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Influence of defects and interface on radiative transition of Ge

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The influences of defects and surface roughness on the indirect bandgap radiative transition of Ge were studied. Bulk Ge has 15 times the integrated intensity of photoluminescence of Ge-on-Si. However, for Ge-on-Si sample, the direct transition related photoluminescence intensity is higher than the indirect transition related one. We affirm that the defects in the Ge-on-Si are responsible for the weak indirect transition and relatively strong direct transition. The scattering of electrons by roughness at Ge/oxide interface can provide extra momentum of the indirect band transition of Ge, and thus enhance the indirect radiative transition. © *2011 American Institute of Physics*. [doi:10.1063/1.3571439]

The optical properties of Ge are of great interest due to the high carrier mobility, strong photon absorption, and possible integration with Si. The direct conduction valley of Ge is only 140 meV above the indirect valleys, and the enhancement of direct transition is possible by increasing the electron population in the direct valley. The approaches to enhance the direct band gap transition reported recently were high electron doping concentration,[1,2] high pumping level,[3] increasing temperature, and tensile strain in Ge.[3,4] Moreover, the direct transition from the electroluminescence (EL) of Ge pn junction was also observed.[5] In this letter, the influence of defects on indirect radiative transition of Ge is studied by comparing bulk Ge and Ge grown on Si samples. The interface roughness scattering is also studied by comparing a Ge metal-insulator-semiconductor (MIS) light-emitting-diode (LED) and an n^+p junction LED.

The Ge-on-Si sample is fabricated by reduced pressure chemical vapor deposition system. A two-step deposition was processed. At the first step, a Ge seed layer was grown on Si at 300 °C in N_2-GeH_4 mixed ambient to form two-dimensional Ge seed layer. The relaxed Ge film was then grown at 550 °C in H_2-GeH_4 mixed ambient. The 550 °C growth temperature is used for accelerating the growth rate of Ge film. In order to improve crystallinity of the Ge layer, several cycles of annealing steps were introduced during the Ge layer deposition process by interrupting the Ge layer growth.[6] The thickness of the relaxed Ge layer is ~2.8 μm with estimated threading dislocation density of $\sim 3.7 \times 10^6$ cm^{-2} observed by optical microscope after Secco etching (Fig. 1).

A (100) p-type Ge wafer with the thickness of 500 μm is used to fabricate the n^+p junction device. The Ga-doped Ge substrate has the resistivity of 1–10 Ω cm and the emitter was formed by implanted phosphorous. The implant dose and implant energy were 1×10^{15} cm^{-2} and 60 keV, respectively. The rapid thermal anneal was performed at 700 °C for 60 s for dopant activation. The junction depth of n^+ region is about 0.8 μm measured by secondary ion mass spectrometry (SIMS).

For the MIS structure fabrication, a 50 °C liquid phase deposition (LPD) was used to form ~2 nm thick gate oxide on p-type Ge.[7] Subsequently, a thin Al film (10 nm) was evaporated on the SiO_2 in a circular area with radius of ~1.2 mm to form a gate electrode. After etching SiO_2 on the backside of the Ge wafer, 100 nm Al was evaporated on the rear surface to form an ohmic contact. Moreover, 2 nm thick Al_2O_3 is also used as gate dielectric to form another MIS structure on an n-type Ge substrate by atomic layer deposition. The Al was evaporated as a gate electrode.

The room-temperature photoluminescence (PL) spectra of the bulk n-type Ge substrate and Ge-on-Si sample are shown in Fig. 2. The laser excitation wavelength is 671 nm and the power density is 360 mW/mm^2. The PL peaks at 695 meV and 780 meV are attributed to the indirect band transition and direct band transition, respectively. The spectra of the indirect and direct band gap emission in both bulk n-Ge and Ge-on-Si sample were fitted by using the electron-

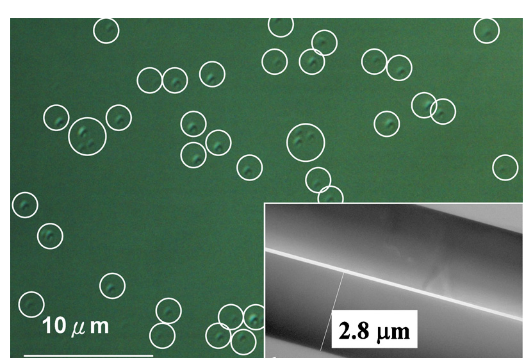

FIG. 1. (Color online) The optical microscope image of Ge-on-Si after Secco etching. The threading dislocation density is $\sim 3.7\times10^6$ cm^{-2}. The defects are marked with circles. The inset is the TEM image of Ge-on-Si.

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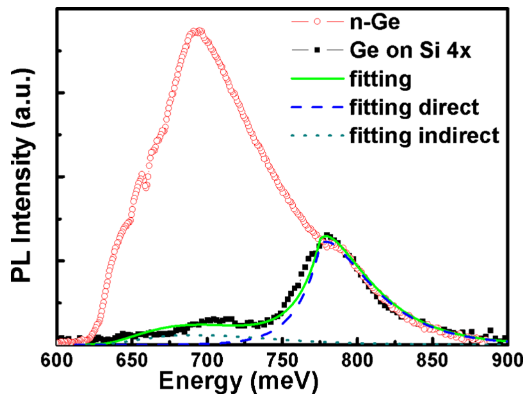

FIG. 2. (Color online) The PL spectra of the bulk Ge and Ge-on-Si at room temperature. The integrated PL intensity ratios of the direct to indirect band gap transition of the bulk n-Ge and Ge-on-Si sample are 0.05 and 2.5, respectively. The bulk Ge is ∼15 times the integrated intensity of PL of the Ge-on-Si sample.

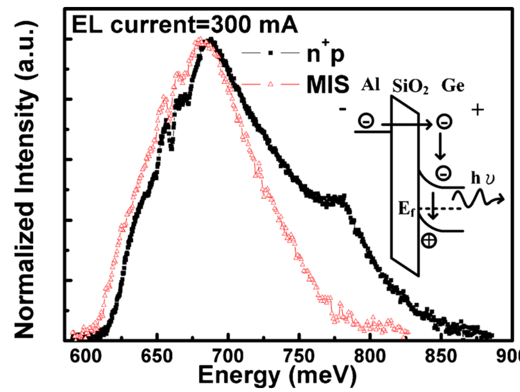

FIG. 4. (Color online) The EL spectra of the n^+p Ge and Ge MIS LEDs at an injection current of 300 mA at room temperature. The roughness scattering conserves the momentum and increases the indirect radiative transition. The inset is the schematic band diagram of the light emission process of the MIS LED.

hole plasma recombination model[8,9] and the direct band gap recombination model,[10] respectively. The band tail of absorption edge model is also taken into consideration in the direct band gap recombination mode.[5] To avoid the intensity enhancement due to highly doped n-type Ge,[10] both bulk n-type Ge and Ge-on-Si had low dopant concentrations. The bulk Ge is Sb-doped with an electron concentration of $\sim 1 \times 10^{15}\ \mathrm{cm}^{-3}$. The epi Ge was grown on boron-doped Si substrate with the resistivity of $5-22\ \Omega$ cm. The n-type epi Ge was unintentionally doped with residual As concentration less than SIMS limit of $1 \times 10^{17}\ \mathrm{cm}^{-3}$. The integrated PL intensity ratios of direct to indirect band gap transition for the bulk n-Ge and Ge-on-Si sample are 0.05 and 2.5, respectively.

The bulk Ge is ∼15 times the integrated intensity of PL of the Ge-on-Si sample indicating that more defects[11,12] in the Ge-on-Si sample increase the nonradiative recombination rate due to Shockley–Read–Hall recombination.[13] Figure 3 shows the models of the indirect band transition in the (a) ideal bulk Ge (without defects) and (b) Ge-on-Si (with defects). For the indirect radiative recombination in bulk Ge, a dominant LA phonon (∼28 meV) is involved to satisfy the momentum conservation between the L valleys and the zone center in the valance band.[14] However, in the Ge-on-Si sample, the large defect density in the Ge film may lead to a spread of trap levels in momentum space. These trap levels enhance the nonradiative recombination rate because the

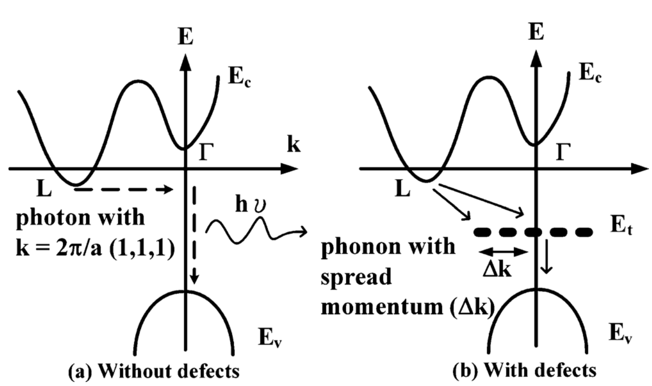

FIG. 3. The schematic band diagram of the Ge (a) without defects and (b) with defects. The large defect density leads to trap levels broadened in momentum space.

more phonons with different momentum can be involved in the momentum conservation [Fig. 3(b)]. Thus, the relative intensity of the indirect band gap transition is lower in the Ge-on-Si sample than in the bulk Ge.

Figure 4 shows the EL infrared emission from a Ge MIS structure with LPD oxide and a Ge n^+p diode at an injection current of 300 mA at room temperature. The EL spectrum of the n^+p diode has two peaks at 688 meV and 780 meV, corresponding to the indirect band gap transition and the direct band gap transition, respectively. However, only the indirect band gap emission is observed in the EL spectrum of the MIS structure. This difference between the two EL spectra is due to the different light emission mechanisms in the MIS and n^+p structures.

For the Ge n^+p structure at the forward bias, the electrons were injected from n^+-Ge to p-Ge, and recombine with the holes at the neutral region of p-Ge substrate. Thus, the radiative recombination occurs deeply away from the Ge surface. For the MIS structure at the negative gate bias, the holes are attracted at the Ge/SiO_2 interface to form an accumulation layer (the inset of Fig. 4). The electrons in the Al gate electrode tunnel through SiO_2 layer and recombine with the holes in accumulation layer.[9] The EL spectra are normalized to unity (Fig. 4). The integrated EL intensity of the MIS diode is ∼7% of that of n^+p diode in our measurement probably because the holes in the Ge injected to the metal electrode cannot cause EL. Moreover, the roughness scattering at Ge/SiO_2 interface can provide the extra momentum in the indirect recombination[15,16] and can significantly enhance the indirect transition rate. The recombination from the direct and indirect band gap transitions is competitive with each other under thermal equilibrium. Therefore, the influence of surface roughness scattering strengthens the indirect radiative transition in MIS, making the direct transition embedded in the indirect one and not observable in Fig. 4.

The influence of roughness scattering was also observed in the Al_2O_3 MIS structure. Figure 5 shows the room temperature PL and EL spectra of the Al_2O_3 device. In the PL spectrum, both the indirect and the direct band transition can be observed. The integrated PL intensity ratio of direct to indirect band transition is ∼8%, while no apparent direct transition was observed in the EL for the Al_2O_3 MIS device. The PL light emission caused by optical pumping is far away

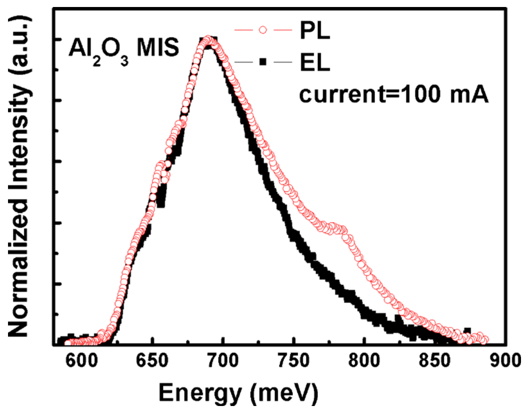

FIG. 5. (Color online) The PL and EL spectra of Al_2O_3 MIS LED at room temperature. There is no direct band transition observed in the EL spectra.

from Al_2O_3/Ge interface. Therefore, the influence of surface roughness is not significant in PL spectrum.

In summary, the direct to indirect transition ratio of the n^+p junction structure is stronger as compared with that of MIS structure. Indirect radiative transition can be enhanced by roughness scattering but be degraded with increasing defect density.

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