The effects of nickel germanosilicide contacts on the biaxial compressive stress in thin epitaxial silicon-germanium alloys on silicon

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When a thin $Si_{1-x}Ge_x$ epitaxial layer is grown on Si, it is under biaxial compression. In this letter, it is shown that a nickel germanosilicide ($NiSi_{1-x}Ge_x$) layer formed on $Si_{1-x}Ge_x$ can significantly reduce the in-plane compressive strain in $Si_{1-x}Ge_x$. It is proposed that the observed reduction is due to the biaxial tensile stress applied by the $NiSi_{1-x}Ge_x$ layer. Because the $Si_{1-x}Ge_x$ bandgap is a strong function of the strain, this is expected to have a strong impact on the metal-semiconductor barrier height and the contact resistivity of the interface if the metal Fermi level is pinned near the $Si_{1-x}Ge_x$ midgap. © *2007 American Institute of Physics*. [DOI: 10.1063/1.2795346]

The recessed $Si_{1-x}Ge_x$ junction technology is currently employed in state-of-the-art metal oxide silicon field effect transistors (MOSFETs) to induce uniaxial compressive stress in the Si channel. This effect has been shown to enhance the hole mobility and that the enhancement is preserved at high vertical electric fields.[1] In these MOSFETs, self-aligned $NiSi_{1-x}Ge_x$ is the preferred contact material on $Si_{1-x}Ge_x$ due to its small substrate consumption, low resistivity, and low formation temperature.

Previous work in this laboratory has shown that another key advantage of the $Si_{1-x}Ge_x$ source/drain technology is its potential to reduce the source/drain contact resistivity.[2–4] For the commonly used silicides formed on Si (e.g., $TiSi_2$ and NiSi), the Fermi level is pinned near the Si midgap resulting in a Schottky barrier height approximately equal to half the Si bandgap. It has been shown that this is also true for the $Ni/Si_{1-x}Ge_x$ system.[5] Since the contact resistivity is an exponential function of the metal-semiconductor barrier height, the contact resistivity can be substantially reduced by forming the contact on $Si_{1-x}Ge_x$, whose bandgap is smaller than Si.[2–5] This is significant because the contact resistivity is the primary contributor to the MOSFET series resistance, which must be limited to a small fraction of the channel "on" resistance.[6] Since the contact resistivity advantage of $Si_{1-x}Ge_x$ is based on bandgap reduction, all factors that can potentially influence the $Si_{1-x}Ge_x$ bandgap must be carefully considered.

Strained epitaxy of $Si_{1-x}Ge_x$ on Si leads to in-plane compression and extension normal to the interface. Epitaxial $Si_{1-x}Ge_x$ layers grown in source/drain areas of MOSFETs are expected to be similarly strained. Much work has been done to understand the impact of strain on the $Si_{1-x}Ge_x$ bandgap and a nice summary of this work can be found in a review paper by People.[7] The strain causes splitting of the conduction and valence bands resulting in a smaller $Si_{1-x}Ge_x$ bandgap. For a Ge fraction of 50%, the reduction is more than 0.2 eV, which is significant considering the exponential dependence of the contact resistivity on this parameter.

The impact of the $Si_{1-x}Ge_x$ composition and thickness on the in-plane compressive strain is well understood. Another factor that can influence the strain in the alloy is the type and thickness of the metal contact used. Previous reports on NiSi contacts formed on Si indicate that the NiSi layer is under tension and the Si underneath is under compression.[8–10] In this work, the influence of a $NiSi_{1-x}Ge_x$ contact layer on the in-plane compressive strain in $Si_{1-x}Ge_x$ has been studied and the results are reported in this paper. The study includes the effects of Ge concentration, thickness of the Ni layer (t_{Ni}) used to form the germanosilicide contact, and boron doping in $Si_{1-x}Ge_x$.

Undoped and *in situ* boron doped $Si_{1-x}Ge_x$ epitaxial layers were grown on *n*-type Si wafers of ⟨100⟩ orientation by ultrahigh vacuum rapid thermal chemical vapor deposition.[11] Epitaxial layers with 28% and 48% Ge were grown at 550 and 500 °C, respectively. Nickel deposition was carried out in an ultrahigh vacuum magnetron sputtering system and the $NiSi_{1-x}Ge_x$ layers were formed by rapid thermal annealing in nitrogen ambient at 350 °C for 30 s. The annealing temperature was optimized by monitoring the sheet resistance of the $NiSi_{1-x}Ge_x$ layers using a Magne-tron M-700, four point probe system. Atomic force microscopy and Raman spectroscopy were used to verify that the layers were stable during rapid thermal annealing. A micro-Raman system manufactured by Horiba Jobin Yvon equipped with an Ar+ laser ($\lambda = 514.5$ nm) was used to measure the amount of in-plane strain in the $Si_{1-x}Ge_x$ layers.

Figure 1 shows the typical Raman spectra obtained from the $Si_{0.52}Ge_{0.48}$ layers between the germanosilicide contact and the Si substrate. The contact layers were formed using different thicknesses of Ni ranging from 0 to 20 nm. The two major peaks around 400 and 500 cm^{-1} correspond to Si–Ge and Si–Si bonds in $Si_{1-x}Ge_x$, respectively. We note that the intensities of both peaks are much reduced when t_{Ni} is increased. In fact, when $t_{Ni} \approx 20$ nm, we can no longer detect any peaks from the $Si_{1-x}Ge_x$ layer. This is not surprising considering the exponential drop in the intensity of the laser beam as it travels through the $NiSi_{1-x}Ge_x$ layer. At $\lambda = 514.5$ nm, the absorption coefficient of NiSi is 0.12 nm^{-1}.[12]

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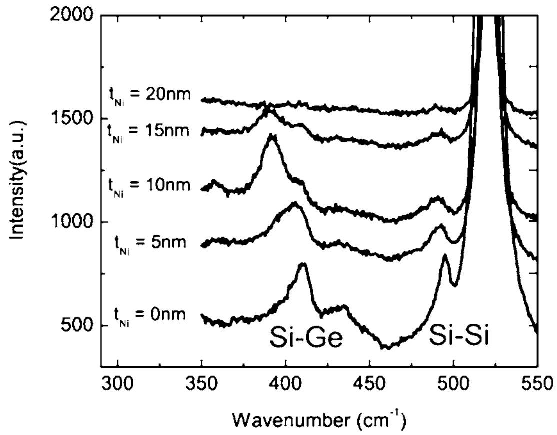

FIG. 1. Raman spectra obtained after forming $NiSi_{1-x}Ge_x$ on 50 nm thick $Si_{0.52}Ge_{0.48}$ using three different Ni thicknesses.

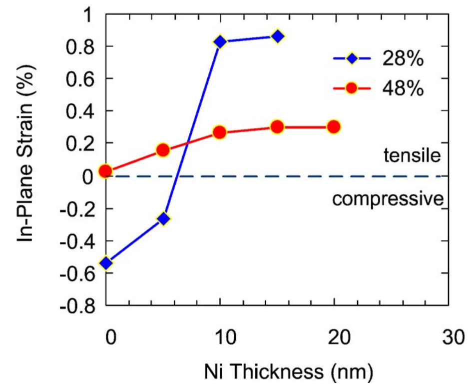

FIG. 3. (Color online) In-plane strain in $Si_{1-x}Ge_x$ alloys with two different Ge concentrations plotted as a function of the Ni thickness used to form the $NiSi_{1-x}Ge_x$ layers. The $Si_{1-x}Ge_x$ layers were fully or mostly relaxed prior to $NiSi_{1-x}Ge_x$ formation.

Assuming that the absorption coefficient of $NiSi_{1-x}Ge_x$ is close to this value, we estimate the laser intensity entering the $Si_{1-x}Ge_x$ to be less than 1% of the incident value on the germanosilicide layer. It can be observed that both peaks shift to the left with increasing Ni thickness, indicative of decreasing compression in $Si_{1-x}Ge_x$.

The in-plane strain in the epitaxial layers was determined from the shifts of the Si–Si peaks using the phenomenological model reported by Dietrich *et al.*[13] and Bhagavannarayana *et al.*[14] In this model, the location of the Si–Si peak ω_{Si} is first calculated for the relaxed, alloylike $Si_{1-x}Ge_x$ and the position of this peak can be approximated by

$$\omega_{Si}(x) \simeq \omega_0 - 0.70x \text{ cm}^{-1}, \tag{1}$$

where ω_0=520 cm^{-1} and x is the Ge fraction in the alloy. The in-plane strain $\varepsilon(x)$ in the pseudomorphic layer is then calculated from the measured shift $\Delta\omega(x)$ of the Si–Si peak from its position in the above equation using

$$\varepsilon(x) = \frac{-\Delta\omega(x)}{\omega_0\left[K_{12}(x) - K_{11}(x)\frac{c_{12}(x)}{c_{11}(x)}\right]}, \tag{2}$$

where the constants K_{ij} and c_{ij} can be estimated from the constants of pure Si and Ge assuming linear dependence on the Ge fraction x.[14]

Figure 2 shows the in-plane strain in $Si_{1-x}Ge_x$ as a function of Ni thickness for the two different germanium concentrations of 28% and 48% used in this study. The $Si_{1-x}Ge_x$ thickness prior to $NiSi_{1-x}Ge_x$ formation was approximately 50 nm for both concentrations. This thickness was chosen to ensure that the $Si_{1-x}Ge_x$ layers were at least partially strained but thick enough to avoid full consumption during $NiSi_{1-x}Ge_x$ formation. Without the germanosilicide contact, the strain measured in the sample with 28% Ge is very close to the value that we would expect to find in a fully strained, pseudomorphic $Si_{0.72}Ge_{0.28}$ layer. On the other hand, the $Si_{0.52}Ge_{0.48}$ layer is partially relaxed. The expected strain for a fully strained film with 48% Ge is about 2%. Nevertheless it can be seen that for both Ge concentrations, the strain in $Si_{1-x}Ge_x$ gradually decreases as the Ni (and hence, the germanosilicide thickness) is increased. This effect can be interpreted in two different ways:

(1) $NiSi_{1-x}Ge_x$ results in additional compressive stress in $Si_{1-x}Ge_x$. This increases the effective strain energy above the critical amount, which leads to strain relaxation and hence, an effective reduction in the measured strain.
(2) $NiSi_{1-x}Ge_x$ results in tensile stress in $Si_{1-x}Ge_x$, which subtracts from the compressive stress originating from the Si substrate.

In order to better understand the role of $NiSi_{1-x}Ge_x$, the above experiment was repeated using mostly relaxed $Si_{1-x}Ge_x$ layers by using the same growth conditions to grow thicker (~150 nm) layers. Figure 3 summarizes the measurement results. It can be seen that the $Si_{0.52}Ge_{0.48}$ layer is fully relaxed without the germanosilicide contact. Interestingly, the measurements suggest that increasing the Ni thickness leads to in-plane tension in this layer. The $Si_{0.72}Ge_{0.28}$ layer is still under compression but it is mostly relaxed prior to the germanosilicide formation. With 5 nm Ni, the in-plane compressive strain is reduced similar to the behavior observed in Fig. 2. With 10 and 15 nm Ni, the underlying $Si_{1-x}Ge_x$ layers are in tension in agreement with our observations for the $Si_{0.52}Ge_{0.48}$ layer. These findings indicate that $NiSi_{1-x}Ge_x$ induces in-plane tensile strain in $Si_{1-x}Ge_x$ and the amount increases with the Ni thickness. Therefore, it is concluded that the reduction of the biaxial compression in $Si_{1-x}Ge_x$ alloys is due to two opposing stress components as opposed to strain relaxation.

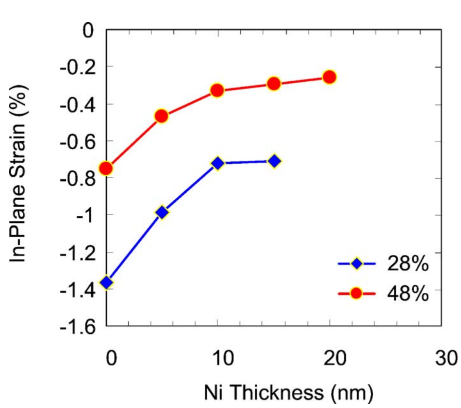

FIG. 2. (Color online) In-plane strain in $Si_{1-x}Ge_x$ alloys with two different Ge concentrations plotted as a function of the Ni thickness used to form the $NiSi_{1-x}Ge_x$ layers. The $Si_{1-x}Ge_x$ layers were strained prior to $NiSi_{1-x}Ge_x$ formation. Negative values indicate compression.

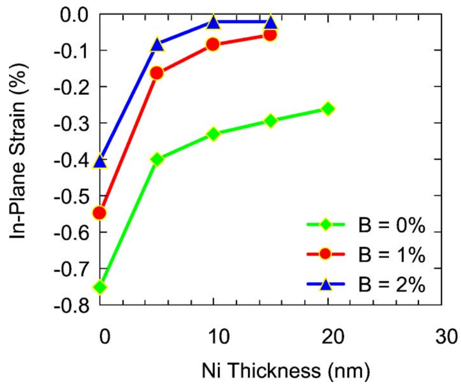

FIG. 4. (Color online) In-plane strain in $Si_{0.5}Ge_{0.5}$ alloys with three different boron concentrations plotted as a function of the Ni thickness used to form the germanosilicide layers.

Since the linear expansion coefficients of NiSi and NiGe are close to each other, thermal expansion cannot explain the different types of in-plane strain obtained with NiSi and $NiSi_{1-x}Ge_x$. One possible explanation is epitaxial stress due to the difference in the lattice parameters. It has been shown in the literature that $NiSi_{1-x}Ge_x$ has an orthorhombic structure, with one of the lattice parameters greater than that of the corresponding $Si_{1-x}Ge_x$ lattice.[15] $NiSi_{1-x}Ge_x$ films formed on $Si_{1-x}Ge_x$ have also been shown to be strongly textured along the ⟨010⟩ axis, as opposed to NiSi, which orients randomly on Si. This texturing suggests a strong epitaxial relationship between its ⟨010⟩ plane and the ⟨001⟩ plane of $Si_{1-x}Ge_x$ and can be the source of the tensile stress component. An interesting observation that can be made from Fig. 3 is that the final in-plane strain is larger when the Ge concentration is lower, which supports this view.

Figure 4 shows the in-plane strain in $Si_{0.5}Ge_{0.5}$ as a function of the nickel thickness for different boron concentrations. It can be seen that boron introduces yet another mechanism for reducing the in-plane compressive strain in $Si_{1-x}Ge_x$. This effect referred to as "boron strain compensation" can be found in previous reports from this laboratory.[11,16] It is important to note that the $Si_{1-x}Ge_x$ layer may lose most of its original strain due to the combined effects of $NiSi_{1-x}Ge_x$ and boron strain compensation.

In summary, the experimental results from this work indicate that $NiSi_{1-x}Ge_x$ contacts formed on strained $Si_{1-x}Ge_x$ layers tend to reduce the in-plane compressive strain in the alloy by introducing a tensile stress component. This finding suggests that upon formation of the germanosilicide, the $Si_{1-x}Ge_x$ epitaxial layer no longer satisfies the pseudomorphic condition. The effect is enhanced with boron strain compensation and it is expected to have a strong impact on the band structure of the $Si_{1-x}Ge_x$ layer. Most importantly, if the metal Fermi level is pinned near the $Si_{1-x}Ge_x$ midgap, the effect can lead to a larger metal-semiconductor barrier height potentially eliminating the contact resistivity advantage of $Si_{1-x}Ge_x$ in field-effect transistors. This requires optimization of all parameters that influence the strain distribution in $Si_{1-x}Ge_x$ including the alloy composition and thickness.

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