Relaxation of strained pseudomorphic Si$_x$Ge$_{1-x}$ layers on He-implanted Si/δ-Si:C/Si(100) substrates

D. Buca,[1,a)] R. A. Minamisawa,[1] H. Trinkaus,[1] B. Holländer,[1] N. D. Nguyen,[2] R. Loo,[2] and S. Mantl[1]

[1]*Institute of Bio- and Nanosystems, Forschungszentrum Jülich, and JARA—Fundamentals of Future Information Technology, D-52425 Jülich, Germany*
[2]*IMEC, Kapeldreef 75, B-3001 Leuven, Belgium*

In this letter we present a method to increase the efficiency of SiGe layer relaxation by He$^+$ ion implantation and annealing. Preferential nucleation of He platelets along a δ-impurity layer grown in the Si substrate below the SiGe layer results in planar localization and homogenization of dislocation loop sources inducing a more uniform distribution of misfit dislocations. We demonstrate this for a thin Si:C layer grown by reduced pressure chemical vapor deposition. The optimization of the conditions for efficient relaxation and layer quality is studied with respect to the position of the Si:C layer and the process parameters. Relaxation degrees up to 85% are obtained for Si$_{0.77}$Ge$_{0.23}$ layers. © 2009 American Institute of Physics. [doi:10.1063/1.3240409]

Tensile strain in Si (sSi) and sSi/Si$_x$Ge$_{1-x}$ heterostructures is well known to enhance carrier mobility for high performance channels in complementary metal oxide semiconductor field effect transistors.[1] A key achievement to fabricate such materials, compatible with industrial processes at wafer level, is the strain induced in Si films grown on strain-relaxed Si$_x$Ge$_{1-x}$ virtual substrates.[2] The advantageous coupling of sSi and silicon on insulator technologies[3,4] allows device fabrication with a better control of the electrostatics and lower power consumption.

We have previously introduced and demonstrated the usefulness of He$^+$ ion implantation and annealing to produce high quality thin ($\sim$200 nm) relaxed SiGe layers.[5,6] This concept is based on the creation of overpressurized He filled cavities of platelet shape in the ion implanted region underneath the SiGe/Si interface during an intermediate stage of annealing. These defects eject interstitial dislocation loops that glide to the SiGe/Si interface. Here, one segment of each loop is hold at the interface as a misfit dislocation (MD) segment while the other is driven by the stress through the SiGe layer to the surface forming by this two threading dislocations (TDs). The motion of the two TDs in opposite directions results in an extension of the MD segment leading to strain relaxation of the SiGe layer.[7] The generation of dislocation loops by overpressurized He platelets has been observed in Si (Ref. 7) as well as in SiC (Ref. 8) after He$^+$ implantation and subsequent annealing. Note that platelet shaped He cavities tend to decay into small spherical cavities in a late evolution stage usually reached during annealing.[9]

The method of relaxing SiGe layers by He implantation and subsequent annealing has limitations at low and high implantation doses. At low doses, due to low spatial density of dislocation sources, unacceptable strain fluctuations have been found in the relaxed layer. In the opposite case, at high doses, even if the high density of He cavities provides a relatively *regular array of dislocation sources*, their *broad depth distribution* [Fig. 1(a)] favors mutual dislocation loop blocking. This limits the effective injection of mobile dislocation loops into the SiGe layer and, consequently, its degree of strain relaxation.

In the present work we concentrate on the mechanism of creating overpressurized He filled platelets. We present a method for preferential nucleation of He platelets in the Si substrate below the SiGe layer which results in *planar localization, homogenization, and alignment of dislocation loop sources*, as illustrated in Fig. 1(b). An analytical model based on He diffusion is proposed which allows the understanding and optimization of the process conditions with respect to an enhanced relaxation of Si$_x$Ge$_{1-x}$ layers.

Two effects are essential: (1) local enhancement of He cavity nucleation at a δ-layer and (2) suppression of cavity nucleation in its surroundings. The first effect can be realized either by reducing the energy associated with cavity formation or by creating additional volume for He accumulation. A reduction in the cavity surface energy (determined by matrix atom binding energies) is obtained by locally alloying Si with Ge, e.g., by growing a SiGe or Ge δ layers.[10] However, this approach has the disadvantage that the effective lattice volume required for the accumulation of He interstitial atoms is reduced. A more genuine approach is the use of a Si:C layer embedded in the Si substrate. Recently, the effects of *interstitial* C on the helium-induced cavities in carbon im-
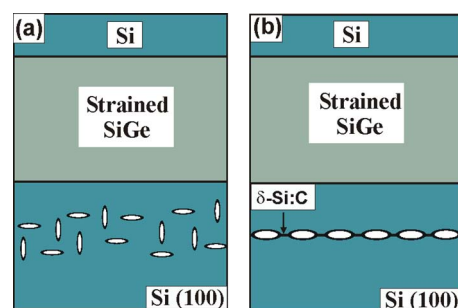

FIG. 1. (Color online) Schematic of the He cavity distribution forming in the Si substrate without (a) and with (b) an epitaxial δ-Si:C layer. The presence of the δ-Si:C layer changes the broad depth distribution of the He platelets (a) to a localized, uniform, and aligned one (b).

a)Electronic mail: d.m.buca@fz-juelich.de.

planted silicon during high-temperature annealing have been described.[11] D'Angelo *et al.*[10] have discussed the role of *substitutional* C on cavity formation at high irradiation conditions. The authors interpret the enhancement of cavity nucleation in relatively thick layers (20 nm) as a consequence of the strain induced by the C incorporation in the Si lattice.[12] However, applications require a detailed experimental and theoretical analysis of the effect of enhanced cavity nucleation along embedded SiGe (Ge) or Si:C layers on the relaxation process of SiGe layers, not available up to date.

Here, we report on the use of a buried ultrathin Si:C layer (δ-Si:C) on the Si(100) substrate to improve the relaxation of epitaxial strained Si_xGe_{1-x} structures. Our goals are to optimize the process parameters with respect to the strain relaxation of SiGe layers and the quality of the heterostructures, and to propose a mechanism of localized He cavity formation in the buried δ-Si:C layer.

180 nm thick strained $Si_{0.77}Ge_{0.23}$ layers were grown on 200 mm *p*-type wafers of pure Si (001) and on wafers containing a single epitaxially grown δ-Si:C (then buried) layer. The δ-Si:C layer had a targeted substitutional carbon concentration of about 1 at. % and a layer thickness of 2 nm. Pure Si spacers of thicknesses h_{SiC}=100, 150, and 200 nm were deposited before the growth of the $Si_{0.77}Ge_{0.23}$ layer. All structures were grown by chemical vapor deposition in an ASM Epsilon® production tool. The SiGe layers were capped with 6 nm Si layers which become tensely strained by plastic strain transfer during the relaxation of the SiGe layers as demonstrated in Ref. 5. A tensile stress of about 1 GPa was obtained in the top Si layer for a degree of relaxation of 70% of the SiGe layer. The heterostructures were implanted at room temperature with He+ ions to doses between 7×10^{15} cm^{-2} and 2×10^{16} cm^{-2} using energies such that the projected range R_p is located above, below and at the δ-Si:C layer position. For easier data presentation, we use the mean ion distribution depth h_p counted from the SiGe/Si interface, $h_p=R_p-(h_{SiGe}+h_{Si})$, where h_{SiGe} and h_{Si} are the SiGe and Si cap layer thicknesses, respectively. After implantation, samples were annealed in a rapid thermal annealing system at a temperature of 850 °C for 600 s in inert atmosphere. Reference wafers without the additional δ-Si:C layer were processed at the same conditions. The degree of relaxation of the SiGe layers (R_{SiGe}) was measured by Raman spectroscopy using a 415 nm wavelength and low laser power density.

The relaxation degrees of the $Si_{0.77}Ge_{0.23}$ layers with and without the δ-Si:C layers grown at h_{SiC}=100, 150, and 200 nm below the SiGe interface, are shown in Fig. 2 as a function of the He-implantation dose, for the case of $h_{SiC}=h_p$. For all the implanted samples, the δ-Si:C layer induces an average increase of about 20% of the SiGe relaxation degree with respect to the reference wafers. We attribute this relaxation increase to an enhanced cavity nucleation in the δ-Si:C layer due to an increase in the volume available for He atoms on the six octahedral interstitial sites nearest to each substitutional C atom (note that, with an atomic volume of 5.68 Å^3, C atoms are small compared to Si matrix atoms having an atomic volume of 20 Å^3).

It is useful here to discuss the proper choice of the intrinsic parameters of the δ-Si:C layer, the C concentration, x, and the layer thickness $d_{Si:C}$, assuming that, for the low implantation doses used in the present experiments, the major
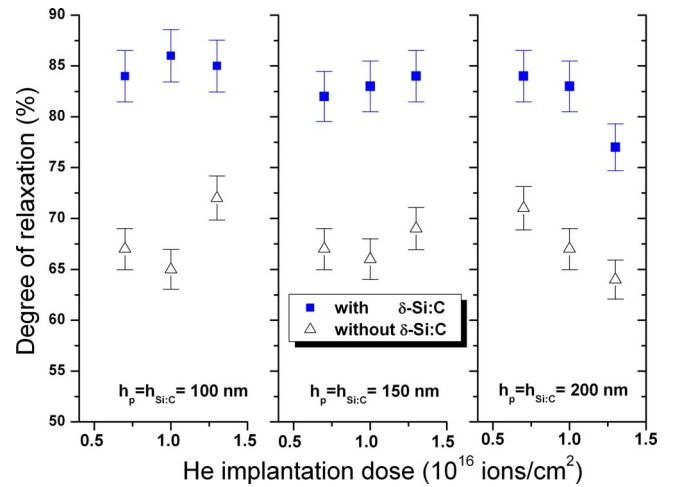

FIG. 2. (Color online) Comparison of relaxation degrees of 180 nm $Si_{0.77}Ge_{0.23}$ layers obtained by He implantation and annealing in the presence (squares) and absence (triangles) of Si:C layers for different layer positions h_{SiC} and implantation depth $h_p=h_{SiC}$ (optimum case) as a function of He+ implantation dose.

part of substitutional C atoms is conserved in the layer after the He+ ion implantation. Localization of cavity nucleation may be considered to become optimal when, before nucleation occurs, a diffusing He interstitial atom penetrating the layer from outside has a significant probability for getting trapped close to a C atom even in the middle of the δ-Si:C layer. This qualitative condition may be quantified by requiring that the mean He diffusion length in the δ-layer is about half of the layer thickness $l_{diff} \approx d_{Si:C}/2$. In a continuum diffusion approach, the mean diffusion length in a medium containing sinks is given by $l_{diff}=1/k$ where k^2 is the strength of the sinks.[13] Approximating the octahedron formed by the 8 interstitial sites around each C atom by a spherical sink of trapping radius $r_{tr}=a/2$ where a is the lattice constant, and using $k^2=4\pi r_{tr}N_{tr}$, where $N_{tr}=N_C=8x/a^3$ is the number density of traps (C atoms), we may write

$$D = d_{SiC}/2l_{diff} \approx 2\sqrt{\pi x}d_{SiC}/a \approx 1. \tag{1}$$

For $D<1$, the Si:C layer is not efficient for He cavity localization while for $D>1$, separate cavity layers must be expected to form at each side of the Si:C layer. The latter situation is confirmed by the cross-section transmission electron microscopy (XTEM) image of a sample with a δ-Si:C layer 200 nm below the SiGe/Si(100) interface, presented in Fig. 3. In the figure inset, locally double cavity layers formed at the δ-Si:C layer position are exemplified. This result indicates that our samples do not fully satisfy the condition for ideal localization of cavity nucleation defined by Eq. (1)
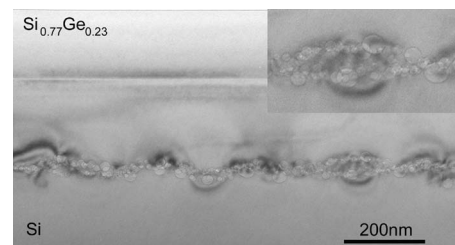

FIG. 3. XTEM image of a 180 nm $Si_{0.77}Ge_{0.23}$ layer relaxed by a 40 keV implantation of 1.3×10^{16} He+ ions/cm^2. The inset shows a magnification of a double cavity layer formed adjacent to the δ-Si:C layer.
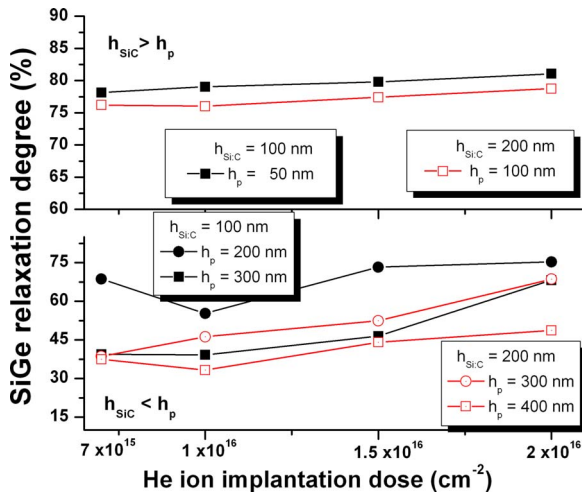
FIG. 4. (Color online) Relaxation degree of $Si_{0.77}Ge_{0.23}$ layers as a function of implantation dose for the nonoptimum conditions: $h_{SiC} \neq h_p$: (a) $h_{SiC} > h_p$ and (b) $h_{SiC} < h_p$. Full and empty symbols correspond to $h_{SiC} = 100$ and 200 nm for various h_p depths, respectively.

which would also fit to the value of $D \approx 1.85 > 1$ obtained using in Eq. (1) $d_{Si:C} = 2$ nm and the targeted value for x.

Trapping of diffusing He interstitial atoms in the δ-Si:C layer is associated with a reduction of the He concentration in regions adjacent to the layer. This results in a reduction of cavity nucleation and dissolution of initially formed cavity embryos in the surroundings of the layer which manifests itself in depleted zones (DZs) at both sides of the layer.[8] The temporal evolution of the width w of these zones depends on the implanted He concentration, c_{He}^{impl}, and the annealing temperature T as[8]

$$wdw/dt \sim D_{He}(T)c_{He}^{int}(T)/c_{He}^{imp}, \qquad (2)$$

where $D_{He}(T)$ is the diffusivity and $c_{He}^{int}(T)$ is the concentration of interstitial He in Si (He in solution). According to Eq. (2), the final width of the DZ can be controlled, via $c_{He}^{int}(T)$, by the He-implantation dose and, via $D_{He}(T)$ and $c_{He}^{int}(T)$, by the annealing temperature. In the ideal case, the total width of the two DZs at both sides of the δ-Si:C layer (plus the δ-Si:C layer width) equals the He distribution profile.

Results for the relaxation degree of SiGe layers obtained for He implantation at depths different from the positions of the δ-Si:C layers ($h_{SiC} \neq h_p$) are presented in Fig. 4(a). For $h_{SiC} > h_p$, where most of the He distribution profile is positioned between the SiGe/Si interface and δ-Si:C layer, the relaxation degree of the SiGe layers is only somewhat lower but less sensitive to the increase in implantation dose than under optimal conditions. In the present case, the interface also acts as a He-getting site in addition to the δ-Si:C layer. We have previously reported[14] that, despite of a high relaxation degree of the SiGe layer, cavities at the interface act as obstacles against the propagation of TDs, thus leading to a dose independence of the relaxation process but also to a strong decrease of the crystalline quality of the relaxed SiGe layer.

For $h_p > h_{SiC}$, the effect of the δ-Si:C layer becomes significant if the implanted He volume density is sufficiently large at the δ-Si:C layer position. Calculations using the SRIM simulation code[15] for the doses applied in this work

yield for $h_{SiC} = 100$ nm and $h_p = 200$ nm densities of 1 to 2×10^{20} He/cm^3 at the δ-Si:C layer position, which are known to be sufficient for He cavity nucleation at interfaces.[14,16] For $h_{SiC} = 100$ nm and deeper implantation $h_p = 300$ nm, only the high dose implantation of 2×10^{16} cm^{-2} fulfills this condition; the low doses result in He densities below 3×10^{19} cm^{-3}. These estimates explain the lower degree of relaxation of the SiGe layer for the case of lower dose and deep implantation, as shown in Fig. 4(b). In addition, for a deeper δ-Si:C layer position, the reduction of the elastic image force pulling the dislocation loops formed at the δ-Si:C layer toward the sample surface decreases the SiGe relaxation degree to similar values obtained in the absence of the δ-Si:C layer.

In summary, we have shown that the relaxation degree of SiGe layers can be increased by introducing a buried δ-Si:C layer in the Si(100) substrates. This enhancement is attributed to localization, homogenization, and alignment of the He cavities along the layer plane improving the dislocation dynamics responsible for strain relaxation. The preferential nucleation of He cavities along a δ-Si:C layer is modeled in terms of the diffusion of He interstitial atoms to the layer and their trapping and agglomeration there. Under optimal implantation conditions, a buried δ-Si:C layer leads to an increase in the relaxation degree of a He-implanted 180 nm $Si_{0.77}Ge_{0.23}$ layer by about 20%, inducing an elastic stress transfer to the top Si epilayer of $\sigma_{si} = 1.35$ GPa.

[1] Y. J. Mii, H. Y. Xie, E. A. Fitzgerald, D. Monroe, F. A. Thiel, B. E. Weir, and L. C. Feldman, Appl. Phys. Lett. **59**, 1611 (1991).

[2] E. Fitzgerald, Y.-H. Xie, M. Green, D. Brasen, A. Kortan, J. Michel, Y.-J. Mii, and B. Weir, Appl. Phys. Lett. **59**, 811 (1991).

[3] C. Mazure and A.-J. Auberton-Hervé, *Proceedings of the 31st European Solid-State Circuits Conference (ESSCIRC 2005)*, Grenoble, France (IEEE, Piscataway, NJ, 2005), p. 29.

[4] M. Reiche, C. Himcinschi, U. Gösele, S. Christiansen, S. Mantl, D. Buca, Q. T. Zhao, S. Feste, R. Loo, D. Nguyen, W. Buchholtz, A. Wei, M. Horstmann, D. Feijoo, and P. Storck, ECS Trans. **6**, 339 (2007).

[5] D. Buca, S. F. Feste, B. Holländer, S. Mantl, R. Loo, M. Caymax, R. Carius, and H. Schaefer, Solid-State Electron. **50**, 32 (2006).

[6] D. Buca, B. Holländer, S. Feste, St. Lenk, H. Trinkaus, S. Mantl, R. Loo, and M. Caymax, Appl. Phys. Lett. **90**, 032108 (2007).

[7] H. Trinkaus, B. Holländer, S. Rongen, S. Mantl, H.-J. Herzog, J. Kuchenbecker, and T. Hackbarth, Appl. Phys. Lett. **76**, 3552 (2000).

[8] J. Chen, P. Jung, and H. Trinkaus, Phys. Rev. B **61**, 12923 (2000).

[9] N. Hueging, M. Luysberg, H. Trinkaus, K. Tillmann, and K. Urban, J. Mater. Sci. **41**, 4454 (2006).

[10] D. D'Angelo, S. Mirabella, E. Bruno, A. Terrasi, C. Bongiorno, F. Giannazzo, V. Raineri, G. Bisognin, and M. Berti, J. Appl. Phys. **103**, 016104 (2008).

[11] V. M. Vishnyakov, S. E. Donnelly, and G. Carter, J. Appl. Phys. **94**, 238 (2003).

[12] D. D'Angelo, S. Mirabella, E. Bruno, G. Pulvirenti, A. Terrasi, G. Bisognin, M. Berti, C. Bongiorno, and V. Raineri, J. Appl. Phys. **104**, 023501 (2008).

[13] A. D. Brailsford and R. Bullough, Philos. Trans. R. Soc. London, Ser. A **302**, 87 (1981).

[14] D. Buca, M. J. Mörschbächer, B. Holländer, M. Luysberg, R. Loo, M. Caymax, and S. Mantl, Mater. Res. Soc. Symp. Proc. **809**, 15 (2004).

[15] J. F. Ziegler, J. P. Biersack, and U. Littmark, *The Stopping Range of Ions in Solids (SRIM—The Stopping and Range of Ions in Matter)* (Pergamon, New York, 1985), http://www.srim.org/.

[16] V. Raineri, P. Fallica, G. Percolla, A. Battaglia, M. Barbagallo, and S. Campisano, J. Appl. Phys. **78**, 3727 (1995).