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Dry thermal oxidation of a graded SiGe layer

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A method for the dry thermal oxidation of a strained SiGe layer is proposed. By oxidation of a graded $Si_{1-x}Ge_x$ layer, the effect of Ge pileup was significantly reduced and the undesirable strain relaxation by defect formation is prohibited. After oxidation, the oxidized SiGe layer was homogenized by postannealing process, and thereby a SiO_2/SiGe interface with good structural properties was obtained. During postannealing, the homogenization was significantly enhanced by strain-induced diffusion, and it was clearly proved by the uphill diffusion. This result can propose an alternative oxidation method of strained SiGe/Si heterostructures. © *2001 American Institute of Physics.* [DOI: 10.1063/1.1415373]

Due to the compatibility with well-known Si technology, SiGe/Si strained heterostructures have been widely investigated for various applications in the field of electronic and optoelectronic devices.[1,2] For device applications of SiGe, growth of a good quality thermal oxide on a strained SiGe is very critical for the fabrication process, such as gate oxide, isolation, and masking.[3] However, producing a high quality thermal oxide layer for gate dielectric of field-effect devices has been very difficult and conventional thermal oxidation has been shown to result in undesired strain relaxation and formation of a Ge pileup layer below oxide layer.[4–6] This Ge pileup layer causes high interface density, high fixed charge, and poor breakdown characteristics.[7]

The dry thermal oxidation behavior of strained SiGe layer is dependent on oxidation temperature, Ge fraction, and ambient.[8–10] When a strained $Si_{1-x}Ge_x$ layer with Ge content ($x<0.5$) is oxidized at high temperature ($T>700$ °C), due to the large difference between the heat of formation of SiO_2 and GeO_2, SiO_2 is more preferentially produced than GeO_2. As a result, the thermally grown oxide is nearly pure SiO_2, and Ge is rejected from the oxide and piled up below the oxide layer. Therefore, conventional thermal oxidation has been shown to result in undesired strain relaxation and formation of a Ge pileup layer below oxide layer.[11] To prevent the pileup effect and undesirable strain relaxation in thermal oxidation of strained SiGe layer, alternative mechanisms for the oxidation of strained SiGe layer have been proposed,[12–18] but thermal oxidation with reduced pileup effect has not yet been reported.

In this letter, a study on the dry thermal oxidation of a graded SiGe layer is proposed. By oxidation of a graded $Si_{1-x}Ge_x$ layer, the effect of Ge pileup was significantly reduced and the undesirable strain relaxation by defect formation is not visible at all. During postannealing after the oxidation, homogenization of the SiGe layer below the oxide was significantly enhanced by strain-induced diffusion, and it was clearly proved by the uphill diffusion with low energy secondary ion mass spectroscopy (SIMS) measurement. This result can propose an alternative oxidation method of strained SiGe/Si heterostructures.

A graded SiGe/Si layer was deposited at 650 °C on Si(001) wafer by reduced pressure chemical vapor deposition using silane and germane. The Ge composition in the graded SiGe layer is nominally linear from the interface to the surface, and the average Ge composition in the layer is about 12.4%. In the graded SiGe layer, the Ge composition at the $Si_{1-x}Ge_x$/Si heterointerface is about 18.5%, and that at the surface is about 6.5%. After deposition, the graded SiGe layers were oxidized at 900 °C under atmospheric pressure with 2*l*/min O_2 gas flow. To homogenize the Ge distribution in the layer, the oxidized samples were postannealed at 900 °C in N_2 ambient. The average composition and remaining strain of the samples were measured by high-resolution x-ray diffractometer (Philips, X'pert), and the transmission electron microscopy (TEM) observations were performed in a JEM 2000 EX transmission electron microscope operating at 200 kV along a [110] zone axis. Ge profiles in the SiGe/Si heterostructures were analyzed with low energy SIMS (Cameca 4*f*) using 650 eV O_2^+ ions under the incidence angle of 75° with an accel–decel system.

Figure 1(a) shows a cross-sectional TEM micrograph of as-deposited SiGe/Si heterostructures, and (b) and (c) show the enlarged high-resolution TEM micrographs of SiO_2/SiGe interface and SiGe/Si interface of an oxidized SiGe/Si het-

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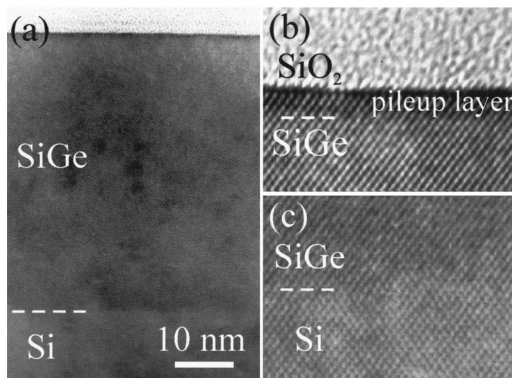

FIG. 1. (a) High-resolution TEM micrograph showing the as-deposited SiGe/Si heterostructure, and enlarged high-resolution TEM micrographs of (b) SiO_2/Ge pileup layer interface and (c) remaining SiGe layer/Si substrate interface of 15 min oxidized SiGe layer.

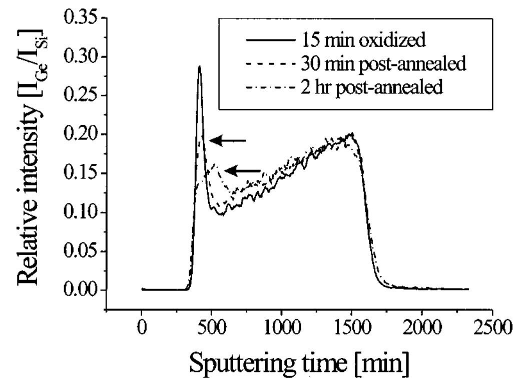

FIG. 3. Low energy SIMS depth profiles of the 15 min oxidized SiGe layers with postannealing time. Leftward arrows indicate the position of the maximum Ge concentration, and it moves toward Si substrate with increasing postannealing time.

erostructure at 900 °C for 15 min, respectively. The thickness of the as-deposited SiGe layer was 45 nm, and there was no evidence of the strain relaxation by defect formation. In oxidized sample, the oxide and pileup layers were clearly defined by atomic number contrast, and the thicknesses of these layers were 12.2 nm (t_{ox}) and 1.3 nm (t_p), respectively. Because the Si consumption rate during oxidation is 0.45 t_{ox}, the Ge atoms distributed in the region from original free surface to 5.5 nm of depth will be rejected from the oxide region and piled up below the SiO_2 layer. In the case of thermal oxidation of a strained SiGe layer with a uniform Ge distribution, the Ge concentration in the pileup region will be at least about five times higher than original concentration $(1+0.45t_{ox}/t_p)$, and it will meet the critical thickness problem, i.e., the defect formation to reduce the strain energy of the strain heterostructure. However, in this experiment, the strain relaxation could not be observed at all, even though in an oxidized heterostructure at 900 °C for 2 h ($t_{ox}=42$ nm, $t_p=5.5$ nm). Therefore, due to the low Ge concentration near surface in the graded SiGe layer, the defect-free oxidation was possible, and the undesirable strain relaxation was negligible.

After oxidation, the oxidized SiGe layers were postannealed at 900 °C in the time range of 30 min–4 h to reduce the inhomogeneity of Ge distribution in pileup region. Figure 2 shows the (004) peak position of the graded SiGe layer relative to (004) peak position of Si substrate measured by high-resolution x-ray diffractometer (HRXRD). In this figure, it is shown that the average strain in the SiGe layer increases with oxidation time. Moreover, the average strain in oxidized sample also increases with the postannealing time, while that in the as-deposited sample is almost constant or slightly decreases with annealing time due to the interdiffusion between Si substrate and graded SiGe layer. By high-resolution TEM measurements, it is observed that there is no defect formation in the postannealed samples, as well as the as-oxidized SiGe layer. Therefore, this result indicates that there is no undesirable strain relaxation by defect formation during postannealing process, and that the postannealing induces the homogenization between a highly strained Ge pileup region and graded SiGe layer.

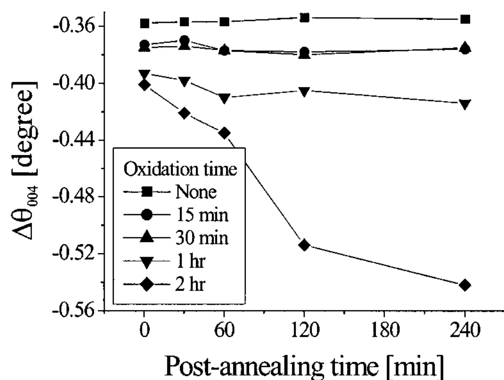

FIG. 2. (004) peak position of the graded SiGe layer relative to (004) peak position of Si substrate measured by HRXRD.

Figure 3 shows the depth profiles of as-oxidized, and postannealed SiGe layers. From the depth profiles, it is clearly shown that the as-oxidized Ge fraction in the pileup region if not severely higher than average Ge fraction in the remaining SiGe layer, and that the Ge fraction in the pileup region rapidly decreases with the postannealing time. By postannealing, the Ge atoms in the pileup region diffuse into the SiGe layer very rapidly, and thereby the graded SiGe layer is almost homogenized after 2 h postannealing. Therefore, the oxidation of a graded SiGe layer with postannealing process can prevent the pileup effect and the undesirable strain relaxation by defect formation.

Moreover, it is clearly shown in Fig. 3 that the position of the maximum Ge concentration in the pileup region (marked by leftward arrows) moves toward the Si substrate. Due to the kinetic barrier of the concentration gradient, the observed uphill diffusion cannot occur in a general diffusion with finite source, such as a dopant diffusion.[19] Therefore, it can be proposed that there should be an additional driving force for the uphill diffusion as well as concentration gradient.[20] In other samples with different oxidation time and postannealing time, the migration of the maximum position of the Ge concentration was consistently observed, and it means that this uphill diffusion can reduce the total energy of the system. In this system, there is much difference of strain energy between the pileup region and the remaining SiGe layer. Due to the high Ge concentration in the pileup region, the strain energy is much higher at the pileup region, and thereby the Ge atoms will preferentially diffuse toward the remaining region of the SiGe layer. Therefore, the diffusion

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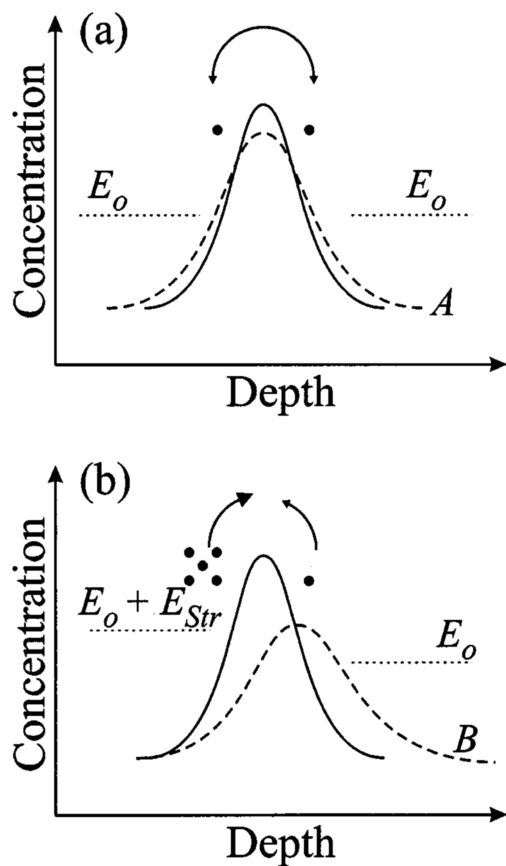

FIG. 4. Schematic diagram showing the uphill diffusion in strained SiGe layer. If the energy states of both sides are identical, thermally activated Ge atoms will diffuse toward both directions with the same amount, and thereby the maximum concentration position will not vary (state *A*). However, due to the thermal oxidation, there is an increment of the strain energy (E_{Str}) in the pileup layer, and it makes the flux toward both directions different and induces the movement of the maximum position toward the direction of low energy state (state *B*).

is significantly enhanced by strain potential gradient, and the strain-induced diffusion can be observed by the migration of the maximum position of Ge concentration.

Furthermore, the migration distance is not linearly proportional to the postannealing time. The distance of the 30 min postannealed sample was about 2 nm and that of the 2 h postannealed sample was about 4.5 nm. It is originated from the decreasing driving force for the uphill diffusion during postannealing process, and this result clearly indicates that the observed uphill diffusion is induced by the strain-potential gradient. Therefore, the homogenization of the SiGe layer is significantly enhanced by strain-induced diffusion during initial stage of the postannealing process.

Figure 4 is a schematic diagram showing a mechanism of the uphill diffusion. During thermal process, an atom will have a chance of overcoming the concentration barrier due to thermal activation. However, if the energy states of both sides are identical, the net flux of the uphill diffusion should be zero, and thereby the maximum position of the concentration profile should not be varied (state *A*), as shown in Fig. 4(a). In this experiment, because the energy state in the pileup region is very high due to the strain energy, as shown in Fig. 4(b), the number of the Ge atoms having a chance of overcoming the barrier will be different at both sides, and Ge atoms will preferentially diffuse toward the region with low energy state. Therefore, the maximum position of the concentration will be changed as state *B*, as shown Fig. 4(b), and this strain-induced diffusion can enhance the homogenization of the SiGe layer.[20]

In conclusion, a method for oxidation of strained SiGe layer was proposed. With graded Ge composition in the SiGe layer, the pileup effect during oxidation process was significantly reduced. By postannealing of the oxidized SiGe layer, a rapid homogenization of the Ge distribution in the layer was possible, and this result can propose an alternative thermal oxidation process without undesirable strain relaxation and pileup effect. Moreover, the uphill diffusion was observed during postannealing, and it can confirm the enhancement of diffusion in strained heterostructure, i.e., strain-induced diffusion.

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[1] Y. H. Xie, Mater. Sci. Eng., R. **25**, 89 (1999).
[2] D. J. Paul, Thin Solid Films **321**, 172 (1998).
[3] D. K. Nayak, J. S. Park, J. C. S. Woo, K. L. Wang, and I. C. Ivanov, J. Appl. Phys. **76**, 982 (1994).
[4] U. König and J. Hersener, Solid State Phenom. **47/48**, 17 (1996).
[5] D. K. Nayak, K. Kamjoo, J. C. S. Woo, J. S. Park, and K. L. Wang, Appl. Phys. Lett. **56**, 66 (1990).
[6] S. J. Kilpatrick, R. J. Jaccodine, and P. E. Thomson, J. Appl. Phys. **81**, 8018 (1997).
[7] L. P. Chen, Y. C. Chan, S. J. Chang, G. W. Huang, and C. Y. Chang, Jpn. J. Appl. Phys., Part 2 **37**, L122 (1998).
[8] J. P. Zhang, P. L. F. Hemment, S. M. Newstead, A. R. Powell, T. E. Whall, and E. H. C. Parker, Thin Solid Films **222**, 141 (1992).
[9] J. Xiang, N. Herbots, H. Jacobsson, P. Ye, S. Hearne, and S. Whaley, J. Appl. Phys. **80**, 1857 (1996).
[10] F. K. LeGoues, R. Rosenberg, T. Nguyen, F. Himpsel, and B. S. Mayerson, J. Appl. Phys. **65**, 1724 (1989).
[11] R. Hull, J. C. Bean, D. J. Werder, and R. E. Leibenguth, Appl. Phys. Lett. **52**, 1605 (1988).
[12] I. Boyd, V. Cracium, and A. Kazor, J. Appl. Phys. **32**, 6141 (1993).
[13] J. M. Madsen, Z. Cui, and C. G. Takoudis, J. Appl. Phys. **87**, 2046 (2000).
[14] R. Sharma, J. L. Fretwell, T. Nagi, and S. Banerjee, J. Vac. Sci. Technol. B **17**, 460 (1999).
[15] G. Lucovsky, S. S. Kim, D. V. Tsu, G. G. Fountain, and R. J. Markunas, J. Vac. Sci. Technol. B **7**, 861 (1989).
[16] L. S. Riley and S. Hall, J. Appl. Phys. **85**, 6828 (1999).
[17] Y. H. Xie, Mater. Sci. Eng., R. **25**, 89 (1999).
[18] A. Agarwal, J. K. Patterson, J. E. Greene, and A. Rockett, Appl. Phys. Lett. **63**, 518 (1993).
[19] W. R. Runyan and K. E. Bean, *Semiconductor Integrated Circuit Processing Technology* (Addison-Wesley, New York, 1990).
[20] Y. S. Lim, J. Y. Lee, H. S. Kim, and D. W. Moon, Appl. Phys. Lett. **77**, 4157 (2000).

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