Kinetics of solid phase epitaxial regrowth in amorphized $Si_{0.88}Ge_{0.12}$ measured by time-resolved reflectivity

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Time-resolved reflectivity has been used to measure the rate of solid phase epitaxial regrowth (SPER) *in situ* during annealing of strained $Si_{0.88}Ge_{0.12}$ epilayers on Si preamorphized by the implantation of Si. The SPER velocities were measured over more than two orders of magnitude at temperatures from 503 to 603 °C. The results confirm that the average SPER velocity in thin, strained $Si_{0.88}Ge_{0.12}$ layers is less than that in pure Si. Furthermore, these real-time measurements demonstrate that the SPER rate for strained $Si_{0.88}Ge_{0.12}$ alloys is not a constant during regrowth at a fixed temperature but varies systematically as a function of the position of the amorphous-crystalline interface. The activation energy barrier of SPER in strained $Si_{0.88}Ge_{0.12}$ is higher than that in pure Si and is also a function of interface position, ranging from 2.94 to 3.11 eV. Cross-section transmission electron microscopy shows that strain-relieving defects are introduced coincidentally with the minimum regrowth rate.

Intensive research effort has been directed toward the applications of SiGe alloys in high performance electronic and optical devices, such as high electron mobility transistors[1] and photodetectors.[2] The advantages of SiGe alloys include higher mobilities and smaller band gaps, compared with Si. In conventional silicon IC processing, amorphization during dopant implantation and subsequent solid phase epitaxial regrowth (SPER) are critical steps for improving activation, minimizing channeling tails, and reducing the densities of extended defects. On the other hand, SPER in SiGe alloys results in poor quality layers.[3] Furthermore, the SPER rate of strained SiGe alloys is reportedly smaller than that of pure Si, while the activation energy is larger.[3–5] Thus, the reduction in the velocity and increase in the activation energy of SPER processes in SiGe relative to Si have been attributed to the existence of strain, although the mechanisms have not been determined. The relationship between strain and SPER rate deserves further study.

The technique of time-resolved reflectivity (TRR), as described by Olson *et al.*,[6,7] permits real-time measurement of the interface position and regrowth velocity during SPER. Besides, TRR measurements are efficient and do not require extensive sample preparation. In this letter, the first extensive set of TRR measurements of the SPER kinetics in SiGe epilayers on Si is described. In addition to confirming and extending previous results obtained by cross-section transmission electron microscopy (XTEM) and ion channeling,[3–5,8] this letter reports the discovery of a previously overlooked phenomenon, namely that the SPER velocity varies systematically with interface position in these strained layers.

Strained $Si_{1-x}Ge_x$ layers were grown on *p*-type, 5–20 Ω cm, 4 in. (100) Si wafers at 550 °C by molecular beam epitaxy at Texas Instruments, Inc. Rutherford backscattering spectrometry and XTEM showed the $Si_{1-x}Ge_x$ layer had a Ge fraction of $x=0.12$ and a thickness of ~2000 Å. This $Si_{0.88}Ge_{0.12}$ epilayer was amorphized to a depth of 3000 Å (including 1000 Å of the Si substrate) by dual-energy implantation of $6\times10^{14}/cm^2$ Si^+ at −100 °C and energies of 75 and 150 keV. As-implanted and partially regrown layers were characterized by XTEM (using a JEOL 4000 FX with a point-to-point resolution of 1.95 Å) and ⟨100⟩-axial ion channeling (2 MeV He+ at a 160° scattering angle).

The technique of TRR has been described extensively elsewhere.[6,7] Briefly, the phase difference between the components of laser light reflected from the surface and from the crystalline-amorphous (*c/a*) interface changes continuously during SPER due to the advance of the *c/a* interface, leading to interference fringes in the reflected light intensity that are used to monitor the progress of the interface position. In these experiments, a He-Ne laser ($\lambda=6328$ Å) source was used, with two Si photodiodes to measure the incident and reflected laser power. Samples were mounted on a low-mass molybdenum holder using a heat-conducting paint, and this holder was then wedged into a larger, heated stage which had been preheated to the annealing temperature in an Ar-filled chamber. The sample temperature was measured by a thermocouple embedded in the sample holder. The sample reached the annealing temperature in less than 1 min after insertion. The temperature was quite stable, with variations of less than ±1 °C after an initial settling period of ~1 min, thus permitting TRR measurements over time scales from several minutes

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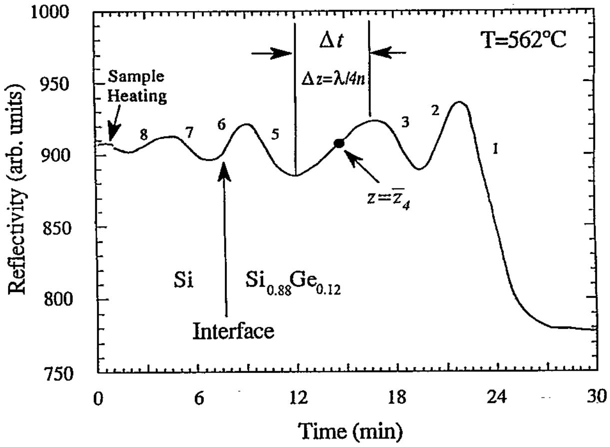

FIG. 1. Time dependence of the reflectivity during regrowth of $Si_{0.88}Ge_{0.12}$/Si at 562 °C. Numerals label sections of the curve corresponding to regrowth stages 1–8.

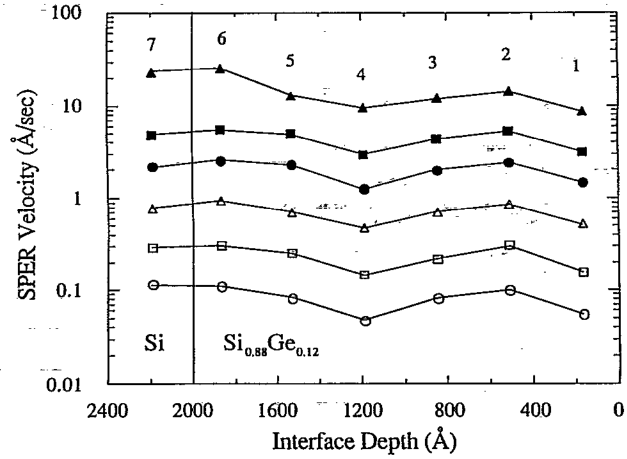

FIG. 2. The SPER rate as a function of a/c interface depth at various temperatures (top to bottom: 603, 580, 562, 543, 523, and 503 °C, respectively). The vertical line marks the Si/SiGe interface. The uncertainties in the measured regrowth rates vary between 3% and 9%.

to tens of hours. In several samples, SPER was interrupted and the thicknesses of the partially regrown layers measured by ion channeling and XTEM, in order to verify the thicknesses determined from TRR.

Figure 1 shows an example of the time dependence of the reflectivity during regrowth of $Si_{0.88}Ge_{0.12}$/Si at 562 °C. The film thickness increment, Δz, between each successive interference maximum and minimum is $\lambda/4n$, where $n=4.65$ is the refractive index of this a-$Si_{0.88}Ge_{0.12}$ layer, as measured by spectroscopic ellipsometry. The SPER rate $v(z)$ is defined as $v=\Delta z/\Delta t=\lambda/(4n \cdot \Delta t)$, where Δt is the time interval between successive extrema. (Thus, v is actually the average rate during the time interval, Δt.) As the c/a interface moves toward the surface, the absorption decreases, and consequently, the amplitude of the reflectivity oscillations is expected to increase. Such behavior is observed in the Si substrate (stages 7–8 in Fig. 1) but not in the strained $Si_{0.88}Ge_{0.12}$ epilayer (stages 2–5), where the amplitude instead decreases slightly. A similar reduction of the interference amplitude has been reported during SPER in GaAs, where it is caused by interface roughening during regrowth.[9] Thus, the reduction of the amplitude in these SiGe layers is ascribed to the presence of a nonplanar interface, as described below. In the case of a nonplanar interface, TRR still reliably measures the mean interface depth (i.e., the interference fringes are not shifted), so long as the roughness is not a strong function of interface position.[9] It is shown below that this condition is satisfied in these alloy layers.

The present results demonstrate that v depends on the c/a interface depth. This can be seen immediately in Fig. 1, where Δt varies for different stages, e.g., $\Delta t_4 > \Delta t_3$. A plot of velocity versus a/c interface depth is presented in Fig. 2. As the interface moves into the $Si_{0.88}Ge_{0.12}$ alloy, the velocity first decreases in stages 5 and 4 to a minimum at $\sim$1200 Å deep, and then increases in stages 3 and 2. Earlier reports did not detect these variations in SPER rate due to experimental uncertainties. However, in retrospect, evidence for such variations might be inferred from the data exhibited in Fig. 4 of Ref. 3 and Fig. 2 of Ref. 4. The interface velocity appears to decrease again in stage 1, but this is at least partly due to the roughness of the c/a interface, which simulations have shown induces a long tail on the last interference fringe.[9]

An Arrhenius plot of the SPER velocity for stages 2–4 is shown in Fig. 3. The SPER rates reported in Ref. 5 for a similar alloy composition are bounded by the lines in Fig. 3. The activation energy determined from these fits varies from 2.94 to 3.11 eV as a function of interface depth. The dependence of activation energy on depth is shown in Fig. 4. It reaches its maximum in stage 4, where the SPER rate is a minimum. At all other depths, the activation energy barrier is approximately constant at $\sim$2.97 eV, to within the experimental uncertainty. This value is $\sim$0.3 eV larger than in pure Si (2.68 eV[6]) and is consistent with values reported earlier for strained SiGe epilayers.[3–5] Based on an analysis of the experimental errors and quality of the Arrhenius fits, the difference between the measured activation energy in stage 4 and the other stages is significant.

XTEM has been used to investigate the relationship

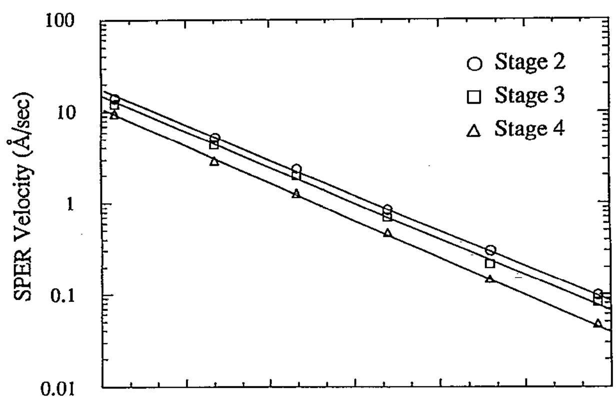

FIG. 3. Arrhenius plot of the SPER velocity for stages 2–4.

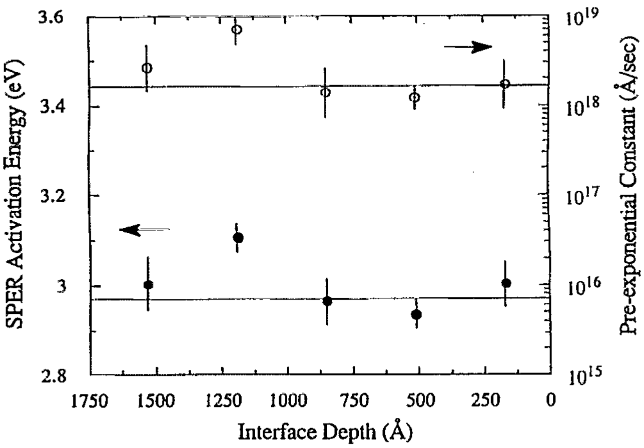

FIG. 4. Activation energy and preexponential factor of SPER velocity as functions of the *a/c* interface position. Error bars represent the standard error of the Arrhenius fits shown in Fig. 3.

between the variable SPER rate and microscopic features of the *a/c* interface. Samples were annealed at 562 °C, and SPER was interrupted at selected stages during TRR measurements. Figure 5(a) shows a cross-section micrograph of such a sample interrupted in stage 2. This figure illustrates (1) the roughness of the *a/c* interface; (2) coherent, relatively defect-free regrowth of the first 400 Å of the alloy near the Si interface; and (3) defects such as stacking faults and dislocations. Such defects relieve strain in these lattice-mismatched epilayers.[5] That they do not appear in the 400 Å of SiGe nearest the Si/SiGe interface is in good agreement with the critical thickness calculations in Ref. 5. Careful examination of a number of micrographs indicated that most such defects originated in the range between 400 and 1000 Å from the Si/SiGe interface. This observation was confirmed by ion channeling on the same samples, illustrated in Fig. 5(b). The channeling spectra exhibit a defect peak indicating that the largest concentration of defects is found in the range between 500 and 1000 Å from the Si/SiGe interface (1000–1500 Å from the surface). Note that this corresponds to the mean depth of the *a/c* interface in stage 4, where the velocity is a minimum. In the channeling spectra of Fig. 5(b), the large peaks on the right correspond to the residual amorphous layer, and the slopes of the left edges of these peaks are indicative of the roughness of the *a/c* interface. Comparison of the spectra (2) and (4) shows that the interface roughness is similar in stages 2 and 4.

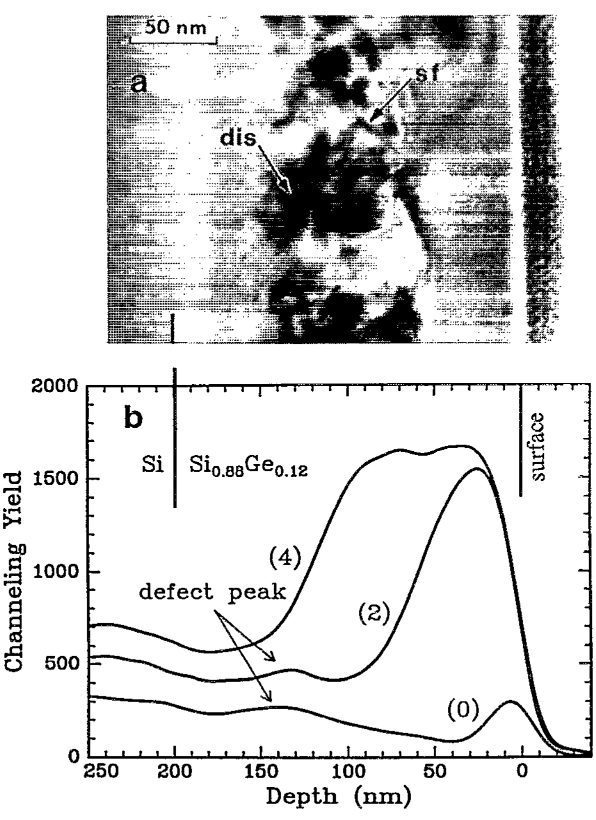

FIG. 5. (a) XTEM micrograph of a partially regrown layer interrupted during stage 2 at 562 °C, showing dislocations (dis) and stacking faults (sf); (b) ion channeling spectra of (0) a fully regrown layer and partially regrown layers interrupted in (2) stage 2 and (4) stage 4. Depth scales in (a) and (b) are identical.

In summary, the first extensive set of measurements of the SPER kinetics in SiGe epilayers on Si has been reported. The main observation from these measurements is that the SPER velocity of strained $Si_{0.88}Ge_{0.12}$ alloys is not a constant, but varies with interface position. The SPER rate reaches a minimum after regrowth of approximately 800 Å of SiGe. This depth corresponds to the region where the majority of strain-relieving defects nucleate. Since it is known that nonhydrostatic compressive strain retards SPER in elemental Si,[10] the present observations suggest the following interpretation: SPER in SiGe alloy epilayers on Si is initially retarded due to compressive strain, but subsequently SPER is accelerated as this strain is relaxed by the introduction of extended defects.

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[1] C. Smith and M. E. Jones, Mater. Res. Soc. Proc. **91**, 277 (1987).

[2] H. Temkin, A. Antreasyan, N. A. Olsson, T. P. Pearsall, and J. C. Bean, Appl. Phys. Lett. **49**, 809 (1986).

[3] D. C. Paine, D. J. Howard, N. G. Stoffel, and J. A. Horton, J. Mater. Res. **5**, 1023 (1990).

[4] Q. Z. Hong, J. G. Zhu, J. W. Mayer, W. Xia, and S. S. Lau, J. Appl. Phys. **71**, 1768 (1992).

[5] D. C. Paine, N. D. Evans, and N. G. Stoffel, J. Appl. Phys. **70**, 4278 (1991).

[6] G. L. Olson and J. A. Roth, Mater. Sci. Rep. **3**, 1 (1988).

[7] G. Q. Lu, E. Nygren, and M. J. Aziz, J. Appl. Phys. **70**, 5323 (1991).

[8] B. T. Chilton, B. J. Robinson, D. A. Thompson, T. E. Jackman, and J. M. Baribeau, Appl. Phys. Lett. **54**, 42 (1989).

[9] C. Licoppe, Y. I. Nissim, C. Meriadec, and P. Krauz, J. Appl. Phys. **60**, 1352 (1986).

[10] M. J. Aziz, P. C. Sabin, and G.-Q. Lu, Phys. Rev. B **44**, 9812 (1991).