Molecular Beam Epitaxial Growth of Si\textsubscript{1-x}Ge\textsubscript{x}/Si Pseudomorphic Layers Using Disilane and Germanium

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Molecular beam epitaxial growth of pseudomorphic Si\textsubscript{1-x}Ge\textsubscript{x}/Si layers using disilane (Si\textsubscript{2}H\textsubscript{6}) and elemental germanium has been studied for the first time. It is found that at a fixed flow rate of Si\textsubscript{2}H\textsubscript{6}, the germanium content in the Si\textsubscript{1-x}Ge\textsubscript{x} alloys is a function of the germanium cell temperature. Heterostructures and multi-quantum wells with good surface morphology, excellent crystalline quality, and abrupt interfaces are demonstrated, indicating little or no source-related transient effects.

Key words: Disilane, Ge MBE source, SiGe/Si

The advent of Si\textsubscript{1-x}Ge\textsubscript{x}/Si hetero-epitaxial structures offers attractive possibilities for integrated, high-performance electronic and optoelectronic devices.\textsuperscript{1} An important key step toward this realization is the successful growth of epitaxial layers which need to be defect-free, of good crystalline quality, and pseudomorphic in many cases. In the case of heterojunctions, the interfaces also have to be abrupt. While growth techniques such as ultra high vacuum/chemical vapor deposition (UHV/CVD)\textsuperscript{2} and rapid thermal chemical vapor deposition (RTCVD)\textsuperscript{3} have been developed to produce epitaxial Si\textsubscript{1-x}Ge\textsubscript{x} materials, molecular beam epitaxy (MBE)\textsuperscript{4} is one of the more common techniques to synthesize the heterojunction structures with abrupt interfaces. The major difference among these techniques, besides the apparatus used, are the silicon and germanium sources used and the chamber pressures during growth. In RTCVD, dichlorosilane (SiH\textsubscript{2}Cl\textsubscript{2}) and germane (GeH\textsubscript{4}) are used and the growth pressure is between 1–10 Torr. In UHV/CVD, silane (SiH\textsubscript{4}) and GeH\textsubscript{4} are the sources and the growth pressure ranges from 10\textsuperscript{-3} to 10\textsuperscript{-1} Torr. Molecular beam epitaxy normally uses elemental silicon and germanium sources. The pressure during growth is approximately 10\textsuperscript{-7} Torr. Molecular beam epitaxy has the ability to grow heterojunction structures with abrupt interfaces because of the extremely low pressures in the growth chamber and the ability to rapidly shutter the source cells.

Gas sources (GS), such as disilane (Si\textsubscript{2}H\textsubscript{6}) and GeH\textsubscript{4}, have been introduced in MBE to replace solid sources to improve the growth process\textsuperscript{5,6} and to eliminate spitting defects which are usually present in layers grown by solid source MBE.\textsuperscript{7} High-quality bulk layers have been recently grown and reported by us.\textsuperscript{6} Despite the success with reduction of defects in the grown layers, there are problems with GSMBE. When GeH\textsubscript{4} is introduced into the chamber, the system pressure takes an extremely long time to reach steady state. As a result, graded composition Si\textsubscript{1-x}Ge\textsubscript{x} layers are usually obtained.\textsuperscript{7} Precracking of GeH\textsubscript{4} is not a very efficient way to solve this problem since metallic germanium will be produced to clog the cell.

We have explored the growth of Si\textsubscript{1-x}Ge\textsubscript{x}/Si using Si\textsubscript{2}H\textsubscript{6} and solid germanium as sources. In this technique, the growing surface is still passivated by hydrogen atoms, as in GSMBE. The chamber pressure, the partial pressure of Si\textsubscript{2}H\textsubscript{6}, and the germanium flux remain very steady as growth proceeds. The germanium cell can be conveniently shuttered to grow

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Fig. 1. Dependence of germanium content in Si$_{1-x}$Ge$_x$ alloys as a function of germanium cell temperature. The composition of the layers with low germanium content were obtained by double crystal x-ray diffraction. The composition of layers with high germanium content were determined from electron microprobe. All compositions were confirmed by Rutherford backscattering spectrometry.

Fig. 2. Double crystal x-ray rocking curves for pseudomorphic Si$_{1-x}$Ge$_x$ layers with various germanium compositions and thicknesses.

Si$_{1-x}$Ge$_x$/Si multilayers with negligible transient effects.

A two-chamber RIBER 32 MBE with a vacuum load lock is used for our experiments. The growth chamber is provided with an ion pump which maintains a background vacuum of 10$^{-1}$ Torr. The cryoshroud temperature is fixed at 77K and additional pumping is provided during growth by a turbomolecular pump. The Si$_2$H$_6$ flow rate is controlled by a precision mass flow controller. Elemental germanium is effused from a resistively heated cell with a PBN crucible. During growth the substrate temperature is monitored by a pyrometer.

Si$_{1-x}$Ge$_x$ epitaxial layers were grown on (100)-oriented, boron-doped, p-type silicon wafers with a resistivity between 2–5 × 10$^3$ ohm-cm. The substrates were sequentially cleaned in (1) 1NH$_4$OH:1H$_2$O$_2$:5H$_2$O, (2) 1HC1:1H$_2$O$_2$:3H$_2$O, and (3) 1HF:50H$_2$O solutions for 10 min, 10 min, and 30 s, respectively. They were rinsed in deionized H$_2$O between each solution. Prior to growth, the surface oxide was removed by heating to 840°C for 10 min. At this point a clear (2 × 1) reflection high energy electron diffraction (RHEED) pattern is observed.

Cu$_{0.3}$ (004) x-ray rocking curve measurements were performed with a double-crystal x-ray diffractometer (XRD). Pendelosung oscillations were observed in the data. From these oscillations, both the perpendicular lattice constant and the layer thickness can be simultaneously determined. The composition and thickness of some of the alloys were confirmed by electron microprobe measurements and Rutherford backscattering spectrometry (RBS). Secondary ion mass spectrometry (SIMS) was also done to determine the germanium concentration profile as a function of depth.

At a fixed Si$_2$H$_6$ flow rate of 7 sccm and a growth temperature of 650°C, the germanium composition in the Si$_{1-x}$Ge$_x$ layers is a function of the germanium cell temperature, as shown in Fig. 1. The thickness of the layers with low germanium compositions is below critical thickness, while those of layers with high germanium content is approximately 1 µm. The thickness for the thin layers was determined from double-crystal XRD rocking curves, as discussed below, and the thickness for the thick layers are measured by optical microscopy. The data of Fig. 1 indicate that alloy composition of the films is largely controlled by the germanium flux.

Figure 2 shows x-ray rocking curves for the Si$_{1-x}$Ge$_x$ layers with various germanium compositions. The growth times are 15, 13, 10, and 8 min, respectively. Despite the high noise/signal ratios, the curves clearly indicate the epitaxial layer lattice constants and Pendelosung oscillations. The latter indicate that the grown layers are of good crystalline quality and pseudo-