# Smoothing of $Si_{0.7}Ge_{0.3}$ virtual substrates by gas-cluster-ion beam

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The planarization of the SiGe virtual substrate surface is crucial for the fabrication of high-performance strained-Si metal-oxide-semiconductor field-effect transistors. In this letter, we report on the smoothing of the inherently crosshatched rough surfaces of SiGe deposited by molecular beam epitaxy on Si substrates by gas cluster ion beams. Atomic force microscopy measurements show that the average surface roughness ($R_a$) of the SiGe layer could be reduced considerably from 3.2 to 0.7 nm without any crosshatched pattern. Rutherford backscattering in combination with channeling was used to study the damage produced by cluster bombardment. No visible surface damage was observed for the normal-incidence smoothed SiGe with postsmoothing glancing angle cluster ion beam etching. © *2005 American Institute of Physics*.
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Strained-Si on strain-relaxed $Si_{1-x}Ge_x$ buffer layers has received a great deal of attention due to its promising prospect in the fabrication of high-performance strained-Si metal-oxide-semiconductor field-effect transistors (MOSFETs). It is expected that strained-channel devices will exhibit enhanced mobility of holes and electrons.[1–3] However, to exploit these advantages, high-quality strain-relaxed $Si_{1-x}Ge_x$ virtual substrates are required. Due to the large lattice mismatch (4.2%) between Si and Ge, strain-relaxed $Si_{1-x}Ge_x$ inherently presents a crosshatch patterned and rough surface generated by the relaxation of strain field during $Si_{1-x}Ge_x$ growth.[4,5] Such surface morphology is deleterious to device reliability and can interfere with device geometry as defined by lithography. Olsen *et al.*[6] observed that the crosshatching roughness play an important role in roughing the $Si/SiO_2$ interface of strained-Si MOSFETs. More recently, both theory and experiment demonstrate that the rough $Si/SiO_2$ interface is a principal carrier mobility-limiting mechanism.[7–10]

Up to now, many approaches for the fabrication of high-quality relaxed $Si_{1-x}Ge_x$ buffer layer with low threading dislocation density and smooth surface have been pursued. Examples include the composition-graded buffer layer method,[11] the low-temperature grown Si layer method,[12] and the impurity-modified strain method.[13] However, the resulting surface roughness is still not comparable to that of Si wafers. Therefore, an alternative method employing a suitable growth technique and postgrowth surface treatment using chemical mechanical polishing (CMP) has been intensively studied and shown to yield a better performance.[9,14]

A limitation of CMP in addition to being a slow and tedious process is surface contamination. Thus, an additional cleaning process is required after CMP. It is necessary to develop a different method to polish the crosshatched surface of relaxed $Si_{1-x}Ge_x$ buffer layers for MOSFETs application. Our smoothing technique using cluster ion beam is reported here.

Recently, gas cluster ion beam (GCIB) bombardment has emerged as a widely applicable surface smoothing technique. GCIB is an ion beam of clusters of gaseous atoms with a cluster size as big as a few thousand atoms or molecules bonded by van der Waals force. The sputtering effects of the cluster ion-solid interaction are quite different from those of monomer ion-solid interaction.[15] In monomer ion sputtering at normal incidence, the roughening of surfaces is well known and extensively studied. In cluster ion beam sputtering, the simultaneous arrival of constituent atoms at the same location produces multiple collisions between incident atoms and the target surface atoms, which results in the lateral sputtering of many target atoms. These laterally sputtered atoms redeposit on surface depressions, leading to the smoothening of the solid surface. Such a unique smoothing effect from a cluster ion beam has been applied to smoothen the surfaces of many materials, including metals,[16] high $T_c$-superconducting YBCO films,[17] and semiconductors.[18] In this work, we describe a method employing an Ar–GCIB, which can smoothen the crosshatched surface of relaxed $Si_{0.7}Ge_{0.3}$ down to an average smoothness of 7 Å or better.

Thin films of $Si_{0.7}Ge_{0.3}$ were deposited on Si substrate, using an UHV molecular beam epitaxy coater. The base pressure of the chamber was below $2\times10^{-10}$ mbar. The samples consist of (a) a thin buffer layer of Si grown at 700 °C, (b) 1000 Å Si grown at low temperature of 450 °C (LT layer), and (c) a 3000-Å-thick $Si_{0.7}Ge_{0.3}$ layer grown at 650 °C. The as-deposited samples were irradiated with 30 keV Ar clusters at normal incidence with several different dosages ranging from $5\times10^{15}$ clusters/cm$^2$ to $1\times10^{16}$ clusters/cm$^2$. The cluster mean size was estimated at around 3000 atoms. Sputtering yields were obtained from the sputtered depth as measured by Rutherford backscattering spectroscopy (RBS). The

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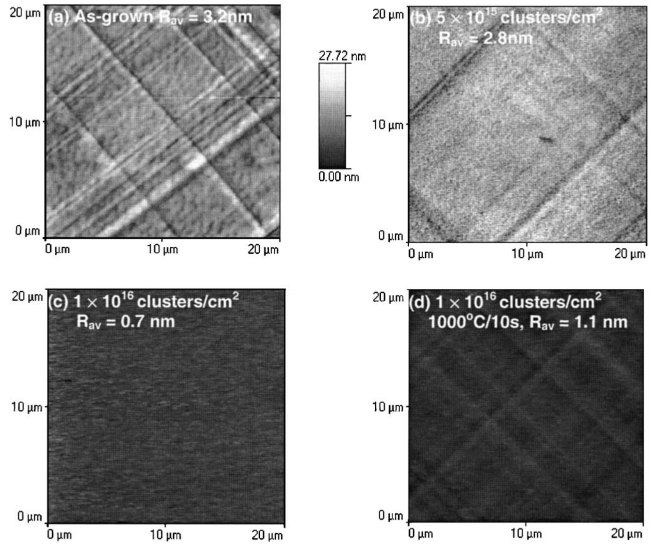


FIG. 1. AFM images of the $Si_{0.7}Ge_{0.3}$ virtual substrates before and after 30 keV Ar gas cluster ion beam irradiation at room temperature: (a) before irradiation, (b) after cluster ion irradiation at $5\times10^{15}$ clusters/cm$^2$, (c) after cluster ion irradiation at $1\times10^{16}$ clusters/cm$^2$, and (d) after cluster ion irradiation at $1\times10^{16}$ clusters/cm$^2$ and rapid thermal annealed at 1000 °C/10 s in nitrogen ambient.

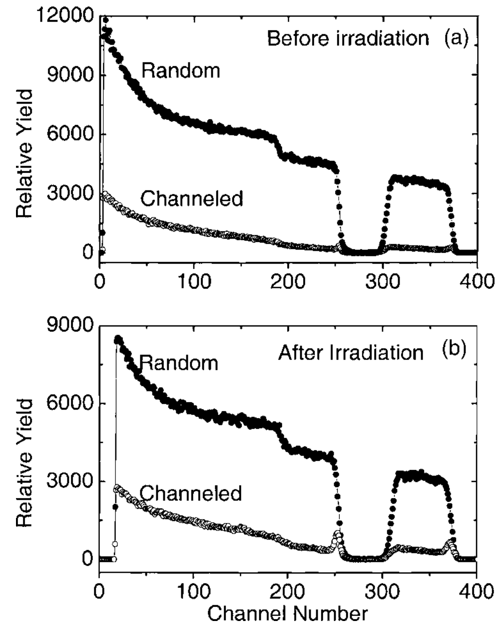


FIG. 2. RBS/channeling analysis of the surface damage in $Si_{0.7}Ge_{0.3}$ virtual substrates induced by Ar gas cluster irradiation: (a) before and (b) after irradiation (30 keV, $1\times10^{16}$ clusters/cm$^2$). The surface peaks are equivalent to disordered layer thickness of 2.0–3.0 and 5.2–6.3 nm for the as-grown and smoothed $Si_{0.7}Ge_{0.3}$ virtual substrates, respectively.

surface morphology and roughness were studied by atomic force microscopy (AFM). Damage production induced by the smoothing process was quantitively studied by RBS/channeling using a 1.7 MV tandem accelerator (NEC, 5SDH) with a 2.0 MeV alpha particle beam.

Figure 1 shows images of the $Si_{0.7}Ge_{0.3}$ virtual substrate surface as observed by AFM before and after Ar–GCIB irradiation at room temperature. Due to the lattice mismatch at the Si/SiGe heterojunction, a crosshatched pattern is observed as shown in Fig. 1(a). The typical average surface roughness ($R_a$) of the as grown $Si_{0.7}Ge_{0.3}$ layer is around 3.2 nm. Figures 1(b) and 1(c) show the surface morphology evolution as a function of dosage of the 30 keV normally incident Ar–GCIB. It is found that the density of the crosshatch lines decrease with increasing Ar cluster dosage. Meanwhile, the average surface roughness of the $Si_{0.7}Ge_{0.3}$ layer is improved gradually from 3.2 to 0.7 nm. The crosshatch pattern was totally removed when the incident cluster ion dose reaches $1\times10^{16}$ clusters/cm$^2$ [see Fig. 1(c)]. Similar improvements are obtained on various samples with different initial surface roughness. The total removed layer was around 66.2 nm after 30 keV Ar cluster irradiation at a dose of $1\times10^{16}$ clusters/cm$^2$ as measured from RBS before and after cluster irradiation.

It is generally accepted that the smoothing effect induced by a normal incident cluster ion beam originates not only from the lateral sputtering effect but also from different sputtering rates at irradiation sites with different slopes. The sputtered atoms migrate to or redeposit in valleys. As a result, cluster ion beams preferentially remove surface protrusions, leading to a smooth solid surface.[19,20] Recent studies show that impact-transient surface diffusion is the primary smoothing mechanism.[21]

Although GCIB improved the surface morphology, we have to consider the side effects of surface damage to the crystalline structure during irradiation. To quantify the damage formation induced by the cluster ion bombardment, RBS/channeling measurements were used. Figure 2 shows the RBS/channeling spectra from both the initial and cluster irradiated $Si_{0.7}Ge_{0.3}$ virtual substrate. For the as-grown sample, it shows very high quality with a $\chi_{min}\approx3.5\%$ and the surface peak in the channeled spectrum corresponded to a layer of 2.0–3.0 nm. After the $1\times10^{16}$ clusters/cm$^2$ cluster ion bombardment, lattice disorder built up near the surface as the $\chi_{min}$ increased to 8.2%. The damaged layer thickness is around 5.2–6.3 nm as assessed from the corresponding channeling spectrum after subtracting the background. It is interesting to note that both the $\chi_{min}$ and the damage layer thickness are independent of the incident cluster ion beam dosage within the range covered in this study (from $5\times10^{15}$ to $1\times10^{16}$ clusters/cm$^2$).

The damaged surface layer has to be removed before further device processing. Otherwise, it will degrade the device performance. Although either chemical etching or physical methods such as postsmoothing annealing can be used to remove or regrow the damaged surface layer, the surface morphologies of the smoothed samples degrade after such treatments. For example, the damaged layer is significantly recovered after 1000 °C 10 s postsmoothing annealing as observed from RBS/channeling spectra. However, the surface shows a crosshatch pattern again after regrowth with the average surface roughness increasing from 0.7 to around 1.1 nm [see Fig. 1(d)]. Similar results have been obtained when we try chemical etching to remove the surface damage layer. Thus a novel alternative method of damaged layer removal while maintaining the surface smoothness has to be developed.

Recently, a molecular dynamics simulation demonstrates that the damage in Si induced by extra large size (>100 000 atoms/cluster) gas cluster bombardment is negligible.[22] This may be a promising way to polish the rough $Si_{1-x}Ge_x$ system without inducing lattice damage during smoothing. However, the extra large size gas cluster ion beams with high beam current for industrial application are

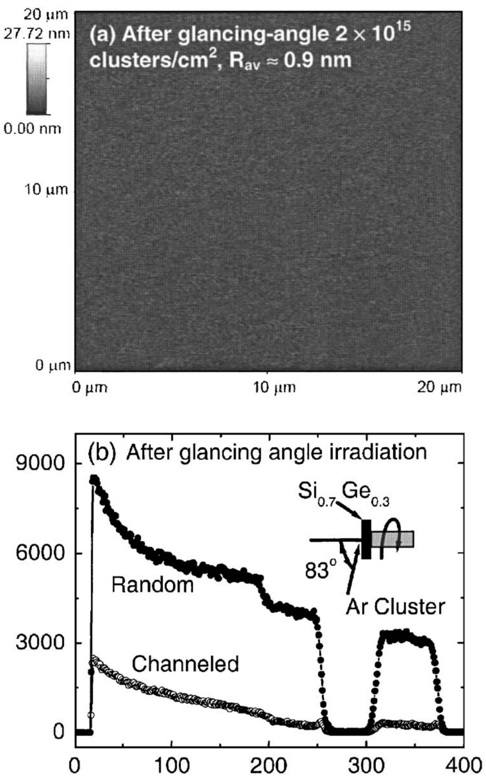


FIG. 3. (a) AFM image and (b) RBS/channeling spectra of $Si_{0.7}Ge_{0.3}$ virtual substrates smoothed by 30 keV $1\times10^{16}$ clusters/cm$^2$ Ar cluster ion beam at normal incidence and followed by 30 keV $2\times10^{15}$ clusters/cm$^2$ Ar cluster ion beam irradiation at glancing angle ($\theta$=83°) with the substrate rotating during irradiation. No visible surface damage is observed.

still under development. In this letter, we describe glancing angle Ar cluster ion beam irradiation on an Ar cluster presmoothed $Si_{0.7}Ge_{0.3}$ virtual substrate as a technique for fabricating smooth surfaces without subsurface damage. The reason to choose glancing angle irradiation is to reduce the cluster energy in the substrate normal direction while etching the surface layer. The experimental setup is shown in the inset of Fig. 3(b). The presmoothed $Si_{0.7}Ge_{0.3}$ sample using 30 keV Ar clusters with dose $1\times10^{16}$ clusters/cm$^2$ was mounted on a holder which rotates during the Ar cluster glancing bombardment. The direction of the incident Ar cluster ion beam is 83° away from the normal of the $Si_{0.7}Ge_{0.3}$ substrate. Figure 3(a) shows the AFM image of the presmoothed $Si_{0.7}Ge_{0.3}$ sample after 30 keV Ar clusters irradiation at glancing angle to a dose of $2\times10^{15}$ clusters/cm$^2$. The surface is atomically smooth without crosshatch pattern and the average roughness is 0.8–1.0 nm. The RBS/channeling measurement confirmed that this postsmoothing glancing angle dry etching thoroughly removed the damaged surface layer produced by the normal smoothing process. The samples smoothed with the normal incidence cluster beam, followed by the oblique cluster smoothing possess good bulk quality with $\chi_{min}\approx3.5\%-4\%$ comparable to the as-grown sample [see Fig. 3(b)]. It is noteworthy that the selection of the angle from sample normal and the glancing angle irradiation dosage are very critical to the whole process. When the glancing angle is less than a critical angle $\theta_{critical}\sim70°$, cluster ion irradiation roughens the sample surface due to the asymmetric distribution of sputtered atoms.[16] A smoothing effect is observed when the glancing angle is larger than $\theta_{critical}$. However, the smoothing efficiency is much lower due to the decreased sputtering yield under the condition of glancing angle irradiation comparing to the normal incidence irradiation.[16,23] The details of the influence of those parameters will be reported elsewhere.

In summary, we have polished the crosshatched rough surfaces of $Si_{0.7}Ge_{0.3}$ virtual substrate by using an accelerated gas cluster ion beam technology. Atomic level smoothness of the $Si_{0.7}Ge_{0.3}$ layer without irradiation damage was achieved by combining normal direction cluster ion beam smoothing with a postsmoothing glancing angle cluster ion beam dry-etching process. This process is important for strained-Si MOSFET devices fabrication without chemical contamination.

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