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Luminescence in Strained $Si_{1-x}Ge_x/Si$ Quantum Wells

S.Fukatsu , N.Usami, and Y.Shiraki
Research Center for Advanced Science and Technology (RCAST),
The University of Tokyo,
4-6-1 Komaba, Meguro-ku, Tokyo 153, Japan

We present an overview of luminescence studies conducted so far by the authors on strained $Si_{1-x}Ge_x/Si$ quantum wells (QWs) and their families grown by solid source and gas source molecular beam epitaxy (MBE). Focus will be placed on, first of all, the growth criterion based on a general finding that the luminescence efficiency depends critically on the epitaxy temperature. Next, general properties of QW luminescence and structural characterization using exciton luminescence is described, paying closer attention to interfacial transience. Application-oriented aspects will be discussed, including modulated structures such as coupled wells, superlattices, and some other interesting topics like room temperature luminescence and electroluminescence.

In this article, several topics regarding strained $Si_{1-x}Ge_x/Si$ quantum wells (QWs) are presented, including molecular epitaxial growth, consisting of a single QW (SQW) and multiple QW (MQW), photoluminescence (PL) and electroluminescence (EL), potential modulated structures, and room temperature luminescence.

1. Growth of strained Si1-xGex/Si QWs

1-1.Growth temperature and PL intensity

Practical criterion of QWs growth was found during the course of study on growth kinetics by gas source MBE. The general trend commonly observed in solid source and gas source MBEs is that PL intensity critically depends on growth temperature (Ts) and PL is effectively quenched below a threshold temperature, Tth. Note, Tth is much higher than those had been conventionally used for strained layers growth in view of strain relief. For Ts>Tth PL intensity of QW was well in excess of Si PL whereas Ts≈Tth, Si luminescence was dominant. Such a trend has been understood in the context of crystal quality, and cross correlated with post-growth annealing experiments. Dramatic recovery of PL intensity was observed for higher anneal temperatures (Ta) in QWs grown at lower Ts, Ts<Ta. This was found to agree well with sharp electron diffraction patterns observed for Ts>Tth. Hence, we can predict that surface adatom kinetics is fully equilibrated. Meanwhile, excitation spectra showed dramatic reduction of nonradiative channels, or carrier killers, as revealed in terms of smaller power exponent observed for higher Ts and Ta in common. Tth was found to be slightly dependent on crystal orientations. For example, Tth=620°C was found for solid source MBE. Surprisingly, no marked signature of strain relief was observed in PL spectra for QWs and SLS for x<0.35. Ts was able to be further extended beyond 850°C, where band edge PL was intense.

1-2. Ge rich quantum wells

In terms of quantum confinement shown below, a larger x is preferred since valence band discontinuity increases linearly with x. Ge rich quantum wells growth, however, appears to be a real challenge from the viewpoint of strain relief so far as we use a higher Ts addressed above. However, we have already demonstrated successful growth of Ge rich QWs with x in excess of 0.6 for Ts>800°C exhibiting clearly phonon-resolved PLs. With increasing Ge content, qualitative change in the actual band lineup is expected to occur for QWs grown on Si(100) due to anticrossover of conduction band edge between the well and the Si barrier. Although this has remained rather theoretical but still hypothetical, we did observe such a change in PL that seems to provide an evidence for type-I to type-II transition.

2. Properties of $Si/Si_{1-x}Ge_x$ QW luminescence

2-1. PL

Quantum confined excitonic PL peak shift have been reported by several authors in $Si/Si_{1-x}Ge_x$ QW systems. We have demonstrated the quantum confinement for QWs grown on Si(100), (110), and (111). Note, conduction band discontinuity in QWs is of type-I whereas on Si(111) it increases monotonically with x, i.e., type-II band lineup (staggered). Confinement barrier is expected to prevent carrier loss, which should manifest itself as thermal activation of PL intensity variation with temperature. The valence band discontinuity was found to essentially dictate the quantum confinement, namely due to holes.

Carrier generation and transport in PL an EL in strained $Si/Si_{1-x}Ge_x$ QWs presents an interesting aspect reflecting its optically indirect nature. Optical absorption length of visible excitation source in PL being rather small, $\approx 10^3 cm^{-1}$, excitation density is orders of magnitude lower than in EL. An extended carrier profile in PL configuration gives rise to dramatic change in carrier collection density in MQWs of different wells depending on the actual arrangement. Accordingly, the first-grown QW is greater in intensity when QWs are set closer to the surface compared to optical penetration depth. Time resolved PL experiments revealed systematic variation of with the location of first grown QW compared to the surface side QW whose location is fixed. Steady state luminescence was in agreement with such observations.

2-2. EL

Electroluminescence is definitely of primary importance for device applications. We have demonstrated EL of QWs grown on various substrates, showing quantum confinement shift in the interband transition rather than excitonic transitions. It is obvious that solid source MBE is superior to gas source MBE in terms of doping controllability and its variation. We developed a novel recipe of doping gas source grown QWs suing solid source MBE by sample transfer through the air, referred to as "hybrid" epitaxy. Exploiting advantages of both MBEs, we reported excellent EL spectra of sharper linewidth and under extremely low excitation density with well-resolved acoustic phonon assisted transition peak which has not been reported in the past. EL from QW with x=0.35 was successfully observed at 60°C, the highest operation temperature of SiGe-based light emitting diode.

3. Interface transience

Heterointerfacial transience in strained $Si/Si_{1-x}Ge_x$ as well as Si/Ge has been a major focus of interest in recent years., since its is obvious that compositional distribution modulates the resultant band structure. Interface mixing would be a serious problem in some extreme cases like monolayer superlattices in which band-gap nature is expected to be converted to what is often referred to as "direct" as a consequence of zone folding.Surface segregation of Ge has been addressed by several groups to be notorious representative giving rise to such intermixing of interface. Copel et al. and Fukatsu et al. developed a recipe to inhibit Ge segregation during growth using dopant adlayers, referred to as surfactant mediated growth or segregant-assisted growth (SAG).

Recently, we performed the first interface characterization using excitonic PL as an angstrom-sensitive probe. PL peak energies were consistently higher than those predicted form a theoretical calculation assuming standard square potential. Such a peak shift was found to be accounted for when we take Ge segregation into account in the calculation. We further demonstrated that application of SAG brings an abrupt potential profile effectively inhibiting Ge segregation.

In contrast, potential profile of QWs grown by gas source MBE in the adsorption/dissociation limited domain was found to be rectangular, i.e. Ge segregation was apparently absent. Segregation-driven peak shift was totally absent. Such compositional abruptness seems to be inherent to gas source growth including other growth schemes, like chemical vapor deposition.

4. Modulated structures

Potential profile modulation which we can introduce artificially by proper arrangement of heterostructures and by appropriate design of doping profiles generally gives rise to substantial change in the electronic and optical properties. Apart from this, nano-fabrication is known to bring substantial change in the optical spectra, as represented by geometries of reduced dimension like quantum dots and wires.

4-1. Coupled wells

Coupled quantum well (CQW), i.e. QWs with thin barrier(s) in between, has emerged as a new class of QW family, whose electronic state is dictated by interwell tunneling of carriers across the intervening barrier. CQW is referred to as symmetric (S) when the wells are identical and asymmetric (A) when the wells are different. Systematic red shift has been observed by the authors upon reduction of Si barrier width in $Si/Si_{1-x}Ge_x$ SCDQWs. In ACDQW, PL profiles were found to be controlled by interwell tunneling. Tunneling time across a Si barrier could be obtained from barrier width dependence of relative intensity profiles of DQW PL, to be of the order of 0.1μsec, obviously competing with radiative recombination rate inside the narrower well. Sequential tunneling was observed in multiply connected QWs with thin tunnel barriers, where only PL of the widest well was observed.

4-2. Superlattices

A superlattice results as repeated extension of CQWs and the associated electronic states are folded together into a miniband. So far, we have observed clearly the evolution of a superlattice state in PL by systematically increasing the number of wells in SCQWs in agreement with Kronig-Penney type calculation. Superlattice state variation was observed in wider range of structures with varying single period length, composition, and Si to SiGe length ratio even for ultrathin superlattices. All of them turned out to be in fair agreement with K-P calculation, showing the validity of envelope function approach within effective mass approximation in this superlattice system. Exciton localization was identified in superlattice, unlike in SQWs, presumably related to potential fluctuation in the growth direction Electroluminescence was also observed in superlattices with a higher survival temperature compared to SQW.

4-3. Interdiffusion

Interdiffusion at heterointerfaces is an important issue to be addressed when we discuss structural integrity. Once diffusion sets in, potential profile is modulated, leading to significant peak blue shift in PL. We evaluated the interdiffusivity around its onset from PL peak shift in SQWs undergoing post-growth anneals. The activation energy was found to be in between what have been reported previously by others.

4-3. Size quantization in nano-structures

Artificially controlled nano-structures with reduced dimension has attracted much attention recently in particular among compound semiconductors. We have demonstrated quantum wire fabrication using gas source MBE on groove-patterned substrates. Considerable peak shift was observed in PL spectra which could be attributed to dimensional reduction.

5. Room temperature luminescence

5.1. EL

As is already shown, valence band discontinuity increases with x independent of substrate orientation. First demonstration of room temperature luminescence was done by Mi et al. in a rather Ge-rich, x=0.35, type-I MQWs of 5 period grown on Si(100). Subsequently, we demonstrated 60°C operation of light emitting diode for a rather challenging system with type-II band lineup of a B-doped type-II MQWs with x=0.35 grown on Si(111). This was extended to other substrate orientations and SQWs. Note, however, in SQWs, Si substrate EL was dominating with a small contribution of QW in contrast with MQW EL.

5.2. PL

Since the excitation density is orders of magnitude different between EL and PL where Si substrate is selectively excited due to finite well width. To obtain QW PL at room temperature, carrier injection efficiency or external quantum efficiency should be optimized by structural modification. Taking into the actual spatial extension of carrier profile dictated by optical penetration depth of incident excitation light, we modified QW arrangement so that the photogenerated carrier will be trapped by QWs most effectively. As a result, we could observe PL due to QWs well surmounting Si PL at room temperature. Quantum confinement was confirmed by spectral shift as in low temperature PL.

Conclusions

We have presented a systematic overview of what we have done in recent years on strained $Si_{1-x}Ge_x/Si$ QWs, though qualitatively stated. We are now extending the research program further toward realizing actual optical element fabrication.

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