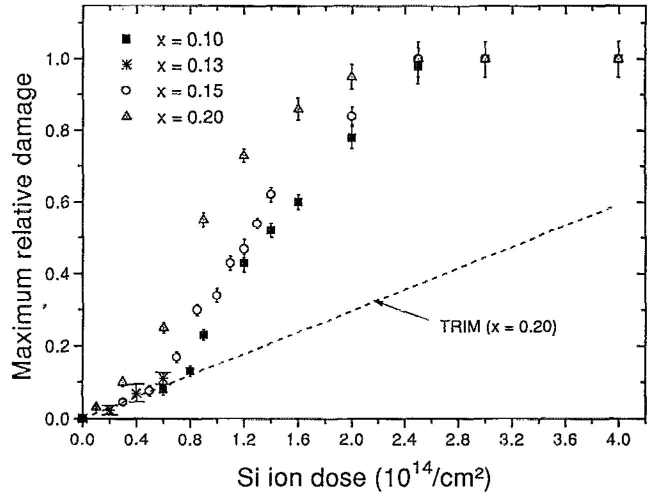

FIG. 4. The maximum relative damage in x=0.10, 0.13, 0.15, and 0.20 irradiated at room temperature by 100 keV Si. The dashed line is the TRIM calculation of the number of displaced atoms in an amorphous x=0.20 irradiated by 100 keV Si at 0 K.

B. Dose dependence of damage

The maximum values of the relative damage profiles for Ge, x=0.10 and Si are plotted in Fig. 3 as a function of irradiation dose. All curves in Fig. 3 exhibit three damage regimes: (I) there is an initially slow increase of the maximum relative damage with dose; (II) the rate of increase of the maximum relative damage accelerates after a threshold level of ~15% is reached, and (III) finally amorphization of the sample is reached beyond a critical dose, $\phi_c(x)$, which is a function of the Ge content. In the case of x=0.10, $\phi_c\sim2.5\times10^{14}$/cm^2, which is a third of that for Si self-irradiation ($\sim7\times10^{14}$/cm^2), even though there is only 10 at. % Ge in the film. It thus appears that a small addition of Ge to Si significantly enhances the retention of irradiation-induced damage. Such an effect can be explained either by an increase in the number of defects initially generated by the impact of an ion or by an increase in the fraction of the defects still present after irradiation. These possibilities are discussed further below. A recent article also showed the existence of these three regimes for

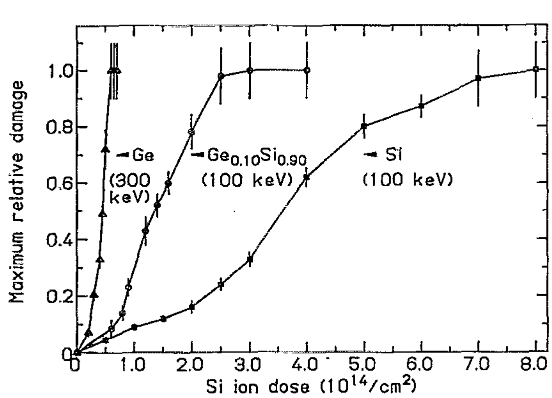

FIG. 3. The maximum relative damage in Si(100) and x=0.10 irradiated by 100 keV Si, and in Ge(100) irradiated by 300 keV Si, plotted vs the Si ion dose. All irradiations were done at room temperature.

the case of Si in an almost identical irradiation experiment.[18] An earlier article on damage in Si produced by 230 keV Si ions also reported a nonlinear increase of damage with dose.[19]

The maximum relative damage obtained from the channeling measurements for x=0.10, 0.13, 0.15 and 0.20 is reported in Fig. 4. We see that all curves exhibit three regimes similar to those identified in Fig. 3. It is thus clear that a nonlinear rise of damage with dose is a general feature of the way damage builds up in the Ge-Si system, under the irradiation conditions applied here. Figure 4 also shows how the maximum relative damage rises with the dose of 100 keV ^{28}Si ions as predicted by the TRIM90 simulation code[20] for an amorphous target of x=0.20 at 0 K. A binding energy of 1 eV and a threshold displacement energy of 15 eV were used as input parameters for the simulation. The computed relative damage does not correctly represent the highly nonlinear data. By concept, TRIM simulation will predict a linear dose dependence because it does not include interactions of defects. The nonlinear dose dependence of the experimental results shows that these interactions are very important. This conclusion is consistent with results reported for pure Ge and Si.[14,21] Thus, TRIM does not serve as a relevant predictor of the retained maximum damage versus dose.

The data in Figs. 3 and 4, as well as the results of other workers,[6–14] show that the retained damage introduced by a given dose of silicon ions increases rapidly with the addition of a relatively small amount of germanium (10%–20%) to pure silicon. It will be demonstrated in Sec. III D below that this increase in retained damage is not related to the initial pseudomorphic strain in the alloy film. The presence of germanium might increase the retained damage in Ge_xSi_{1-x} alloys by increasing the average energy per ion in the collision cascades, and/or by decreasing the mobility of the defects in the cascades, resulting in higher damage re-

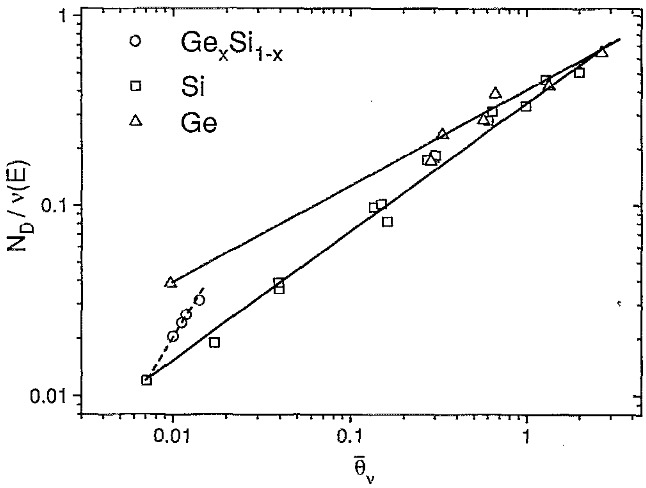

FIG. 5. The total number of displaced atoms, N_D, divided by $\nu(E)$, the component of ion energy dissipated in elastic collisions, is plotted vs the averaged energy density deposited into the collision cascade per atom, $\bar{\theta}_v$ (eV/atom). The two solid straight lines were drawn using the least-mean-square fitting over all data points for bulk Ge (above), or for bulk Si (below). The dashed line is to indicate the trend as x increases in 100 keV Si irradiated $x=0.10$, 0.13, 0.15, and 0.20.

tention at a given bombardment temperature, as discussed in the remainder of this section.

Thompson and Walker have shown that in a given material the stability of ion bombardment damage is dependent on $\bar{\theta}_v$, the average energy density per atom in the collision cascades produced by the bombarding ions.[22] This quantity is given by

$$\bar{\theta}_v=0.2\nu(E)/N_V V_R. \tag{1}$$

$\nu(E)$ is the component of ion energy dissipated in elastic collisions, which can be evaluated using the results of Winterbon.[23] N_v is the number of atoms contained within a spheroid defined by the longitudinal and transverse straggling of the statistical damage distribution, which can also be calculated using Winterbon's tables. V_R is the ratio of an individual cascade volume to the transport cascade volume. This quantity can be estimated by using the results in Fig. 4 of Ref. 24.

We have calculated values of $\bar{\theta}_v$ for 100 keV Si ions incident on silicon and on Ge_xSi_{1-x} alloy for $x=0.10$, 0.13, 0.15, and 0.20. The value of $\bar{\theta}_v$ increases from 0.0072 eV/atom in pure silicon to 0.0142 eV/atom when $x=0.20$. In order to assess the effect that this increase in $\bar{\theta}_v$ may have on damage in these materials, we have plotted data obtained in the present work together with data from Thompson and Walker and Davies[25] in Fig. 5. N_D in this figure is the number of displaced atoms per incident ion determined in samples in which only a few percentages of the atoms have been displaced. N_D was obtained by integrating the damage profiles extracted from the channeling spectra. In the present work this corresponds to the low dose regime I. Straight lines have been drawn using a least square fit in the figure to indicate the trend of the data for pure silicon and pure germanium. These lines give a good representation of the damage retained in silicon or germanium bombarded at room temperature using a variety of different ions and bombarding energies. If the only effect of a small percentage of germanium were to increase the density of retained defects as a result of the increase in the value of $\bar{\theta}_v$, the points for $x=0.10$, 0.13, 0.15, and 0.20 would be expected to fall very near to the line through the silicon data points. However, the points for the Ge_xSi_{1-x} alloys fall significantly above this line indicating that the effect of the germanium in the alloys is to both increase the damage as a result of the increase in $\bar{\theta}_v$ and to reduce the mobility of the defects in the collision cascades resulting in an increase in damage retention. Inspection of Fig. 5 suggests that these two effects make roughly equal contributions to the observed damage increases with respect to pure silicon.

A dashed line has been drawn in Fig. 5 to indicate the trend of the points as x increases. The extension of the dashed line intersects the line drawn for the germanium data points at a $\bar{\theta}_v$ value corresponding to $x=0.35$. It is interesting to note that Haynes and Holland[11] found that for $x=0.50$ the alloy accumulates damage at about the same rate as pure germanium. These results suggest that the incremental damage accumulation decreases with increments of x above $x=0.20$.

It is worth pointing out, as has been done in Ref. 25, that the ordinate in Fig. 5 can also be given a scale corresponding to an effective threshold energy, E_d^{eff}, by using the modified Kinchin–Pease formulation[26]

$$N_D=0.42\nu(E)/E_d^{\mathrm{eff}}. \tag{2}$$

Application of this formula to the silicon data points in Fig. 5 yields an effective threshold energy ranging from about 35 eV for the data point at the lowest value of $\bar{\theta}_v$ to 0.65 eV at the point with the highest value of $\bar{\theta}_v$. This wide variation in effective threshold is a further indication of the inadequacy of damage calculation programs, such as TRIM, which make use of a single value for the displacement energy.

C. Perpendicular strain versus dose

Figure 6 shows the maximum values of the perpendicular strain, $\epsilon_{\max}^{\perp}$, plotted as a function of the Si ion dose for Ge, $x=0.10$ and Si. The dashed line is the component of the strain in the pseudomorphic film that is added to the initial strain as a result of the Si irradiation. Although derived from a different analytical method, the dose dependence of the irradiation-induced perpendicular strain resembles that of the damage shown in Fig. 3. Three dose regimes exist here too: first the induced perpendicular strain builds up slowly up to $\sim$0.15%; then the induced strain rises at an accelerated rate; finally samples are amorphized. The x-ray method becomes ineffective prior to amorphization due to the loss of x-ray diffraction intensity resulting from the damage.

Figure 7 shows the maximum perpendicular strain for $x=0.10$, 0.15, 0.20 versus the Si irradiation dose. In all three cases the dependence of maximum perpendicular strain on dose has the same characteristics as displayed for

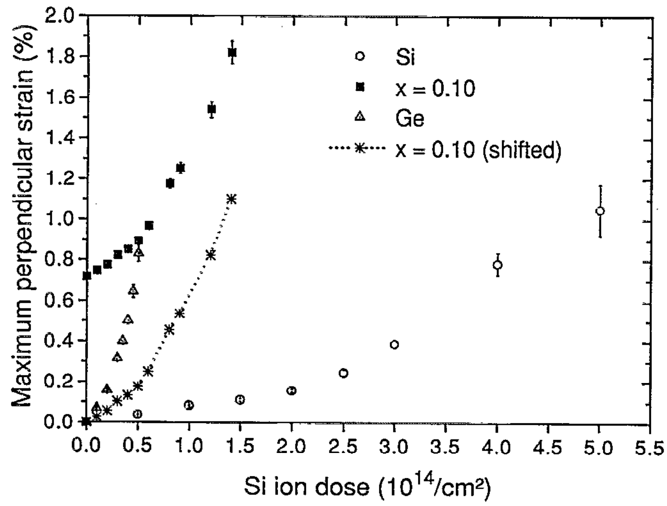

FIG. 6. The maximum perpendicular strain in Si(100) and in $x=0.10$ irradiated by 100 keV Si, and in Ge(100) irradiated by 300 keV Si, plotted vs the Si ion dose. The shifted dashed line shows the *induced* maximum perpendicular strain of the 100 keV Si irradiated $x=0.10$. All irradiations were performed at room temperature.

pure Si and Ge in Fig. 6. We thus conclude that in general the perpendicular strain rises nonlinearly with the dose in the Ge-Si system in much the same way as does the damage (previous section, Figs. 3 & 4).

D. Damage versus strain

We have shown in the previous sections and in Refs. 14 and 21 that the irradiation-induced perpendicular strain and damage are related. Also, the uniform strain in an unirradiated pseudomorphic film does not create damage measurable by channeling. These facts strongly suggest that it is the retained damage that induces the strain.

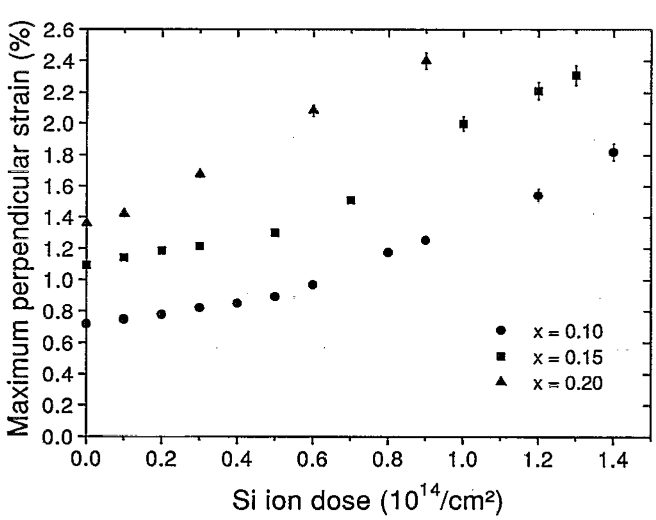

FIG. 7. The maximum perpendicular strain plotted vs Si ion dose of $x=0.10$, 0.15, and 0.20, all irradiated by 100 keV Si at room temperature.

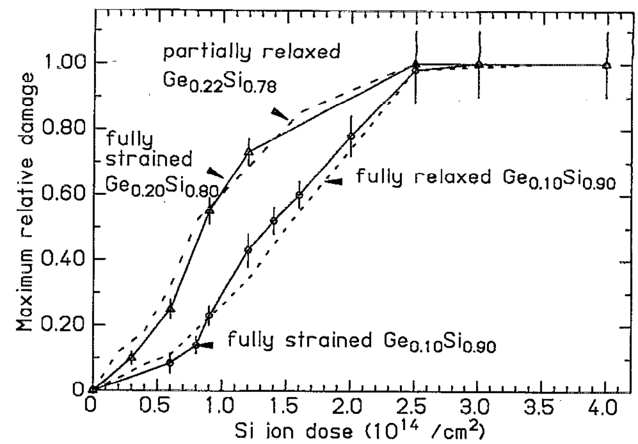

FIG. 8. The maximum relative damage of $x=0.10$ and $x=0.20$ irradiated by 100 keV Si at room temperature were plotted vs the Si ion dose (solid lines). The maximum relative damage of a fully relaxed $x=0.10$ and a partially relaxed $x=0.22$, both irradiated at the same condition as described above, were also plotted here (dashed lines) for comparisons.

1. Influence of initial strain

We now consider how the uniform strain, present initially in epitaxial films, affects the retained damage generated by Si irradiation. Epitaxial Ge_xSi_{1-x} films with different amounts of strain relaxation offer a convenient opportunity to investigate this question. We have done so using samples of $x=0.10$ for both fully relaxed and fully strained layers, and with partially relaxed and fully strained samples of almost the same composition ($x=0.22$ and 0.20, respectively). Figure 8 shows that the initially uniform strain of the Ge_xSi_{1-x} samples does not alter the induced damage levels significantly. For both pseudomorphic and fully relaxed $x=0.10$ layers, the curves of maximum relative damage versus the Si ion-dose are similar. The damage-dose relationships among pseudomorphic $x=0.20$ and partially related $x=0.22$ films are close to each other as well.

We suggest that the reason the initial strain does not play an important role here is because the elastic energy density in the film is small compared with the average energy density per atom deposited into the atomic collision cascade by the energetic ions. To see this quantitatively, the elastic energy density of an elastically isotropic material is given by

$$U_{\text{elastic}}=2\mu\epsilon_0^2(1+\nu)/(1-\nu), \quad (3)$$

where μ is the elastic shear modulus, $\epsilon_0 \approx -0.042x$ is the elastic mismatch of the strained film, and ν is its Poisson ratio. For $x=0.10$ and taking μ about 70 Gpa,[27] Eq. (3) gives

$$U_{\text{elastic}} \approx 5\times 10^{-4} \text{ eV/atom},$$

which is about 5% of the average energy density deposited in the collision cascade during 100 keV Si irradiation of the same film. Thus the pre-existing pseudomorphic strain is unlikely to strongly affect the defect accumulation/

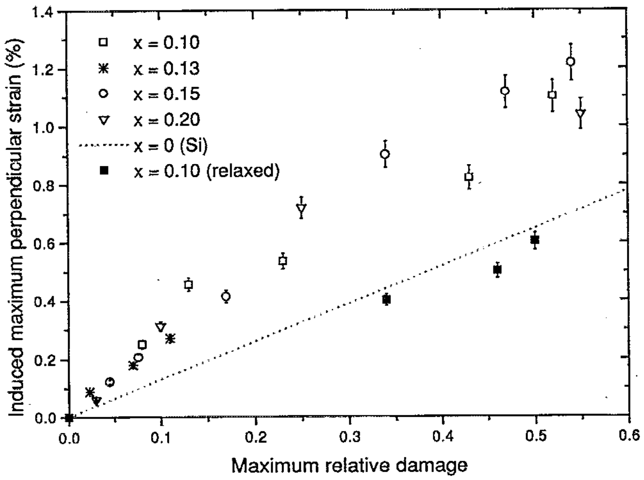

FIG. 9. The induced maximum perpendicular strain is plotted vs the maximum relative damage for $x=0.10$, 0.13, 0.15, and 0.20 irradiated with 100 keV Si (both fully strained and fully relaxed). The dashed line is the relationship between the maximum perpendicular strain and the maximum relative damage for bulk Si irradiated with 100 keV Si.

annihilation mechanism. Vos *et al.*[12] have also suggested that the initial strain of the film may not result in damage enhancement in Ge_xSi_{1-x}.

2. Damage versus induced strain

The results presented in Sec. III D 1 show that a uniform pseudomorphic strain has little effect on the retained damage measured in Ge_xSi_{1-x} at room temperature. This does not prove (in general) that a nonuniform strain will not affect the retained damage. It has been shown that in pure Ge and Si the maximum perpendicular strain generated by Si ion irradiation at room temperature is approximately linearly related to the maximum relative damage, with a proportionality constant of ~ 0.013.[14] This result was interpreted as meaning that in both Si and Ge it is the damage that creates strain and that equal increments of damage produces roughly equal increments of strain.[14,19] It is interesting therefore to relate the measured maximum perpendicular strain with the maximum relative damage for Ge_xSi_{1-x} as well (Fig. 9). The significant dislocation density in the initially relaxed layers broadens their diffraction peaks and makes the maximum radiation-induced strain difficult to determine. Therefore, only three data points at high doses are plotted for the fully relaxed $x=0.10$ film. Also shown is the linear dependence for the 100 keV Si sample self-irradiated at room temperature.

There is a significant difference in Fig. 9 between the points for pseudomorphic Ge_xSi_{1-x} and the dotted line for Si. Because of the scatter in the data points for Ge_xSi_{1-x} it is not possible to determine whether or not there is a consistent dependence of the relation between strain and damage on the value of x. It is clear however that for values of x as small as 0.10, there is significantly higher strain per unit damage in the alloy than in pure silicon. It is possible that this increased strain is associated with the stabilization of defects by Ge discussed in Sec. III B, but the present work does not permit any conclusions about the details of such an association.

The points for the fully relaxed film with $x=0.10$ fall significantly below those for the unrelaxed alloy films and slightly below the linear relation for pure Si. A fully relaxed layer has dislocations that are absent in its pseudomorphic counterpart (and whose density is approximately $8\times10^8/cm^2$ for $x=0.10$).[28] The difference in strain accumulation with damage between pseudomorphic and relaxed films may be associated with this difference in the initial dislocation density of the sample, but speculations on detailed mechanisms are not warranted at the present time.

IV. CONCLUSIONS

(1) The nonlinear increase of the maximum relative damage with dose is a general property of the Ge-Si system irradiated with Si ions at room temperature.

(2) Increasing the Ge content in the film strongly enhances the damage.

(3) The increase in relative damage with Ge content in the films is due to both an increase in the average energy density per ion deposited in the collision cascade and a stabilization of the damage, in roughly equal proportions.

(4) As the relative damage increases with the dose and Ge content, so does the induced maximum perpendicular strain.

(5) There is greater induced maximum perpendicular strain in pseudomorphic Ge_xSi_{1-x} films than in Si or Ge for the same maximum relative damage, but not in relaxed Ge_xSi_{1-x} films.

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