

WELL-RESOLVED BAND-EDGE PHOTOLUMINESCENCE FROM
STRAINED $\text{Si}_{1-x}\text{Ge}_x$ LAYERS GROWN BY
RAPID THERMAL CHEMICAL VAPOR DEPOSITION

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ABSTRACT

Well resolved band-edge luminescence of excitons in silicon-germanium alloy strained layers, quantum wells, and superlattices has been observed in films grown by Rapid Thermal Chemical Vapor Deposition. The signal is due to bound excitons at low temperatures and free excitons at higher temperatures, and has a strong no-phonon signal which is caused by alloy scattering. Bandgaps inferred from photoluminescence agree well with those measured by absorption spectroscopy, inferring that a no-phonon process dominates the band-edge absorption.

INTRODUCTION

The optical properties of silicon-germanium strained layers for potential application as optical emitters have recently been of extreme interest. Photoluminescence efficiencies of over 10% have been reported in strained layers (not superlattices) grown by MBE, but at energies substantially below the bandgap (~ 120 meV) and with a very broad linewidth (~ 80 meV) [1]. Theoretical work has predicted the possibility of achieving pseudo-direct gap structures by the zone-folding concept [2,3]. Experimental results on such structures [4,5] have been far from convincing and subject to dispute, however, in large part because of the high density of dislocations in those structures [6]. In this paper the first clearly identified optical transitions from the band-edges in strained silicon germanium structures with germanium fractions up to 0.4 is reported.

RAPID THERMAL CHEMICAL VAPOR DEPOSITION

The RTCVD technique is a combination of susceptorless lamp-heating and chemical vapor deposition, and is similar to Limited Reaction Processing (LRP) [7], except that the gas flow and not the wafer temperature is used to switch the growth reaction on and off. The growth is done at 6 torr in using dichlorosilane and germane in a hydrogen carrier. After chemical cleaning, a 1000 °C H₂ bake and a 1000 °C Si buffer layer, silicon layers are grown at 700 °C and Si_{1-x}Ge_x at 600-625 °C. The growth temperature is controlled to within a few degrees centigrade during growth by in-situ measurement of the infrared absorption in the silicon substrate [7]. The structure of all samples reported in this paper was confirmed by x-ray diffraction and/or transmission electron microscopy (TEM). All samples were fully strained to match silicon substrates with threading dislocation densities $\sim 10^3/\text{cm}^{-2}$ and misfit dislocation spacing $\geq 10 \mu\text{m}$. Other growth system details can be found in ref. 8. The degree of control made possible by the technique is demonstrated by a cross-section TEM of a 50 period Si(23 Å)/Si_{0.82}Ge_{0.18} (23 Å) superlattice in which the individual layers are clearly resolved (fig. 1).

PHOTOLUMINESCENCE SPECTRA

A typical low temperature (2K) photoluminescence (PL) spectrum (in this case for a sample with 10 isolated 29 Å -Si_{0.82}Ge_{0.18} quantum wells) is shown in fig. 2. The excitation was provided by an Ar⁺ laser with a spot size of several mm, and a power density from 1-10 W/cm². The spectrum is most easily interpreted by comparing it to results on *bulk* unstrained Si_{1-x}Ge_x, which have been studied previously in great detail [9]. The highest energy signal is due to non-phonon (NP) recombination of bound excitons, and the lower energy signals are due to phonon-assisted recombination (phonon replicas). By comparison with the work of Weber and Alonso [9], the phonons may be identified as the transverse acoustic (TA) and the transverse optical (TO) phonons. The TO is separated into three peaks corresponding to the different local vibrational nodes depending on nearest neighbor pairs. The phonon energies (difference between the NP signal and the phonon replicas) are in excellent agreement with the previous bulk alloy results, implying that strain has little effect on the phonon dispersion curves. The FWHM of the NP line is ~ 5 meV, which agrees well with the previous best reported results in bulk alloys of ~ 4 meV [9], implying good uniformity throughout the films. The linewidths are an order of magnitude wider than those in silicon because of the random alloy nature of the films.

At higher germanium fractions, the PL energies are reduced because of the lower bandgap, but the TO phonon energies do not change within the experimental resolution. At higher germanium fractions, however, the relative intensity of the various TO phonon replicas changes to reflect more Ge-Ge and fewer Si-Si bonds. The spectra in uniform films, quantum wells, and superlattices (period > 45 Å) are also qualitatively similar, except for the appropriate quantum confinement increase in the bandgap. For narrow wells however (< 30 Å) the relative strength of the TO replicas is shifted towards a lower x than is representative of the composition of the well only [10]. This is thought to be due to the

fact that the exciton wavefunction penetrates substantially into the Si barriers, so that some fraction of the phonon-assisted radiative recombination actually takes place in the silicon.

Similar well-resolved band-edge luminescence of strained $\text{Si}_{1-x}\text{Ge}_x$ layers has been reported for single $\text{Si}_{1-x}\text{Ge}_x$ layers grown by MBE only for germanium fractions up to $x = 0.04$ (4% Ge) [11], and not at all for superlattices. At present it is not known why such spectra have not been reported by MBE for larger germanium fractions.

At higher temperatures (> 20 K), the excitons are no longer bound to shallow impurities and become free excitons. The spectra remain similar, except for shifts in energy due to temperature dependence of the bandgap, the exciton binding energy, and thermal broadening [10]. Typical spectra at 77 K, in the case of a single $\text{Si}_{0.6}\text{Ge}_{0.4}$ quantum well, are shown in fig. 3. The various phonon replicas have broadened to form a single peak, and the strong NP line is still present. This NP line of the free excitons is of great interest. While it is sometimes observed with bound excitons in silicon (due to localization of the exciton), it is not observed for free excitons in silicon due to the indirect bandgap. The NP free exciton signal is strong in our samples, however, and increases as the Ge fraction is raised to $x = 0.4$. (Contrast, for example, the relative NP/TO strengths in figure 2 ($x = 0.2$) vs. figure 3 ($x = 0.4$)). Similar results have been reported in bulk unstrained alloys [9]. This signal is not due to superlattice or zone folding effects but simply due to the *random* nature of the alloy [12]. The randomness breaks the translational symmetry of the lattice, with the result that crystal momentum k is no longer a "good" quantum number. Therefore an electron in the indirect conduction band valley also possesses some k component at all other k 's, including $k=0$ for a NP transition. As x increases towards $x = 0.5$, this randomness and hence the NP strength should increase. This random nature of the Si and Ge atomic location is also what physically causes alloy scattering.

BANDGAP AND COMPARISON TO ABSORPTION DATA

By observing the NP line as a function of composition, the bandgap of the $\text{Si}_{1-x}\text{Ge}_x$ alloys can be determined (fig. 4). This is in principle more precise than absorption measurements such as those by Lang [13] since the absorption energy edge may differ from the true band-edge in indirect materials because phonon emission or absorption may be required for an optical transition. The actual data plotted in ref. 13 is the measured absorption edge, with no correction made for phonon energies. The excellent agreement between the reported absorption edge of ref. 13 and the true bandgap as measured by PL in the strained silicon-germanium alloys implies that the dominant optical absorption process in $\text{Si}_{1-x}\text{Ge}_x$ alloys is by a no-phonon process. This is consistent with the observed PL spectra since absorption is the inverse of the photon-emission process. Dominant no-phonon absorption in the alloys is however in direct contradiction with one of the major conclusions of Braunstein et al. [14], which is commonly accepted to give the bandgap of the relaxed $\text{Si}_{1-x}\text{Ge}_x$. This work concluded that optical absorption in the alloys proceeded by a phonon-assisted process, and then subtracted a phonon-energy to the measured absorption edge to obtain the bandgap.

Our work then suggests that the relaxed bandgap energies reported in [14] are underestimated by a phonon energy or some weighted average of various phonon energies.

It has been assumed for several years that the bandgap offset in strained $\text{Si}_{1-x}\text{Ge}_x$ alloys on bulk Si is of type I configuration for small x [15] (up to $x = \sim 0.7$ according to Ref. 16), while that of relaxed $\text{Si}_{1-x}\text{Ge}_x$ vs. strained Si is type II (lower E_C in the Si) [17]. Recently, however, optically detected magnetic resonance experiments have suggested that strained $\text{Si}_{0.65}\text{Ge}_{0.35}$ on relaxed Si might already be type II, although the strain of the superlattice was not made clear and the results were not conclusive [18]. If the type II case were assumed for our samples, the PL measurements at $x \sim 0.4$ would measure an energy less than that of the bandgap, and certainly less than the absorption edge independent of whether phonon emission was part of the absorption process. To within the resolution of our measurements (± 30 meV due to uncertainties in the well width and hence the confinement energy), this was not observed.

CONCLUSION

Well resolved band-edge photoluminescence of excitons in single strained $\text{Si}_{1-x}\text{Ge}_x$ layers, quantum wells, and superlattices with $x = 0.4$ has been reported for the first time. The spectra are characterized by a NP transition and various phonon replicas. Comparisons with absorption measurements suggest that the dominant absorption in $\text{Si}_{1-x}\text{Ge}_x$ alloys is by a no-phonon process. That such well-resolved PL signals are observed also confirms the excellent minority carrier properties and uniformity of $\text{Si}_{1-x}\text{Ge}_x$ layers grown by Rapid Thermal Chemical Vapor Deposition.

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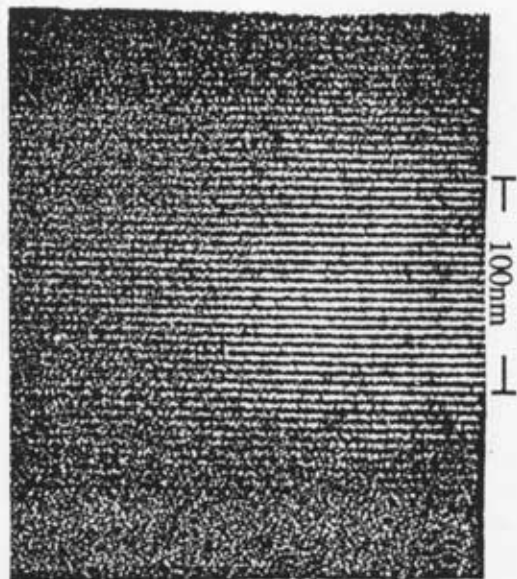


Fig. 1. Cross section TEM of a 50 period 23 Å Si/23 Å Si_{0.82}Ge_{0.18} superlattice.

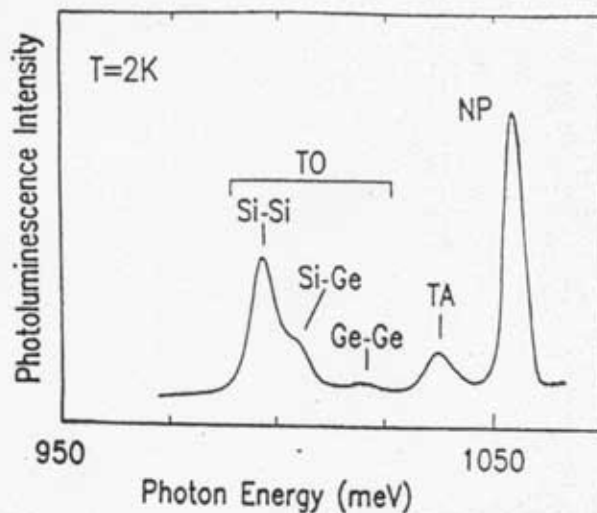


Fig. 2. 2K photoluminescence spectrum of a sample with 10 isolated strained Si_{0.82}Ge_{0.18}-23Å quantum wells.

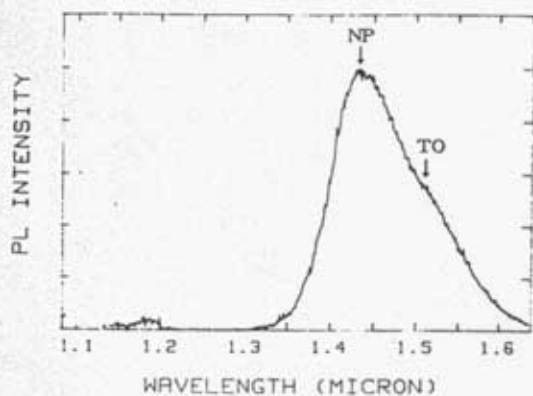


Fig. 3. 77K photoluminescence spectra of a sample with a single strained Si_{0.6}Ge_{0.4} quantum well (~80 Å).

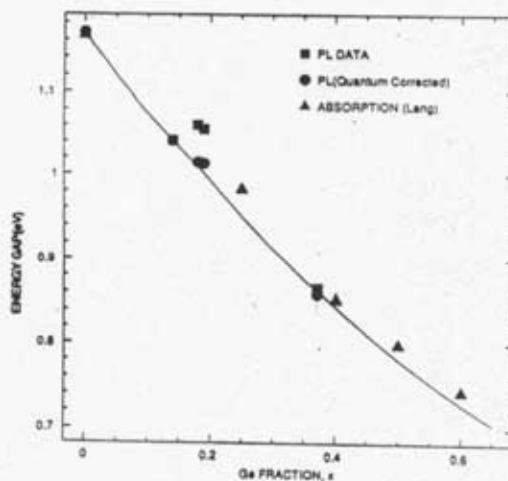


Fig. 4. Bandgap of strained Si_{1-x}Ge_x as determined by the NP PL line. The data has been corrected for quantum confinement effects (indicated) and excitonic binding energies, and adjusted to give the bandgap at 0 K. Also shown is the bandgap determined by photocurrent spectroscopy (Lang [13]) (adjusted to 0 K).