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Analysis of tensile strain enhancement in Ge nano-belts on an insulator surrounded by dielectrics*

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Ge nano-belts with large tensile strain are considered as one of the promising materials for high carrier mobility metal–oxide–semiconductor transistors and efficient photonic devices. In this paper, we design the Ge nano-belts on an insulator surrounded by Si_3N_4 or SiO_2 for improving their tensile strain and simulate the strain profiles by using the finite difference time domain (FDTD) method. The width and thickness parameters of Ge nano-belts on an insulator, which have great effects on the strain profile, are optimized. A large uniaxial tensile strain of 1.16% in 50-nm width and 12-nm thickness Ge nano-belts with the sidewalls protected by Si_3N_4 is achieved after thermal treatments, which would significantly tailor the band gap structures of Ge-nanobelts to realize the high performance devices.

Keywords: Ge nano-belts, FDTD, Si_3N_4 or SiO_2, uniaxially strain

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1. Introduction

Over the past decade, germanium has been demonstrated to be a very promising candidate in nanoscale electronic and photonic device applications due to its high carrier mobility, quasi-direct band gap nature, and its excellent compatibility with current Si technology.[1] Nanoscale Ge structures on insulators with low dimensionality such as quantum wells, nanowires, and nanocrystals have attracted much attention for their possible applications in scaling metal–oxide–semiconductor field effect transistors and photonic devices.[2–6] Moreover, the introduction of uniaxial strain can further increase the carrier mobility through strain-induced band splitting that reduces intervalley scattering events and further lowers the carrier effective mass. On the other hand, proper tensile strain can potentially transform Ge into a direct bandgap semiconductor with a quicker shrinkage of the direct bandgap in relation to the indirect bandgap.[7] Thus it can be seen that strain is a powerful parameter to control the physical properties in semiconductors. It paves a possible way for realizing an Si-based light source with Ge under large tensile strain.[8–11]

So far, several methods have been proposed to reach tensile strain in Ge thin films for the purpose of attaining strong direct band luminescence. The first method is to epitaxially grow Ge on Si substrate, which is able to obtain a maximum of 0.25% tensile strain in Ge due to thermal expansion coefficient mismatch between Ge and Si.[12–14] Recently, more than 2% tensile strain was demonstrated in Ge grown on lattice-relaxed InGaAs/GaAs buffer layers by molecular beam epitaxy[15] and a thin Ge layer on a polyimide film using high-pressure gas.[16] The second method is to use the micromechanical technique and tensile strain as large as 1.13% in a 1.6-μm thick Ge membrane is achieved with a tungsten stressor.[17] The third method is to fabricate GOI materials by layer transfer techniques or the Ge condensation method, but only 0.19% maximum tensile strains is presented.[18–20] The big challenge is that the tensile strain values introduced in Ge are too small or the techniques are incompatible with Si technology.

In this work, we investigate uniaxial tensile strained Ge nano-belts on insulator with various dielectrics (Si_3N_4 or SiO_2) protected on the sidewall by finite difference time domain (FDTD) simulations. The different dielectrics are introduced to compare the uniaxial tensile strain in Ge nano-belts. The effects of width and thickness of the Ge nano-belts on tensile strain are discussed and optimized.

2. Analysis model of Ge nano-belts with sidewalls protected by SiO_2 or Si_3N_4

We have reported on a CMOS-compatible approach to introduce a biaxial tensile strain as large as 0.67% on a 32-μm diameter circular ultra-thin (12 nm) germanium-on-insulator (GOI) by selective oxidation of patterned SiGe with sidewalls protected by SiO_2.[21] This large tensile strain leads to the significant enhancement of direct band photoluminescence from

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the circular Ge layer and the peak position shifting toward longer wavelengths. In this work, we propose and design the Ge nano-belts on an insulator with sidewalls protected by various dielectrics, which may lead to much larger tensile strain. The tensile strain profile in the Ge nano-belts will be analyzed by FDTD simulation.

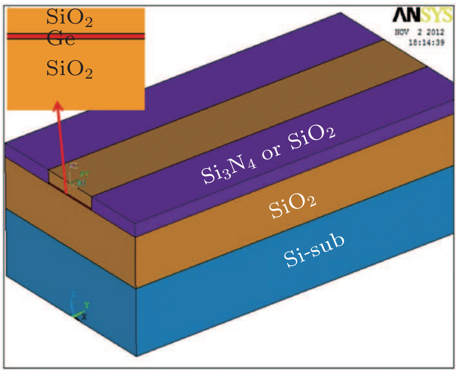

Fig. 1. (color online) Three-dimensional finite element model of one periodic pattern Ge nano-belt. The grating structure is composed of 500-nm wide stripes and 500-nm spacing, and the length of the periodic pattern is 3 μm. The thickness values of the Si substrate, BOX, Ge layer and top SiO_2 are 500 nm, 380 nm, 12 nm, and 90 nm, respectively. And the thickness of sidewalls protected by Si_3N_4 or SiO_2 is 102 nm.

Table 1. ANSYS material parameter configuration.

Materials	Young's moduli/Gpa	Poisson's ratios	Thermal expansion coefficient/10^{-6} °C^{-1}
Si	162.9	0.28	2.6
SiO_2	73.1	0.17	0.5
Ge	103	0.28	8.51
Si_3N_4	304	0.24	3.3

The strain distribution in GOI nano-belts is simulated by a finite element-modeling program (ANSYS software). A three-dimensional finite element model of one periodic pattern is created in ANSYS as shown in Fig. 1. In this model, the grating structure is composed of 500-nm wide stripes (Ge) and 500-nm spacing (SiO_2 or Si_3N_4) with a 3-μm length of the periodic pattern. The thickness values of the Si substrate, buried oxide (BOX), Ge layer and top SiO_2 are 500 μm, 380 nm, 12 nm, and 90 nm, respectively. Besides, the thickness of sidewalls protected by Si_3N_4 or SiO_2 is 102 nm. A non-uniform finite element grid is chosen such that the grid size is fine (1 nm) near the Ge layer region and larger (10 nm) at locations far from the Ge layer, to achieve accurate results.[22] The boundary conditions of the silicon substrate, tractions at the free surface and the middle position of the wide stripes are rigid, zero, and zero horizontal displacements, respectively. In order to reduce the computational complexity, the isotropic approximation is used in the calculation of strain in the finite element-modeling. The Young's moduli, thermal expansion coefficients, and Poisson's ratios of the materials are listed in Table 1.[23–26] It should be noted that the equivalent hydrostatic strain will not be considered in the simulations, which strongly depends on the Si_3N_4 deposition parameter, the geometry and the orientation of Ge layer.[27]

3. Results and discussion

The thermal expansion mismatch processes of a three-dimensional finite element model are simulated from 900 °C[20] cooling down to 25 °C. Strain distributions along the x and y directions of the Ge nano-belts with and without various dielectrics (SiO_2 or Si_3N_4) protected on the sidewall are shown in Fig. 2. The strain components ε_{xx} and ε_{yy} in Ge layer of nano-belts without dielectric protected are approximately 0.60% and 0.51% as shown in Figs. 2(a) and 2(b), respectively. When Ge nano-belts are protected by Si_3N_4, the average strain along the x direction of Ge layer increases to 0.88%, but the strain along the y direction is 0.50% as shown in Figs. 2(c) and 2(d). It can be seen that the strain component ε_{xx} increases sharply, while the strain component ε_{yy} remained nearly constant. These ANSYS simulation results suggest that the strain in the Ge nano-belts is uniaxial strain, in addition, the Ge nano-belts with sidewalls protected by Si_3N_4 has a lager strain along the x direction, and the protected material almost merely increases the ε_{xx} strain component.

A large uniaxial tensile strain of 0.88% in the x direction for the Ge nano-belts with Si_3N_4 protected on the sidewalls is obtained compared with that of without dielectrics. Simultaneously, the tensile strain profile in the Ge nano-belts with SiO_2 protected on the sidewalls is simulated, and the strain components ε_{xx} and ε_{yy} in Ge layer are approximately 0.71% and 0.51%, respectively. It suggests that the choice of strain dielectrics (SiO_2 or Si_3N_4) to protect sidewalls of GOI is important. In order to obtain the biggest possible strain, we vary the width of Ge nano-belts, with other parameters kept constant. The average strain in the x direction in Ge nano-belts, which is dependent on width changing from 20 nm to 980 nm, is shown in Fig. 3(a). It is observed that the strain in the x direction in Ge layers with the sidewalls protected by Si_3N_4 increases drastically with the decrease of Ge width. When Ge width decreases nearly to 50 nm, the strain reaches a maximum value of approximately 1.16%. Nevertheless, the strain in the x direction increases gradually with the increase of Ge width for the Ge nano-belts with sidewalls protected by SiO_2 or nothing. The strain value in Ge nano-belts with the sidewalls protected by Si_3N_4 is much larger than that protected by SiO_2 or nothing for the same width less than 980 nm, the strain of Ge nano-belts with the sidewalls protected by SiO_2 decreases with width increasing, which is similar to that without dielectric surrounded. The average strain in the y direction in Ge layer with the width change from 20 nm to 980 nm is shown in Fig. 3(b). The strain value merely ranges from 0.48% to 0.53%. The variation tendency of strain curve in the x direction is exactly contrary to that in the y direction.

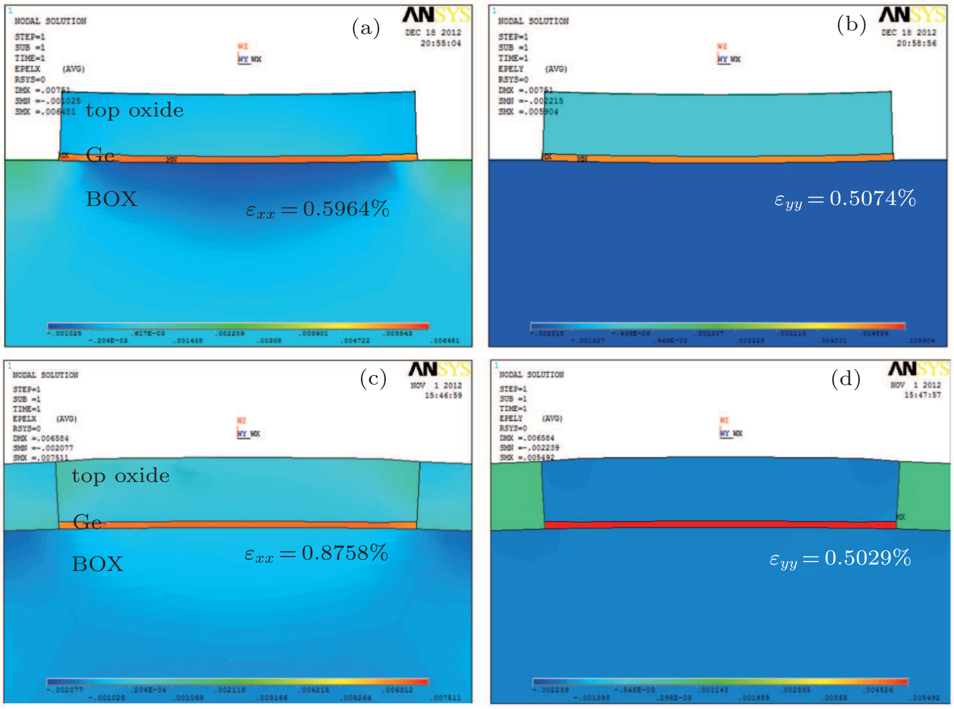

Fig. 2. (color online) Profiles of the strain in the *x* direction and the *y* direction of the Ge nano-belts without and with Si_3N_4 protected on the sidewalls. The bottom scale corresponds to the amplitude of strain component. Tensile strain is positive, and compressive strain is negative. (a) The average strain along the *x* direction of Ge layer without the sidewalls protected is 0.60%, and (b) the strain along the *y* direction is 0.51%. (c) The average strain along the *x* direction of Ge layer with the sidewalls protected by Si_3N_4 is 0.88%, but (d) the strain along the *y* direction is 0.50%.

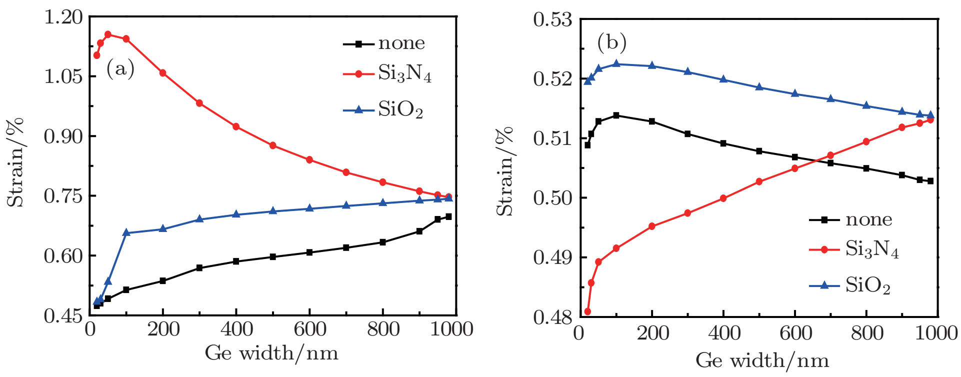

Fig. 3. (color online) (a) Strains in the *x* direction of Ge layer versus Ge width. The red curve (with solid circles), blue curve (with solid angles), and black curve (with solid squares) show the strains in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively. When Ge width decreases nearly to 50 nm, the strain reaches a maximum value of approximately 1.16%. (b) Strains in the *y* direction of Ge layer versus Ge width. The red curve (with solid circles), blue curve (with solid angles), and black curve (with solid angles) show the strain in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively. The strain values are just in a range from 0.48% to 0.53%.

From the simulation results stated above, the strain in Ge nano-belts without a surrounding dielectric is approximately 0.45%∼0.69%, which is far greater than that without defining patterns (0.30%),[21] and the strain in the *x* direction for the Ge nano-belts with sidewalls protected by SiO_2 is slightly larger than that without protection. It can be seen that Ge nano-belt structure has big effect on the improvement of strain in Ge layer, which plays a leading role in increasing the strain in the *x* direction. The average strain of the *x* direction in Ge nano-belts, depending on the thickness of top SiO_2 and BOX layers, is shown in Fig. 4. It can be observed that the strain in the *x* direction in Ge layer with the sidewalls protected by Si_3N_4 or SiO_2 increases with the thickness of top SiO_2 or BOX layer changing from 12 nm to 100 nm. When the thickness of top SiO_2 or BOX layer is more than 100 nm, the average strain in the *x* direction in Ge nano-belts almost remains unchanged. In addition, the strain value in Ge nano-belts with the sidewalls protected by Si_3N_4 or SiO_2 is much larger than that without any protection under the condition of the same thickness. Therefore, it can be inferred that the top SiO_2 and BOX layers of a Ge nano-belt structure interact with the sidewalls of Si_3N_4 or SiO_2, bringing about large tensile strain in the Ge layer.

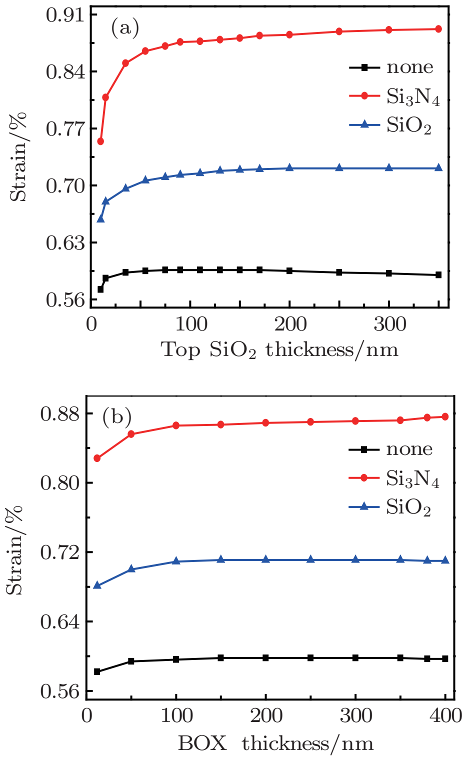

Fig. 4. (color online) (a) Strains in the x direction of the Ge layer versus top SiO_2 thickness. The red curve (with solid circles), blue curve (with solid angles), and black curve (with solid squares) show the strains in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively. (b) Strains in the x direction of Ge layer BOX layer thickness. The red curve (with solid circles), blue curve (with solid angles), and black curve (with solid squares) show the strain in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively.

During the annealing process from 900 °C to 25 °C, the Ge layer trends to expand laterally and interacts with the viscous buried SiO_2 and the Si_3N_4 or SiO_2 sidewalls. When the samples are cooled down to room temperature, the shrinkage of Ge is much larger than SiO_2 and Si_3N_4, due to the thermal expansion coefficient of Ge (8.51×10^{-6} °C^{-1}) larger than those of SiO_2 (5.0×10^{-7} °C^{-1}) and Si_3N_4 (3.3×10^{-6} °C^{-1}), giving rise to large tensile strain in the Ge layer. To analyze the mechanism of uniaxial strain by protecting dielectrics, we use a schematic model for strain analysis from a perspective analogy to lattice mismatch as shown in Fig. 5. Because the strain in the x direction is close to that in the y direction of Ge nano-belts without sidewall being protected as shown in Figs. 2(a) and 2(b), and the strain value in the y direction merely ranges from 0.48% to 0.53%, it can be inferred that the strains in the x and y directions are mainly affected by the top oxide and the BOX, which leads to the uniform distribution of strains in the y direction. The top SiO_2 and BOX layers of Ge nano-belt structure have a significant influence on the improvement of strain in Ge layer, which plays a leading role in increasing the strain in the x direction. Thus the strain in the x direction increases gradually with the increase of Ge width for the Ge nano-belts with sidewalls protected by SiO_2 or nothing, as shown in Fig. 3(a). When the sidewalls of nano-belts are protected by Si_3N_4 or SiO_2, the lattice in the x direction becomes longer, which leads to a drastic increase of strain in the x direction. Nevertheless, the strain in Ge layer with the sidewall surrounded by Si_3N_4 is much larger than that surrounded by SiO_2, due to the Si_3N_4 sidewalls subjected to the actions from the viscous BOX and top SiO_2 layer, and the blocking of the shrinkage of Ge in the x direction. On the other hand, the Young's moduli of Si_3N_4 (304 Gpa) is much larger than that of SiO_2 (73.1 Gpa), so under a certain stress, the dependent variable of Si_3N_4 is smaller than that of SiO_2, which blocks the shrinkage of Ge in the x direction to a greater degree. Thus the strain in the x direction increases gradually with the decrease of Ge width for the Ge nano-belts with sidewalls protected by Si_3N_4, which is contrary to the variation tendency of sidewalls surrounded by SiO_2. But if Ge width reduces to below 50 nm or so, the decreasing effect of top SiO_2 on Ge layer is stronger than the increasing effect of Si_3N_4, giving rise to a reduction of the total strain in the x direction. For the reasons presented above, it is easy to understand the variation tendencies of strain curves in Fig. 3.

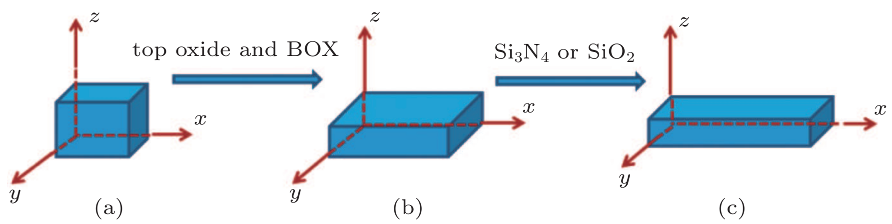

Fig. 5. (color online) Schematic model for strain analysis from a perspective analogous to lattice mismatch. Panel (a) shows the primary lattice, panel (b) the lattice affected by top oxide and BOX, and panel (c) exhibits that the lattice in the x direction becomes longer due to the influence from the sidewalls of Si_3N_4or SiO_2.

We vary the thickness of Ge layers while keeping other parameters constant in order to investigate the effect of Ge thickness on strain. The average strains in the x and y directions in Ge layer with the width changing from 5 nm to 30 nm are shown in Figs. 6(a) and 6(b), respectively. The results indicate that with the increase of Ge thickness, the strain decreases almost linearly, while the slopes of none, SiO_2, and Si_3N_4 in the x direction are 0.00269%/nm, 0.00292%/nm, and

0.00125%/nm, respectively. The strain in the x direction is larger than that in the y direction at the same thickness, which is consistent with the variation tendencies of strain curves in Fig. 3.

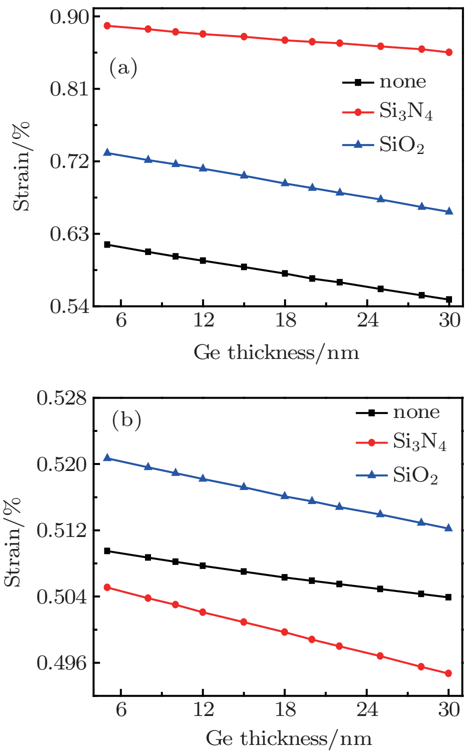

Fig. 6. (color online) (a) Strains in the x direction of Ge layer versus Ge thickness. The red curve (with soled circles), blue curve (with solid angles), and black curve (with solid squares) show the strains in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively. (b) Strains in the y direction of Ge layer versus Ge thickness. The red curve (with soled circles), blue curve (with solid angles), and black curve (with solid squares) show the strains in Ge nano-belts with sidewalls protected by Si_3N_4, SiO_2, and nothing, respectively.

4. Conclusions

In this paper, we investigate the tensile strains of the Ge nano-belts on an insulator with sidewalls protected by various dielectrics (Si_3N_4 or SiO_2) on SOI substrate. When the Ge width decreases to about 50 nm with the sidewalls protected by Si_3N_4, a large uniaxial tensile strain ($\varepsilon_{xx} = 1.16\%$, $\varepsilon_{yy} = 0.49\%$) in Ge layer can be obtained. The strains in the x and y directions are mainly affected by the top oxide and the BOX. The strain in the Ge layer with the sidewall surrounded by Si_3N_4 is much larger than that surrounded by SiO_2, due to the Si_3N_4 sidewalls subjected to the actions from the viscous BOX, top SiO_2 layer, and Young's moduli (304 Gpa), and the blocking of the shrinkage of Ge in the x direction. The strains in the Ge layer decrease linearly with the Ge thickness increasing with the slopes of none, SiO_2, and Si_3N_4 in the x direction being 0.00269%/nm, 0.00292%/nm, and 0.00125%/nm, respectively. The results should be considered for improving the carrier mobility in advanced Ge channel MOSFETs and Si-based Ge light emission efficiency using selective oxidation of SiGe nano-belts to Ge nano-belts with sidewalls protected by Si_3N_4.

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