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Parametric Investigation of $Si_{1-x}Ge_x$/Si Multiple Quantum Well Growth

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$Si_{0.8}Ge_{0.2}$/Si multiple quantum wells (3 nm/30 nm) have been grown by molecular beam epitaxy and have been characterized using photoluminescence (PL), secondary ion mass spectrometry, and transmission electron microscopy. A parametric investigation relating the growth conditions to the PL was initiated. The existence of sharp, phonon-resolved PL appears to be strongly related to the background impurity concentration. The connection between sharp PL and substrate growth temperature is probably due to the temperature dependent incorporation of impurities. The correlation of the broad PL with Ge-rich platelet density is probably due to the gettering of impurities at the platelets. A high temperature (710 °C) anneal removes the broad PL while having no effect on the platelet density.

1. INTRODUCTION

There has been extensive investigation into the growth and characterization of $Si/Si_{1-x}Ge_x$ multiple quantum wells (MQW). The motivation for this work has been two-fold. The first is the search for efficient optical devices (both emitters and detectors) in Si-based materials which overcome the restrictions established by the indirect electronic band structure of Si. The second motivation is that the optical properties of these heterostructures are very sensitive to growth conditions, thereby providing a window for the understanding of fundamental growth phenomena. Initial investigations of MBE-grown SiGe MQW using photoluminescence (PL)[1,2] revealed a broad (full width at half maximum (FWHM) of ~ 60 - 80 meV) luminescence peak located 90 - 120 meV below the strained alloy band gap. More recent work has shown sharp, phonon-resolved PL with MBE-grown material[3-7], as well as with MQW grown by chemical vapor deposition (CVD)[5,8,9]. Brunner *et al.*[6] have found that elevated growth temperature greatly increases layer quality and that phonon-resolved PL with FWHM below 5 meV can be achieved at growth temperatures around 700 °C. It is curious that the broad luminescence peak is only observed with MBE-grown material. The mechanism for this is not well understood. One group has observed a correlation between the concentration of platelets in the quantum wells and the intensity of the broad PL and has proposed a model based upon exciton recombination at the platelets[7]. Another group has a model relying upon donor-acceptor recombination[10]. This model is based upon optically detected magnetic resonance measurements which show that the recombining holes derive from the strain-split $M_J = \pm 3/2$ valence band in the $Si_{1-x}Ge_x$ layers. In this paper we study the origins of the two types of PL peaks by a parametric investigation of the growth of SiGe MQW.

2. EXPERIMENTAL PROCEDURES

The SiGe MQW were grown on 3 in. (100) Si wafers using MBE. Details of the growth system have been reported earlier[11]. The Si and Ge molecular beams were obtained from elemental sources in electron gun evaporators. Prior to growth the substrates were cleaned either by the Shiraki process[12] or by a modified Shiraki process[13] which resulted in a H-terminated surface. Throughout this work the same nominal MQW structure was fabricated: five QW composed of $Si_{0.8}Ge_{0.2}$, 3 nm wide, separated by 30 nm of Si. Growth parameters explored were substrate temperature, buffer layer thickness, Si encapsulation thickness, growth rate, and substrate cleaning procedure. In addition, the effect of post-growth anneal was studied. The primary characterization techniques were PL, secondary ion mass spectrometry (SIMS), and transmission electron microscopy (TEM).

3. RESULTS AND DISCUSSION

It has been shown by previous researchers[4,6], and confirmed here, that the substrate temperature during growth is a critical parameter determining heterostructure quality. PL of MQW grown at 550, 650, and 710 °C are presented in Fig. 1. Each of these samples underwent a Shiraki clean prior to growth. The oxide was desorbed at 900 °C for 10 min. and a 170 nm Si buffer layer was grown at 710 °C. The growth rate was 0.05 nm/s for the Si and 0.015 nm/s for Ge. A 200 nm Si cap was grown on top of the MQW at the growth temperature of the MQW. Sharp, phonon-resolved PL peaks were detected only on the sample grown at 710 °C. The broad PL peak was observed from the sample grown at 550 °C. In support of the exciton recombination at Ge-rich platelet model, plan-view TEM of these samples revealed no platelets in the sample grown at 710 °C, which translates into an upper limit of the platelet density of ~10^6/cm^2. The platelet concentration was ~10^8/cm^2 in the remaining two samples. However, after a one hour anneal at 710 °C in a N_2 atmosphere the broad PL of the 550 °C sample vanished while there was no change in the PL of the 710 °C sample. In addition, there was no change in the platelet concentration in the 550 °C sample after the anneal. This implies that, while the platelets may be a factor in the broad PL, there must be another contributing agent, such as impurity gettering at the platelets.

SIMS was used to determine the background impurities in the MQW as a function of growth temperature. All of the MQW had measurable background concentrations of B, Cr, Ta, and Al. The B was found at the initial growth interface, with a sheet concentration of 1.4x10^{12}/cm^2, as expected, on samples cleaned with the Shiraki process. The B level in the region of the MQW was below the detection limit of 2x10^{15}/cm^3. Both the Cr and Ta had maximum concentrations, coordinated with the Ge concentration, in the SiGe QW of 10^{17} and 4x10^{17}/cm^3, respectively. Only the Al concentration was different among the three samples. In Fig. 2 it is seen that the average Al concentration increased from 10^{16} to 6x10^{16}/cm^3 as the growth temperature decreased from 710 to 550 °C. It is also seen that the maxima of the Al are in the SiGe MQW for growth temperature of 650 and 710, but are found in the Si spacer layers for the growth temperature of 550 °C. The higher concentration of Al, which is an acceptor, in the MQW of the sample grown at 550 °C is consistent with the donor-acceptor recombination model for the broad PL. The concentration of Sb, the suspected residual donor, is at or below the SIMS detection limit of 5x10^{15}/cm^3.

In the course of this work, the liquid nitrogen cryoshroud in the MBE growth system developed a microcrack. During the repair the MBE growth system was dismantled and cleaned and a new Si source was loaded. The same MQW structures described above were grown in the refurbished system. The optical properties of these structures were substantially different from the previous set, Fig. 3. Phonon-resolved PL was observed in all samples, including the sample grown at 550 °C, although some weak, broad PL was also seen in this sample. TEM detected the same concentration of platelets in the new 550 °C sample as in the earlier one. The substrate growth temperature has not changed since it is calibrated with respect to the eutectic temperature of Al on Si. SIMS analyses of the new set of samples show that the Cr, Ta, and Al background impurities were substantially reduced. In the 550 °C sample, the Cr and Ta are localized in the SiGe QWs at maximum values of 2x10^{16} and 6x10^{16}/cm^3, respectively. The average Al concentration is 7x10^{15}, 5x10^{15}, and 4x10^{15}/cm^3 for the 710, 650, and 550 °C samples, respectively. While there are measurable Al peaks in the SiGe QWs in the 710 and 650 °C samples, the Al peaks in the 550 °C specimen are found in the surrounding Si.

The source of the background impurities is uncertain. Two samples were specifically grown for SIMS analysis. The first sample had a series of Si layers, 150 nm thick, grown at temperatures of 710, 650, 550, and 350 °C, and a top layer, 250 nm thick, grown at room temperature. The second sample was similar but the layers were $Si_{0.6}Ge_{0.4}$ and on top of the $Si_{0.6}Ge_{0.4}$ layer grown at room temperature was a 100% Ge layer grown at room temperature. Two key features from these SIMS profiles must be noted. The SIMS analysis of Si and Ge deposited at room temperature shows increased levels of B, Al, Cr, Ta, and Cu in the Ge film, suggesting that either the Ge source material or the e-beam deposition of Ge is a primary source of background impurities. Secondly, it is observed that the incorporation of the impurities into the epitaxial film is a function of the temperature-dependent segregation of the individual impurities. At growth temperatures below 550 °C, there are substantial increases in the background concentrations of most impurities.

Growth parameter space was further investigated using our standard MQW structure (5 QW, $Si_{0.8}Ge_{0.2}$, 3 nm wide, separated by 30 nm of Si) grown at 710 °C. The following parameters were changed independently: thin Si cap (30 nm total), modified Shiraki cleaning process, fast growth rate (0.2 nm/s), thin buffer (50 nm), all of the preceding modifications, and B doping (10^{17}/cm^3). In each of these cases, sharp, phonon resolved PL was observed, however the intensity of the PL of the B-doped sample was substantially less than the other samples.

4. SUMMARY

In this parametric investigation of the growth of SiGe MQW, we have found that the most sensitive parameter determining the nature of the PL is the background impurity concentration. Identical structures, grown at 550 °C, having the same platelet concentration, have radically different PL correlated with impurity concentration. The apparent correlation with growth temperature is likely due to the decreased impurity incorporation at the higher growth temperatures.

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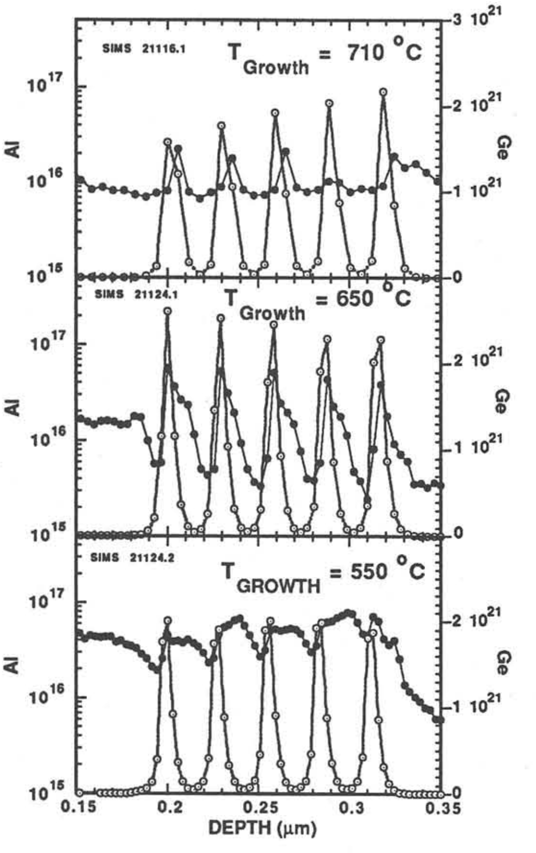

Fig. 2. SIMS profiles of $Si_{0.8}Ge_{0.2}$ quantum wells grown at 550, 650, and 710°C. The solid circles represent Al and the open circles represent Ge.

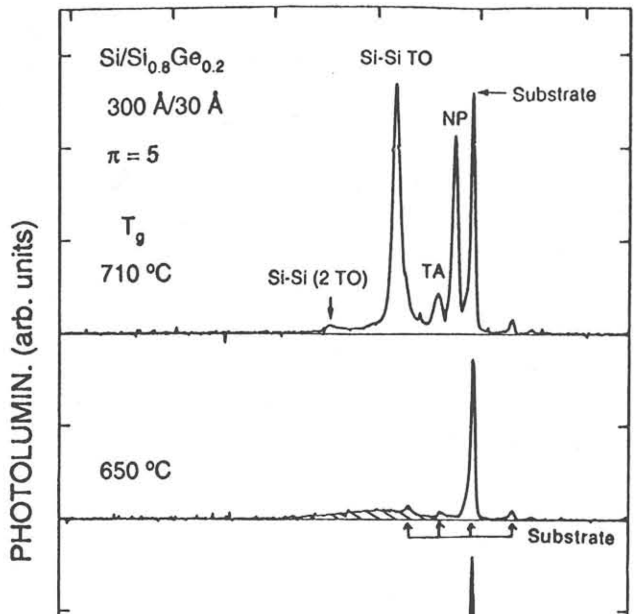

Fig. 1. PL of SiGe heterostructures composed of five 3 nm $Si_{0.8}Ge_{0.2}$ quantum wells separated by 30 nm Si. grown at 550, 650, and 710°C. PL was measured at 1.6 K.

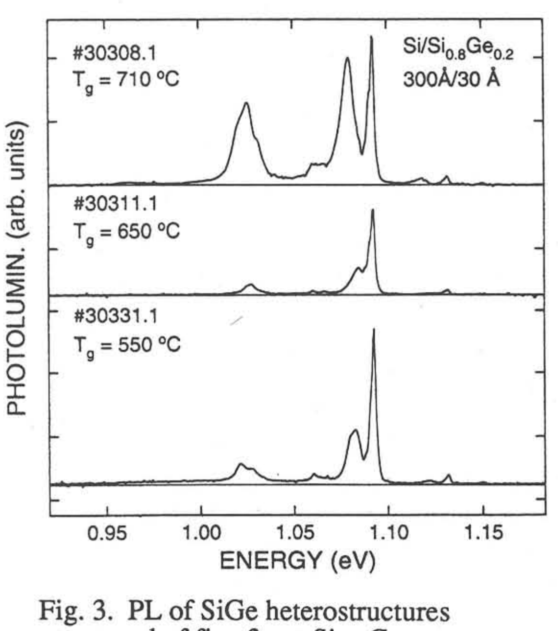

Fig. 3. PL of SiGe heterostructures composed of five 3 nm $Si_{0.8}Ge_{0.2}$ quantum wells separated by 30 nm Si. grown at 550, 650, and 710°C **after growth system repairs**. PL was measured at 1.6 K.