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# Interaction of Pd with Strained Layers of $Si_{1-x}Ge_x$ Epitaxially Grown on Si(100)

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The interaction of thin Pd films deposited on strained layers of $Si_{1-x}Ge_x$ epitaxially grown on Si(100) was studied. A highly textured, ternary compound ($Pd_2Si_{1-y}Ge_y$) formed concurrently with the PdGe phase, at annealing temperatures between 200 and 550°C. Above 550°C, a region of high Ge concentration formed between the fully reacted compound region and the unreacted $Si_{1-x}Ge_x$ layer. Current-voltage investigations showed that Pd on $Si_{1-x}Ge_x$ samples have a lower Schottky barrier height than Pd on pure Si.

As the techniques for epitaxial growth of coherently strained $Si_{1-x}Ge_x/Si$ heterostructures become more advanced, the metallization of these layers for device applications becomes increasingly relevant. While the interactions between thin films of Pd and single crystalline Si or Ge have been well documented in the literature, the interaction of Pd with single crystalline $Si_{1-x}Ge_x$ films remains unreported. In the Pd-Si system[1], the only low temperature (below 650°C) thin film phase is the hexagonal $Pd_2Si$, and above this temperature, the orthorhombic PdSi phase forms. In the Pd-Ge system[2] both $Pd_2Ge$ and PdGe are stable at low temperatures. The structures of the germanide phases are isomorphous with the corresponding silicides.

In this work the interaction between Pd thin films and n-type $Si_{1-x}Ge_x$ layers epitaxially grown by MBE on Si(100) was studied as a function of heat treatments in a vacuum furnace in the temperature range of 250 - 550°C. The Ge content in the epilayers, x, was 0.09 and 0.18, and the corresponding thicknesses were 3000 and 2300Å. Strain in the $Si_{1-x}Ge_x$ layers in the as grown state and following the applied heat treatments was measured by Double Crystal X-ray Diffractometry (DCD). The $Si_{1-x}Ge_x$ layers in the as grown state were found to be commensurate with the substrate.

Compound formation was analyzed by X-ray Diffraction and by Energy Dispersive Spectroscopy (EDS) in the Transmission Electron Microscope (TEM). The X-ray diffraction pattern shown in Fig. 1 shows existence of a dominant peak (at $2\theta=53.74°$), identified as arising from the (002) reflection of the hexagonal ternary compound, $Pd_2Si_{1-y}Ge_y$. This peak being high in intensity over the entire temperature range studied, shows that the compound was highly textured. In addition, Fig. 1 shows that a relatively small amount of PdGe formed as well. The first indication that we have a ternary phase (not a mixture of two binaries) is from the observation that we found a single peak of the (002) plane (seen in Fig. 1), rather than a doublet. From this, however, we cannot unambiguously establish that the compound was ternary. To answer that question, we employed EDS analysis in the TEM; an EDS spectrum was collected while electrons were confined to a single grain region. The resulting spectrum was comprised of signals from all three elements, Pd, Si and Ge, arising entirely from atoms in the single grain. Based upon these results, we established that the compound was indeed ternary.

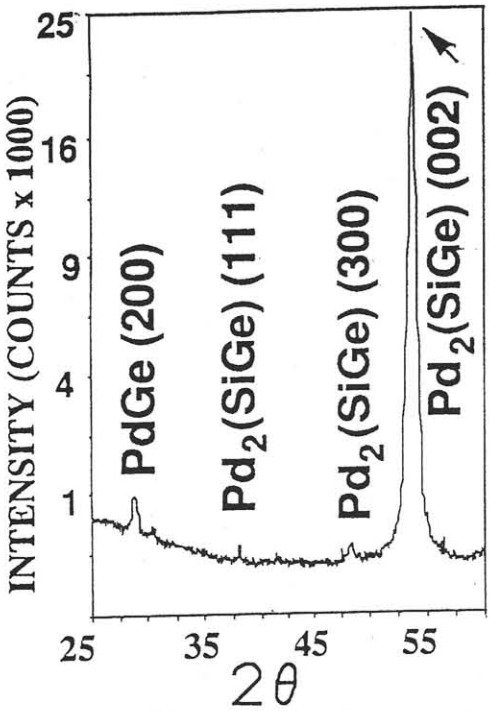


Fig 1. X-ray diffraction spectrum of $Pd/Si_{0.82}Ge_{0.18}$ following annealing at 450°C for 4 hours.

The interaction between Pd and $Si_{1-x}Ge_x$ at low and high temperature heat treatments was followed by the Auger Electron Spectroscopy (AES) depth profiles seen in Fig. 2. Figures 2a, b and c show three depth profiles recorded under the same experimental conditions of (a) an unreacted sample, and samples reacted at 250°C (b) and at 550°C (c) for 4 hours. At the low reaction temperature (250°C) the concentration of Ge in the fully reacted region appears to be slightly lower than its concentration in the unreacted layer. The AES depth profile of the sample reacted at 550°C (Fig. 2c), shows a region of high Ge concentration at the interface between the $Pd_2Si_{1-y}Ge_y$ compound and the unreacted $Si_{1-x}Ge_x$ layer. Again, we note that the signal of Ge from within the compound region was even lower than for the sample reacted at 250°C. Fig. 2 demonstrates that the Ge concentration in the ternary compound decreased as the reaction temperature was increased, while a Ge rich layer formed between the compound and the unreacted $Si_{1-x}Ge_x$.

The formation of the Ge rich layer was accompanied by the creation of defects (seen by TEM by and peak broadening in the DCD measurements), and by relaxation of the strained epitaxial layer. Fig. 3 shows a TEM bright-field image showing planar defects (stacking faults or microtwins) within a ~500Å layer of Ge rich $Si_{1-x}Ge_x$. EDS analysis of this layer showed the Ge atomic concentration in it was approximately 40%.

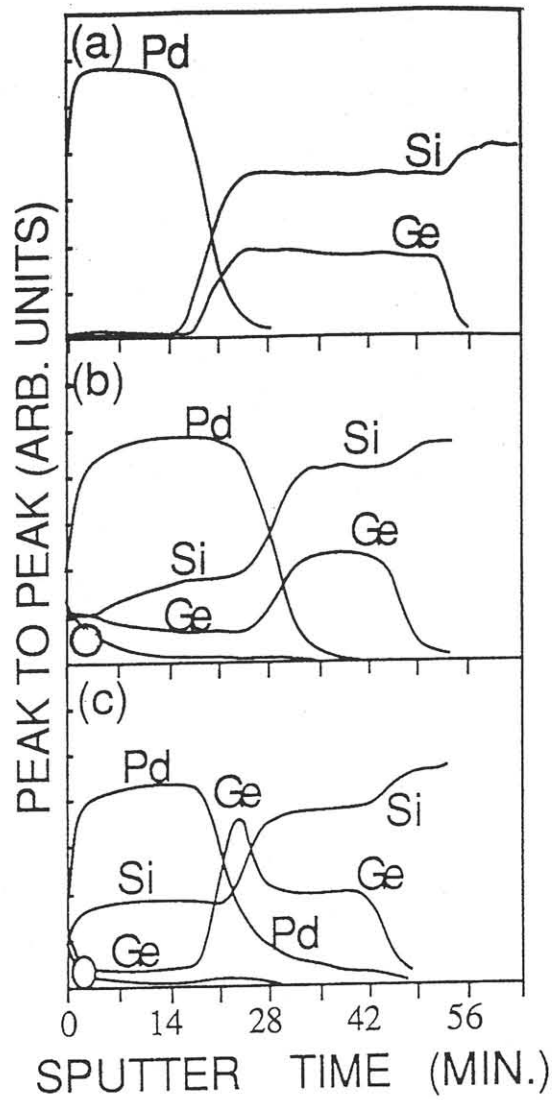


Fig 2. AES depth profiles of $Pd/Si_{0.82}Ge_{0.18}$ in an as deposited state (a), and following annealing at: 250°C, 4 hrs (b), and at 550°C, 4 hrs (c).

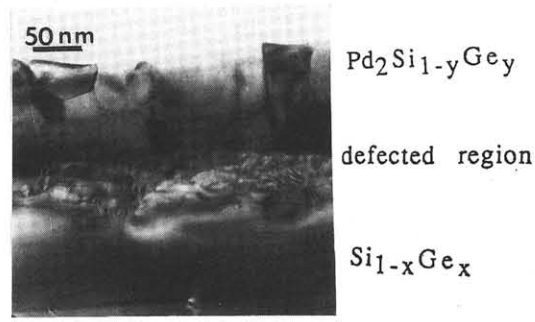


Fig 3. Bright-field TEM cross sectional image of a $Pd/Si_{0.82}Ge_{0.18}/Si$ sample, reacted at 550°C for 4 hours. Note the defected region between the compound and the unreacted $Si_{1-x}Ge_x$ layer.

The double layer structure formed at the higher temperature range can be explained by either a one stage or a two stage reaction mechanism. The one stage mechanism could be the preferential reaction of Pd with the Si atoms in the $Si_{1-x}Ge_x$ layer, thus causing a "snow plow" effect with the Ge atoms in the layer (assuming low solubility of Ge in the $Pd_2Si$ lattice), which eventually leads to the double layer structure seen in Fig. 2c. On the other hand, a two stage reaction mechanism may also be proposed, whereby in the first stage of the reaction, the ternary phase $Pd_2Si_{1-y}Ge_y$ forms, and at a later stage it rejects Ge atoms back on the unreacted $Si_{1-x}Ge_x$ layer, leading thus to the formation of the double layer structure.

The electrical properties (Schottky barrier height) of the Pd contacts to these heterojucntions were investigated by current-voltage measurements. Schottky barrier diodes with Pd metallization were prepared on three differnt type substrates using standard photolithographic techniques: on pure n:Si(100), on $n:Si_{0.91}Ge_{0.09}/n^+$:Si(100), and on $n:Si_{0.82}Ge_{0.18}/n^+$:Si(100). The diodes were heat treated in a vacuum furnace at 250°C for 15 minutes, sufficient conditions for the formation of the $Pd_2Si$ or $Pd_2Si_{1-y}Ge_y$ phases on the repective semiconductors. The current-voltage characteristics of the diodes under forward and reverse bias are shown in Fig. 4. The Schottky barrier height ($\phi_b$) of $Pd_2Si$/n-Si(100) was 0.75 eV, in agreement with values published in literature. The barrier heights of the diodes formed on $Si_{1-x}Ge_x$ with x=0.09 and x=0.18 were 0.67 and 0.65 eV, respectively. The magnitude of the lower values of $\phi_b$ with the addition of Ge is neither identical to the magnitude of the bandgap lowering for the strained $Si_{1-x}Ge_x$ layers ($\Delta E_g$ = 0.13 and 0.21 eV, for x=0.09 and 0.18, respectively) nor is it identical to the conduction band discontinuity, $\Delta E_c$, which is approximately 0.02 eV and does not vary with Ge concentration[3]. The mechanism of the Schottky barrier height lowering is currently under investigation.

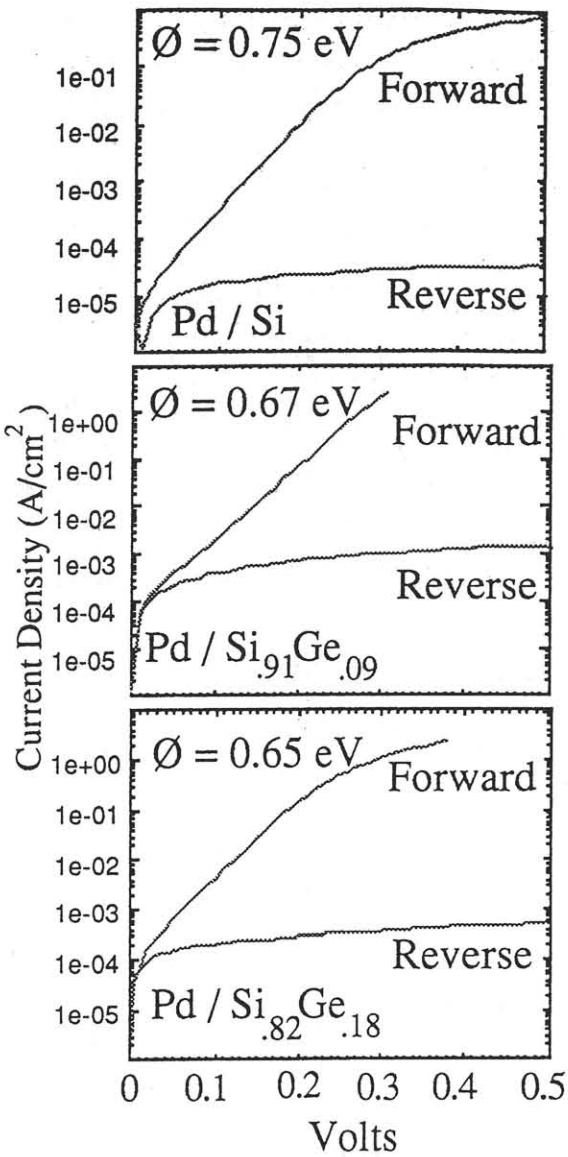


Fig 4. Characteristic current-voltage behavior of diodes for Pd/Si (a), $Pd/Si_{0.91}Ge_{0.09}$ (b), and $Pd/Si_{0.82}Ge_{0.18}$ (c).

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