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Near band edge photoluminescence from pseudomorphic tensially strained $Si_{0.985}C_{0.015}$ alloy

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Abstract

Band edge related low temperature photoluminescence of a strained $Si_{0.985}C_{0.015}$ bulk alloy layer grown by molecular beam epitaxy on a Si (100) substrate has been investigated. The high quality layer was grown to a thickness of 1500 Å and was found to be pseudomorphic and tensially strained. We report two dominant features, a well-resolved band-edge luminescence consisting of a no-phonon and a transverse optical phonon replica, and an intense deep level luminescence peak around 0.778 eV. The band edge feature is attributed to a no-phonon free excitonic recombination in the binary alloy. We also observe a red shift of the energy gap of $Si_{0.985}C_{0.015}$ alloy with respect to Si, contrary to what is predicted according to the bulk alloy effect.

Keywords: Alloys; Molecular beam epitaxy; Photoluminescence

1. Introduction

Alloys of group IV elements have been under investigation recently as potential material systems for novel Si-based heterostructure device applications [1]. The $Si_{1-x}Ge_x$ material system [2,3] has received the most attention, with lesser efforts directed towards the growth and characterization of Sn-based [4] and C-based alloy layers. Lately, the C-based alloy systems of $Ge_{1-x}C_x$ [5,6], $Si_{1-x-y}Ge_xC_y$ [7], and $Si_{1-x-y-z}Ge_xC_ySn_z$ [8] have been receiving attention, especially $Si_{1-x}C_x$ [9,10]. However, in the past few years there has also been a number of investigations into the growth and characterization of $Si_{1-x}C_x$ alloy [11,12]. Two growth processes have mainly been used to grow $Si_{1-x}C_x$ alloys, chemical vapor deposition (CVD) [9,13], and molecular beam epitaxy (MBE) [14]. These two processes have been used to synthesize crystalline $Si_{1-x}C_x$ alloys and heterostructures containing a few percent of carbon. They indicate that only $Si_{1-x}C_x$ alloys which contain a few percent of C can be grown pseudomorphically on a Si substrate. This can be directly attributed to the following. Carbon has an extremely low solubility in Si, about 10^{-4} at.% at 1420°C, the melting point of silicon [15]. Additionally, there is a 40% mismatch in the bond lengths of Si and C. The mismatch would result in large local strain around the substitutional carbon atoms. Also, according to the Si–C phase diagram stoichiometric SiC is the only stable compound. Therefore, the substitutional incorporation of carbon above the solid solubility limit requires far from thermodynamic equilibrium growth conditions, such as MBE. The incorporation of isoelectronic carbon into silicon will offer new possibilities, for bandgap engineering, silicon compatible wide bandgap material, and large band offsets.

There have been a few theoretical investigations on the bandgap and electronic structure of $Si_{1-x}C_x$ alloys, but these studies come to conflicting conclusions. Soref [16], uses Vegards law and performs an interpolation giving a monotonic variation in the bandgap of $Si_{1-x}C_x$ alloys, between the constituent elements. Ab initio calculations were made by a some groups [17,18], revealing that for the addition of small carbon concentrations the $Si_{1-x}C_x$ bandgap reduces below Si, turns semi-metallic around 10% C, and then finally increases above Si beyond 10% C.

2. Experimental details

The details of the solid source MBE growth of the $Si_{1-x}C_x$ layer are described elsewhere [14]. The samples were grown using solid source MBE. Silicon was evaporated using a conventional electron beam evaporator and the carbon co-evaporated using a high purity pyrolytic graphite filament

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housed in a water cooled source assembly. The C flux is controlled using the heating current through the filament. Calibration of the heating current was established using secondary ion mass spectroscopy (SIMS). The substrate temperature was maintained at 500–600°C depending on the carbon concentration of the layer grown. A thin 20 nm Si buffer layer was grown initially followed by the growth of the $Si_{1-x}C_x$ layer. By increasing the carbon concentration while growing an epitaxial silicon layer a tensially strained pseudomorphic $Si_{0.985}C_{0.015}$ alloy layer was obtained. The $Si_{0.985}C_{0.015}$ layer was grown to a thickness of 150 nm, and the growth conditions were optimized to maximize the incorporation of C on Si lattice sites. The layer composition and strain were measured by Rutherford backscattering spectrometry (RBS) and confirmed by X-ray diffraction analysis (XRD). X-Ray analysis confirmed the layer to be pseudomorphic, tensially strained, and the carbon was substitutionally incorporated in the lattice.

Photoluminescence spectra were recorded in standard lock-in configuration, using a dispersive 1 m high-resolution Jarell–Ash (Czerny–Turner) monochromator and detected by a liquid-nitrogen cooled Ge p–i–n photodetector (North Coast EO-817L). The samples were mounted on a cold finger in a temperature variable helium-flow cryostat. The excitation was provided by a multi-line cw argon laser (488–514 nm) focused to a sample area of approximately 2 mm^2, with pump intensities between 0.3 and 5 W cm^{-2}. Data collection, and lock-in amplification were controlled by a desktop computer.

3. Results and discussion

To the best of our knowledge, we know of only two other reports of PL from $Si_{1-x}C_x$ alloys. Boucaud et al. [9] reported PL from a $Si_{1-x}C_x$ bulk alloy layer grown by RTCVD which consisted of a deep level luminescence and was attributed to defects. Recently, Brunner et al. [19] reported near band edge luminescence from pseudomorphic $Si_{1-x}C_x$/Si multiple quantum well structures. Our PL measurements of bulk $Si_{1-x}C_x$ reveal both band edge luminescence and deep level luminescence.

Low temperature PL spectra at 5 K for the $Si_{0.985}C_{0.015}$ bulk alloy sample is presented in Fig. 1. The luminescence consists of an intense deep-level luminescence and two edge peaks. The most intense peak at 1.0599 eV is ascribed to a no-phonon (NP) transition whereas the second peak at 1.0019 eV is red-shifted by about 58 meV and corresponds to its transverse optic (TO) Si–Si phonon replica. The NP transition is shifted 93 meV below that observed in pure Si [20], and is additionally shifted about 159 meV below an expected 1.2182 eV luminescence position using Vegard's Law for a $Si_{1-x}C_x$ alloy composition with 1.5% C. We attribute this red shift to both the lattice distortion within the alloy due to highly localized strain around the carbon atoms, and residual strain between the pseudomorphic alloy layer and the substrate. The lowering of the bandgap due to the pseudomorphic strain

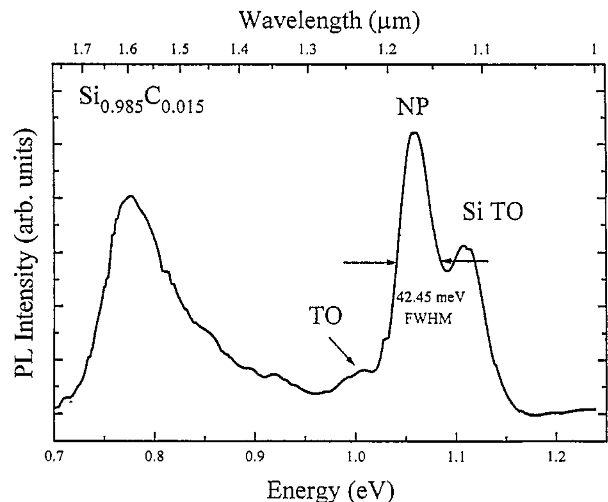

Fig. 1. PL spectra at 5 K of a 1500 Å $Si_{0.985}C_{0.015}$ alloy layer grown by MBE on (100) silicon substrate showing band-edge (NP) and deep level luminescence.

energy in the layer is not enough to explain the large red shift alone. The observed luminescence peak at 1.1089 eV is attributed to a Si TO phonon transition within the Si substrate. Also, an intense deep-level broad band luminescence is observed around 0.7776 eV. Similar deep-level broad band luminescence has been observed in $Si_{1-x}Ge_x$ [21], $Si_{1-x-y}Ge_xC_y$ [7], $Si_{1-x}C_x$ [9], and $Ge_{1-x}C_x$ [23] layers grown by MBE, and were attributed to localized excitons in a strain field created by Ge platelets [21], the emission of deep pseudo-acceptors [22], or to carbon–oxygen complexes [9,23], respectively.

Temperature dependence of the PL spectra was also measured. The luminescence of the deep level peak persisted up to 250 K but was degraded in intensity, while the luminescence of the high-energy PL peaks persisted up to room temperature. As the temperature was increased, the PL intensity decreased, the peak position shifted linearly to higher energy, and the linewidth broadened in the direction of higher energy. This type of linewidth behavior is characteristic of the Maxwell–Boltzman distribution. The laser power dependence of the band-edge luminescence at 5 K show a linear increase in PL intensity with increasing excitation. Linear power dependence is a characteristic of a no-phonon free-exciton recombination. The deep-level band exhibited an almost linear increase in intensity with increasing laser power at low excitation levels, but as the power was increased to higher excitation levels, the luminescence saturates and a sub-linear almost square-root dependence is observed. This is indicative that a recombination center may be involved in the recombination process, and similar deep-level luminescence have previously been attributed to carbon–oxygen complexes [9,23].

4. Conclusions

In conclusion, we have reported low temperature photoluminescence of a pseudomorphic tensially strained

$Si_{0.985}C_{0.015}$ alloy layer grown by solid source MBE. Two general features have been observed, a deep-level broad band luminescence and a band-edge luminescence consisting of a NP and TO replica. Temperature dependent PL analysis of the band-edge feature indicated an exponential temperature dependence, characteristic of free excitonic recombination. The band-edge feature exhibited a linear power dependence with increasing laser excitation. The high-energy PL peaks persisted up to room temperature while the deep level peak persisted up to about 250 K but was severely degraded in intensity. The red-shift of the energy gap was attributed to lattice distortion within the alloy and residual strain between the alloy layer and the substrate.

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