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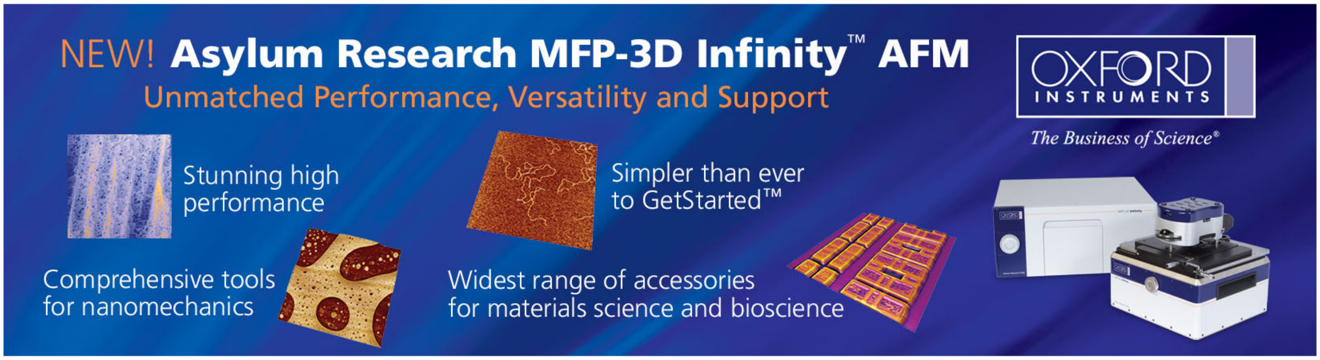

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Use of Si^+ pre-ion-implantation on Si substrate to enhance the strain relaxation of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer layer for the growth of Ge layer on Si substrate

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Si^+ pre-ion-implantation combined with a $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer structure for the growth of Ge layer on Si substrate is proposed. Enhanced strain relaxation of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer layer on Si substrate was achieved due to the introduction of the point defects by heavy dose Si^+ pre-ion-implantation. Because of the strain relaxation enhancement and the interface blocking of the dislocations in the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer structure, the total thickness of the buffer layers was only 0.45 μm. No cross-hatch pattern was observed on the Ge surface and the dislocation density for the top Ge film was only $7.6\times10^6\ \mathrm{cm}^{-2}$. © *2007 American Institute of Physics*.

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Due to the higher mobility of its carriers and its narrower band gap as compared to those of silicon (Si), Ge is now emerging as a viable candidate to supplement Si for complementary metal oxide semiconductor devices and 1.3–1.55 μm optoelectronics applications.[1,2] As a result, it is essential to develop methods for the heteroepitaxial growth of Ge on Si. Such growth is not straightforward because of the large lattice mismatch (4%) between Ge and Si, which limits the quality of the epitaxial layers grown. After reaching a critical thickness, the Ge layer usually contains many misfit and threading dislocations, making it unsuitable for any practical applications.[3]

This study reports on a high dose Si^+ pre-ion-implantation technique which is used to enhance strain relaxation at the interface between the metamorphic buffer layers and the Si substrate in order to facilitate the growth of a high quality Ge on the Si. The epitaxial structure in this study is illustrated in Fig. 1. The composition of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer layers was carefully formulated to block the dislocations in the lower layers. The Ge compositions in the two metamorphic buffer layers were intentionally grown to 80% and 90% each. Because the point defects were introduced by a Si^+ pre-ion-implantation on the surface of the Si substrate, the level of relaxation was enhanced, the thickness of the metamorphic buffer was greatly reduced, and the surface morphology was improved. More interestingly, the dislocation density of the top Ge layer was effectively reduced to $10^6\ \mathrm{cm}^{-2}$.

The experiments in this work can be divided into two parts. The first part involves the growth of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer layers on the Si substrates without Si^+ ion implantations. The growth of the $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ and Ge layers was carried out using an ultrahigh vacuum, chemical-vapor deposition system with a base pressure of less than 2×10^{-8} Torr. After RCA cleaning of the 4 in. Si (100) substrate surface, a $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer structure, in-

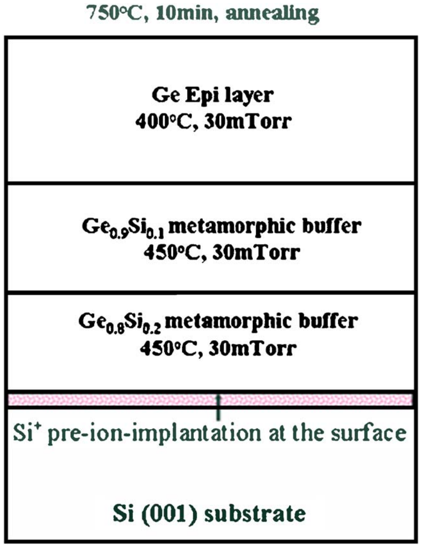

FIG. 1. (Color online) Layer structure and the growth conditions for the Ge film grown on the Si substrate with $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ metamorphic buffer layers. Note that $\mathrm{Ge}_x\mathrm{Si}_{1-x}$ was grown at two growth rates, the Ge composition set at 80% and 90%, and the Si substrate implanted with high dose Si^+ ions.

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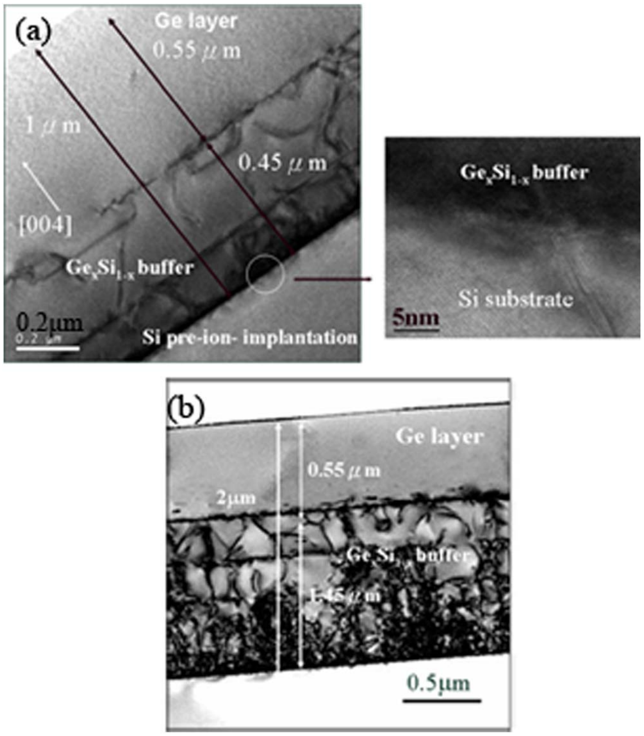

FIG. 2. Cross-sectional TEM images of sample (a) with a Si^+ pre-ion-implantation into the Si substrate; the inserted image is the high-resolution TEM image at the interface between the Ge_xSi_{1-x} metamorphic layer and the Si substrate. (b) The Ge_xSi_{1-x} metamorphic grown on the Si substrate without a Si^+ pre-ion-implantation into the Si substrate.

cluding one $Ge_{0.9}Si_{0.1}$ layer and one $Ge_{0.8}Si_{0.2}$ layer, was grown at 430 °C.[3] Then a pure Ge top layer was subsequently grown at 400 °C with the same vapor pressure and with a constant GeH_4 flow rate of 10 SCCM (SCCM denotes cubic centimeter per minute at STP). After the Ge growth was finished, *in situ* annealing at 750 °C for duration of 15 min was employed to improve the crystalline quality of the epitaxial layers. The optimum thickness of the Ge_xSi_{1-x} metamorphic buffer layer should be larger than 1.45 μm for strain relaxation to occur so that a high quality pure Ge film can be achieved.[3]

The second part of this work focuses on the study of the effect of Si^+ pre-ion-implantation on the growth of the Ge_xSi_{1-x} metamorphic layer. As mentioned above, the Ge_xSi_{1-x} buffer structure was grown with the same Ge composition as that of the Si^+ implanted Si substrate. The implantation involved a Si^+ dose of 5×10^{15} cm^{-2} administered at an acceleration voltage of 50 keV. Figures 2(a) and 2(b) show the bright-field, cross-sectional transmission electron microscopy (TEM) images of the samples with and without the Si^+ pre-ion-implantation, respectively. Figure 2(a) was taken by using a diffraction vector $\mathbf{g}=[004]$, and the surface of the Si substrate was modified with a Si^+ pre-ion-implantation. By contrast, Fig. 2(b) was taken by using a diffraction vector $\mathbf{g}=[004]$, and the Si substrate was not implanted. The top Ge layer and the Ge_xSi_{1-x} metamorphic buffer are clearly shown in both images. In Fig. 2(a) a dark region can be observed at the interface between the Ge_xSi_{1-x} buffer and the Si substrate, this region is associated with the defects induced by the Si^+ pre-ion-implantation. The thinner buffer layers were observed in the Ge_xSi_{1-x} metamorphic buffer layers with a pre-ion-implantation, and the optimized

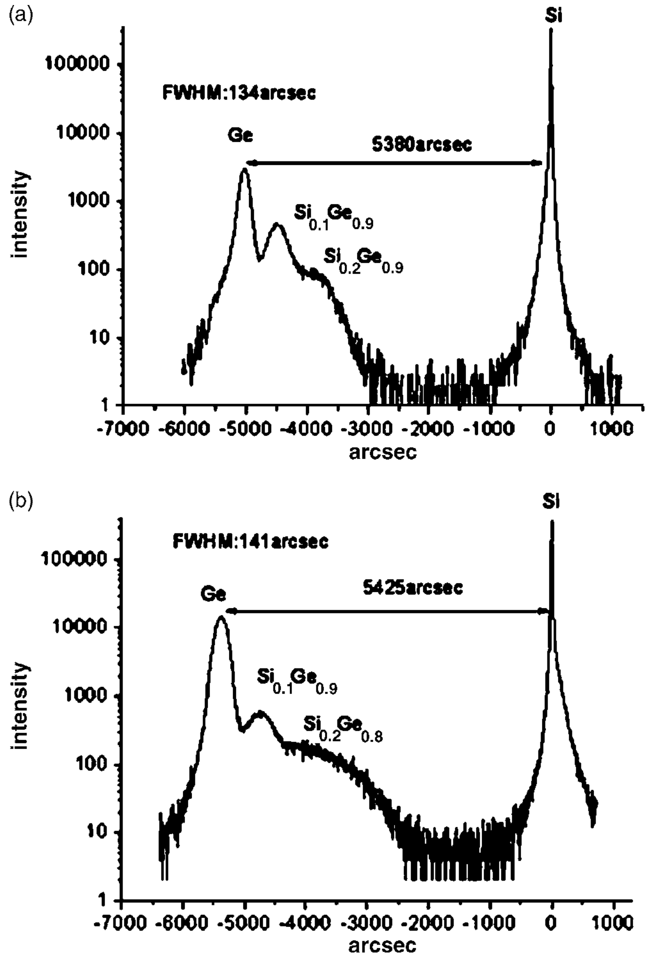

FIG. 3. (a) Double crystal x-ray data indicating variations at a [004] orientation for the Ge_xSi_{1-x} metamorphic buffer layer on the Si substrate with a Si^+ pre-ion-implantation. (b) Double crystal x-ray difference data indicating variations at [004] orientation for the Ge_xSi_{1-x} metamorphic buffer layer on the Si substrate without a Si^+ pre-ion-implantation.

thickness of the Ge_xSi_{1-x} metamorphic buffer required for the growth of a high quality Ge film was only 0.45 μm. By contrast, in Fig. 2(b), in order to obtain a high-quality Ge top layer, a thicker metamorphic buffer layer was required to relax the strain energy for the sample without pre-ion-implantation. In this case, the optimized thickness of the Ge_xSi_{1-x} metamorphic buffer for the growth of high quality Ge film was larger than 1.45 μm.

In Fig. 3(a), the single crystalline peak for the top Ge layer (θ_{Ge}) is clearly visible with a strong intensity. It separated from the Si substrate peak (θ_{Si}) with a distance of θ_{Si}-θ_{Ge}=5380 arc sec, which indicates that the top Ge layer is close to full relaxation (in case of full relaxation, θ_{Si}-θ_{Ge} =5366 arc sec). Other smaller additional peaks are shown on the right side of the Ge peak. These smaller peaks correspond to the different Ge_xSi_{1-x} layers in the metamorphic buffer. Because the Ge composition in the buffer begins at $x=0.8$ (rather than at $x=0$), these peaks are also a great distance from the Si substrate peak. The dislocation density (D) in the top Ge layer can be estimated from the full width half maximum (FWHM) of the x-ray Bragg peak by using the equation[4,5]

$$D=\Delta\varphi^2/(9b^2), \qquad (1)$$

where b is the length of the Burger vector of the dislocations and $\Delta\varphi$ is the FWHM. Assuming that the dislocations contained in the Ge layer are the 60° dislocations, then the value $b=\sqrt{2}\mathbf{a}$, where $\mathbf{a}$ is the lattice parameter. From Fig. 3(a), $\Delta\varphi=134$ arc sec can be obtained. With these values, the dislocation density in the Ge film grown with a Si^+ pre-ion-implantation is calculated to be $D=7.6\times10^6$ cm^{-2}.[6]

Figure 3(b) shows the Ge_xSi_{1-x} metamorphic buffer grown on the Si substrate without Si^+ pre-ion-implantation. The highly intense peak for the top Ge layer (θ_{Ge}) is also clearly visible. It is separated from the Si substrate peak (θ_{Si}) by a distance of θ_{Si}-$\theta_{Ge}=5425$ arc sec, which indicates that the top Ge layer has higher strain than the Ge layer grown on the Si substrate with pre-ion-implantation.[7] This result indicates that the Si^+ pre-ion-implantation induced point defects in the Si substrate clearly result in the reduction of strain in the buffer layer.[8] Other smaller peaks in Fig. 3(b) are broader than their counterpart peaks in Fig. 3(a), which can be attributed to more dislocations generated at the lower layer of the metamorphic buffer when grown on the Si substrate without pre-ion-implantation. It is postulated that this is due to the increased density of defect nucleation sites arising from point-defect condensation to form incipient dislocation loops.[9] These nucleation sites then help the system to overcome the high nucleation barrier which would exist in the absence of the implantation. It is the enhanced dislocation nucleation which is responsible for the accelerated relaxation of the implanted structure. Once nucleated, it is favorable for the dislocations to propagate energetically, thus relaxing the structure. Consequently, the density of threading dislocations is reduced.[10–12]

An atomic force microscopy image of the surface of the Ge film grown on the Si substrate with Si^+ pre-ion-implantation is shown in Fig. 4. The surface is smooth and no cross-hatch pattern is visible. For the current case, the disappearance of the cross-hatch pattern is because the metamorphic buffer takes a three-dimensional growth mode in its initial stage, and the resulted behavior of the dislocations is different from that in the conventional composition graded GeSi layers.

In summary, a thin Ge_xSi_{1-x} metamorphic buffer layer for the growth of a high-quality Ge film on a Si substrate was achieved by using a Si^+ on implantation on the Si substrate before the growth of the Ge_xSi_{1-x} metamorphic buffer layers. The enhanced level of relaxation can be attributed to the introduction of point defects in the Si substrate with a heavy dose Si^+ pre-ion-implantation. Due to the use of the pre-ion-implantation technique and the interface blocking of the dislocations in the Ge_xSi_{1-x} metamorphic buffer structure, the total thickness of the Ge_xSi_{1-x} metamorphic buffer layer was greatly reduced to a thickness of 0.45 μm, which is much thinner than in the previous report.[3] Because the formation of the dislocation pileups in the Ge_xSi_{1-x} metamorphic buffer layer was eliminated, the surface of the Ge film grown was very smooth, no cross-hatch pattern could be observed and the dislocations in the top Ge layer were reduced to about 7.6×10^6 cm^{-2}. The approach described in this letter can be used to grow high-quality Ge film on a Si substrate and can also be easily applied to the fabrication of the Ge metal oxide semiconductor field effect transistors and optoelectronic devices on Si substrates.

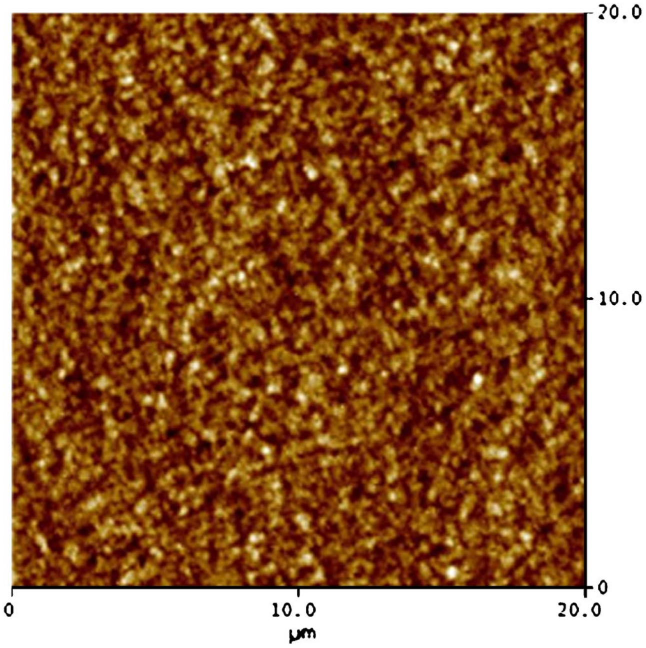

FIG. 4. (Color online) Atomic force microscopy image of the surface morphology of the sample with a Si^+ pre-ion-implantation. The root mean square (rms) of the roughness is 0.38 nm.

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