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Band-edge exciton luminescence from Si/strained $Si_{1-x}Ge_x$/Si structures

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Well-resolved band-edge exciton photoluminescence has been observed in strained $Si_{1-x}Ge_x$ layers grown on Si(100) by rapid thermal chemical vapor deposition. The luminescence is due to shallow-impurity bound excitons at low temperatures (under 20 K) and is an excellent probe of quantum confinement effects in narrow quantum wells. At higher temperatures, the luminescence is due to free excitons or electron hole plasmas, depending on the pump power. Experiments with single and multiple quantum well structures indicate that most of the $Si_{1-x}Ge_x$ luminescence is from carriers which were generated in the silicon substrate and subsequently were trapped in the quantum wells.

I. INTRODUCTION

Strained $Si_{1-x}Ge_x$ layers grown commensurate on Si(100) substrates have been under intense investigation for nearly ten years as a possible candidate for the development of silicon-based heterojunction semiconductor devices. Band-edge exciton luminescence in these strained layers has been reported only recently, however.[1,2] Previous reports of luminescence from strained $Si_{1-x}Ge_x$ layers were all from material grown by molecular-beam epitaxy (MBE). In these reports, the luminescence was either from intentionally introduced impurities[3] or deep levels of unknown origin[4] in single films or quantum wells (QWs), or from Si–Ge short-period "zone-folded" superlattices.[5,6] However these superlattices typically contained high densities of threading dislocations (10^8–10^{10} cm^{-2}), and it now seems more likely that the emission was related to the dislocations rather than a property of the superlattice itself.[7,8]

In this article, the well-resolved band-edge luminescence of excitons in strained $Si_{1-x}Ge_x$ layers grown by rapid thermal chemical vapor deposition (RTCVD) will be reported. The growth process will be briefly reviewed, and then typical spectra for both narrow QWs and thicker films will be described. Finally, the transport of generated excitons to the quantum wells and their ability to move from one well to another will be investigated.

II. RTCVD

The structures described in this article were grown by RTCVD.[9] A schematic diagram of the reactor is shown in Fig. 1. A silicon wafer is suspended on quartz pins inside a cylindrical quartz tube which is externally cooled by forced air. The wafer is introduced through a load lock and is heated radiatively by a bank of tungsten-halogen lamps located outside the reaction chamber. The process gases are dichlorosilane or silane as a silicon source and germane as a germanium source in a hydrogen carrier. Typical growth pressures are 6 Torr, with the reactor being exhausted by a rotary vane pump. The reaction chamber is not an "ultrahigh vacuum" (it contains several *o*-ring seals), but with extreme attention to gas purity and sample loading procedures it is possible to achieve high quality epitaxial layers. Typical growth temperatures are 600–625 °C for the $Si_{1-x}Ge_x$ alloys and 700 °C for silicon layers. Note that there are no substrate heaters, susceptors, etc., inside the reaction chamber which could be a source of contamination at high temperature.

Because the growth is a chemical as opposed to a physical process (cf. MBE), accurate knowledge of the substrate temperature is required to control the growth rate. (A 30 °C change in temperature corresponds to a factor of two change in the silicon growth rate). This is a problematic issue in such lamp-heated systems without susceptors. Thermocouples will not accurately measure the wafer temperature unless intimately attached to the wafer, which is inconvenient and risks contamination. Pyrometry requires knowledge of the emissivity, which itself depends on wavelength, temperature, wafer polish, etc. We therefore infer the silicon substrate temperature by measuring its infrared absorption (at 1.3 and 1.5 μm) *in situ* during growth (Fig. 1). This method allows extraction of the absolute wafer temperature to within a few degrees centigrade and is not affected by the presence of $Si_{1-x}Ge_x$ layers under a thickness of ~ 1 μm for x less than 0.5.[10] Further details of the growth system are given in Ref. 9.

III. PHOTOLUMINESCENCE (PL) SPECTRA

Typical 2 and 77 K spectra of nominally undoped strained $Si_{0.8}Ge_{0.2}$ layers with ~ 150 Å Si caps are shown in Fig. 2 for $Si_{0.8}Ge_{0.2}$ layer thicknesses of 33 and 500 Å. Omitting the Si cap layer in general has been found to reduce the emitted intensity by over a factor of 10, presumably due to surface recombination. In general, the 2 K spectra are very similar to those observed by Weber and Alonso in their study of bulk (unstrained) $Si_{1-x}Ge_x$ layers,[11] except for an appropriate shift to lower energy because of the reduction in band gap in our samples due to the strain.[12] At 2 K, we attribute the luminescence as being due to an exciton bound to a shallow impurity site. The assignment of the different features is labeled in Fig. 2. The

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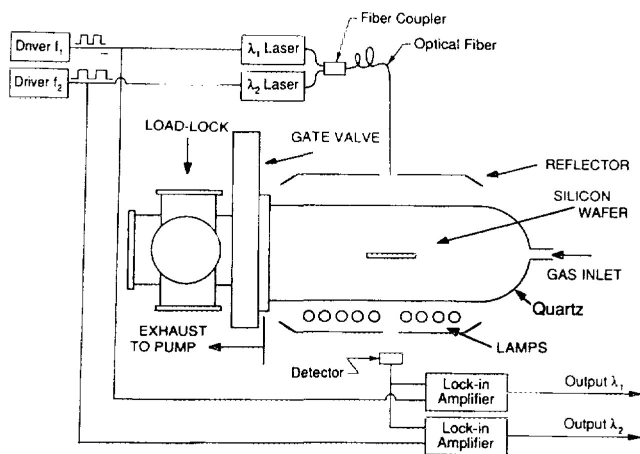

FIG. 1. Schematic diagram of the RTCVD Reactor with temperature measurement by infrared transmission.

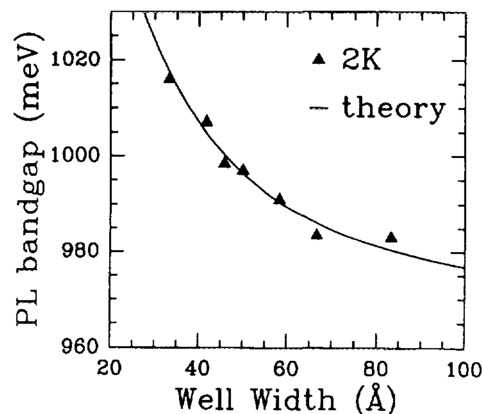

FIG. 3. Bound exciton NP energy as a function of well width for a Si/strained $Si_{0.8}Ge_{0.2}$/Si QW.

highest energy feature is a no-phonon (NP) transition, and the lower energy features are phonon replicas. The transverse optical (TO) phonon replica splits into three peaks because of the three different nearest neighbor interactions in the random alloy. Qualitatively similar spectra have also been observed in $Si/Si_{0.8}Ge_{0.2}$ superlattices grown in our lab with periods down to 45 Å.[2] The relative height of the different TO replicas varies with x (higher x gives more Ge–Ge, less Si–Si, etc.) and agrees well with the bond-

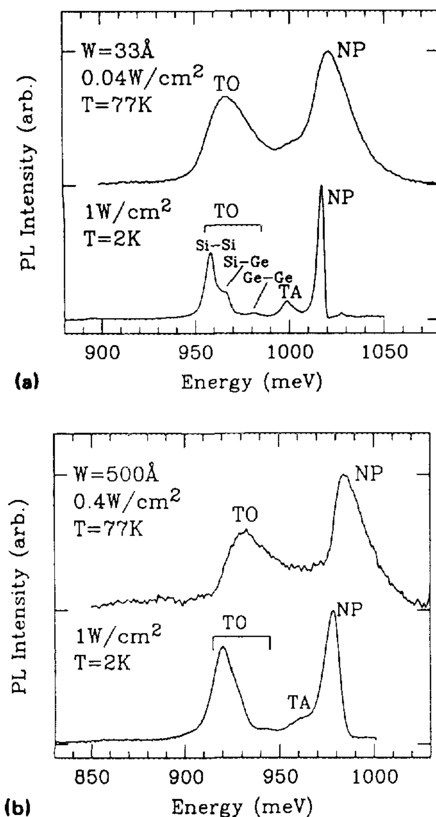

FIG. 2. PL spectra of Si/strained $Si_{1-x}Ge_x$/Si potential wells of width (a) 33 Å and (b) 500 Å at both 2 and 77 K.

counting model of Weber and Alonso.[11] In very thin QWs, the Si–Si replica is higher than expected; this is attributed to penetration of the exciton wavefunction into the Si barriers.[2] As the temperature is raised a clear transition from bound exciton (BE) to free exciton (FE) luminescence is seen, with an energy increase of the NP feature of 5 ± 2 meV. Excitation spectroscopy also confirms the higher temperature signal as a free exciton.[2] The binding site of the bound excitons is not known definitively, but is thought to be either substitutional B or P. They are used as dopants in the growth reactor, and background dopant levels are typically 10^{16} cm^{-3}. The decay time of the bound exciton has been measured to range from 375 to 420 (± 50) ns. This compares to ~ 270 and ~ 1050 ns for P and B centers in Si, respectively.[13]

The energy shift between the 2 K PL spectra of the 33 and 500 Å wells (~ 45 meV) is attributed to quantum confinement effects. Figure 3 shows the shift for a set of fully strained $Si_{0.8}Ge_{0.2}$ wells with the width varying from 33 to 80 Å. The solid line in Fig. 3 is a calculation of the expected change of the hole ground state energy of the QW.[14] That good agreement is found considering only valence band effects is consistent with the fact that the conduction band offset is thought to be small.[15]

Unlike pure silicon, the free exciton spectra (Fig. 2) exhibit a strong NP peak. The physical origin for this transition in an indirect band gap material is the alloy randomness, which breaks the perfect translational symmetry of the lattice and hence relaxes the requirement for momentum conservation.[11,16] In previous work on unstrained $Si_{1-x}Ge_x$,[11] the bound exciton NP peak was largest for $x = 0.5$ when it was roughly an order of magnitude larger than the phonon replicas. A similar trend is seen for both the free exciton and bound exciton NP signal in our strained films grown by RTCVD (for $x < 0.5$). At higher pump powers, the high density of carriers collected in the QWs lead to an electron-hole plasma (EHP) as opposed to discrete excitons. The signature of such a plasma is a broadening of the linewidths as the quasi-Fermi levels move into the conduction and valence bands at high carrier densities.[17] At a power of 100 W/cm², EHPs with esti-

mated carrier densities in the wells $\sim 10^{18}$ cm^{-3} have been observed in both the 33 and 500 Å $Si_{0.8}Ge_{0.2}$ QWs at 77 K.[18] This EHP luminescence has a weak temperature dependence, and PL at room temperature is readily observable in wells with $x > 0.3$.

Such well-resolved band edge exciton luminescence in strained $Si_{1-x}Ge_x$ layers was first reported by Terashima *et al.* in MBE films[1] only for $x = 0.04$; higher Ge fractions resulted in either relaxed films or a broad deep ($E_g - 100$ meV) PL[19] similar to that described by Noël *et al.* in Ref. 3. The first reported band-edge exciton PL for higher Ge fractions ($x = 0.2$) and for QWs and superlattices was in films grown by RTCVD.[2] The exact reason for the sharp band-edge PL of the RTCVD material is not clear, although it may be due to an absence of deep levels within the band gap. The RTCVD growth procedures were refined for optimum heterojunction bipolar transistor (HBT) performance, a device which is very dependent on minority carrier lifetime. We have since found that good HBT performance with ideally low base currents requires material exhibiting good PL.[20] Recently, band-edge exciton luminescence has also been observed in MBE-grown films for $x \approx 0.2$ for very thin layers (few nanometers),[21] but thicker layers still often yield a deep luminescence of uncertain origin.

IV. EXCITON TRANSPORT

It was noticed in our early experiments with two adjacent strained $Si_{1-x}Ge_x$ layers (with no silicon between them) that no luminescence at 2 K was ever seen from the wider band gap material. This implied that the excitons could move considerable distances (> 0.1 μm) by diffusion at 2 K to become trapped in the region of lowest potential. This phenomena was further probed by a triple potential well structure, consisting of a 100 Å strained $Si_{0.75}Ge_{0.25}$ QW sandwiched between two 100 Å $Si_{0.87}Ge_{0.13}$ QWs. A 240 Å Si spacer separated each of the wells (Fig. 4). The 2 K PL spectrum (Fig. 4) shows emission only from the silicon substrate and the $x = 0.13$ wells. Given a pump absorption length in the silicon substrate of ~ 1 μm (green Ar^+ ion laser) and assuming a $Si_{1-x}Ge_x$ absorption coefficient at this wavelength not substantially different than that of Si, one expects only a small fraction of the generated carriers to be created directly in the $Si_{1-x}Ge_x$ QWs, which were all within 0.1 μm of the surface. The excitons generated in the substrate were then apparently collected by the lower $x = 0.13$ well. Because of the large band gap shift between the Si and the well (~ 120 meV), the collected excitons could not escape from this $x = 0.13$ well, explaining why the dominant $Si_{1-x}Ge_x$ PL was from the $x = 0.13$ well and no luminescence from the central $x = 0.25$ well was observed. Note that the PL intensities from the substrate and $Si_{0.87}Ge_{0.13}$ well are comparable, giving evidence of considerable transport of excitons from the Si to the outer QW.

As the temperature is raised, the excitons captured in the $x = 0.13$ well now have enough energy to thermally hop out of the well, and can then be captured by the deeper $x = 0.25$ well (Fig. 5). While at 77 K all PL is still from

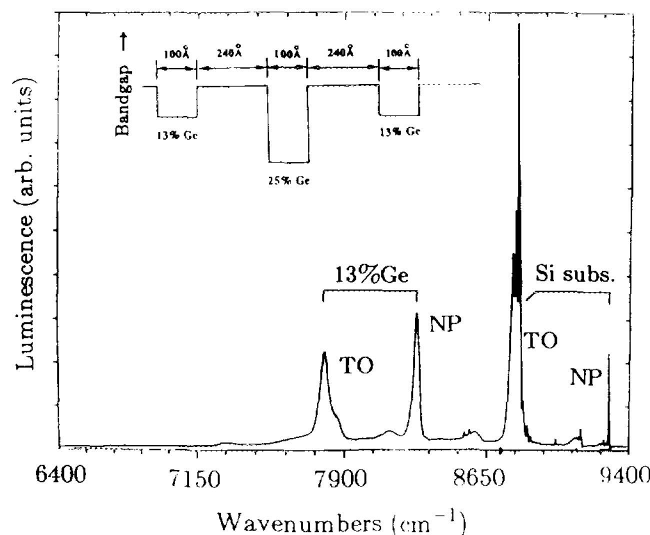

FIG. 4. 2 K luminescence spectra of a triple QW structure ($x = 0.13$, 0.25, 0.13) with 240 Å Si barriers between wells. No $x = 0.25$ luminescence is seen, indicating carriers are collected in the outer $x = 0.13$ wells.

the $x = 0.13$ well, by 120 K all carriers leave the $x = 0.13$ well before luminescencing and only luminescence from the $x = 0.25$ well is observed. Measurements of the hopping rate versus temperature, as probed by the relative strength of the PL from the two wells, show an activation energy of 133 meV. This is in good agreement with the expected barrier height (band gap shift) between Si and strained $Si_{0.87}Ge_{0.13}$ of ~ 120 meV. Also note the relatively much smaller silicon substrate signal at 77 K or higher compared to 4 K. This indicates that the $Si_{1-x}Ge_x$ QWs are even more efficient at collecting excitons generated in

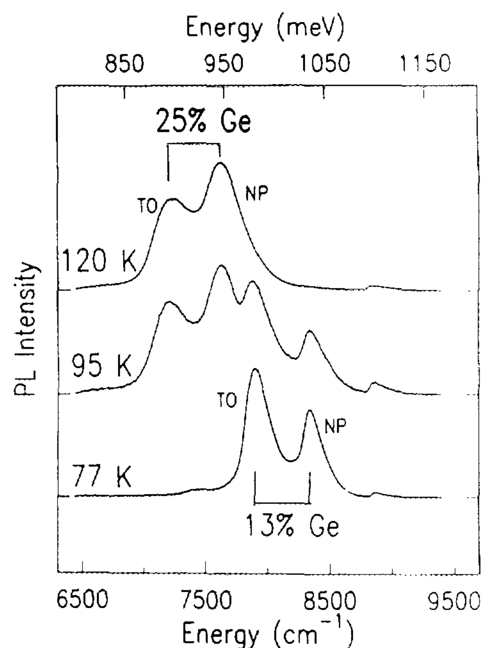

FIG. 5. High-temperature luminescence of the triple well structure of Fig. 4. Note at 95 K and above the excitons thermally hop out of the $x = 0.13$ wells and are captured by the central $x = 0.25$ well.

the Si at 77 K than at 4 K, presumably due to the thermal dissociation of bound excitons at these elevated temperatures.

V. CONCLUSIONS

Well-resolved band-edge luminescence in strained $Si_{1-x}Ge_x$ QWs in silicon grown by RTCVD has been described. At low temperatures, the emission is due to recombination of shallow-impurity bound excitons; at higher temperatures the emission is from free exciton recombination at low densities or an electron-hole plasma at high densities. Finally, most of the observed PL from narrow $Si_{1-x}Ge_x$ layers occurs from the recombination of carriers which are generated far from the well in cladding layers, and are subsequently collected by the QW.

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