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Direct evidence of free-carrier induced band-gap narrowing in Ge

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Abstract

We demonstrate free carrier-induced band-gap narrowing in Ge for the first time. Photoluminescence (PL) measurement was carried out on ultra-thin GeOI FETs, in which the carrier density was intentionally controlled by the gate bias. An intuitive model of the free carrier induced band gap narrowing is proposed from the viewpoint of the covalent bonding weakened by free carriers in Ge.

1. Introduction

It is well known that heavily doped semiconductors show the band gap narrowing (BGN). In fact, an empirical model for device modeling in bipolar transistor performance has been proposed and utilized in simulation [1]. Experimentally, the BGN has been reported in both p-type and n-type heavily-doped Si and Ge [2-4], while theoretically, many models considering electron-electron or electron-phonon interactions have been also proposed [5]. However, since it is hard to experimentally distinguish effects of dopant atoms from those of free carriers in heavily-doped semiconductors, no experimental evidence for distinguishing between them have been reported to our knowledge. On the other hand, it is reported that FETs on heavily doped SOI or GeOI work well as junction-less FETs [6, 7], in which free carriers can be fully depleted by applying the gate bias.

Based on above background, the objective of this work is to experimentally distinguish the free carrier effect on BGN from the dopant atom one in Ge, using FETs on GeOI.

2. Experimental

Both lightly (~1x10^{15} /cm^3) and heavily doped (~1x10^{19} /cm^3) p-type thin GeOI wafers were used. The device structure is schematically shown in **Fig. 1**. This is basically the back-gated GeOI MOSFET, in which the carrier density can be controlled by the back gate (Si substrate). The top surface of Ge was covered with Y_2O_3 to minimize the interface defects [8]. The device fabrication process was described elsewhere [7]. To estimate the band gap of Ge, PL measurement was performed with the second harmonic of Nd:YVO_4 laser (λ=457 nm, 4 mW) at room temperature. The key point in this measurement is that gate bias was applied during the PL measurement. In this work, the direct band gap was characterized instead of the indirect one, because the direct transition PL is sensitive to the electronic structure thanks to the fast recombination rate.

3. Results and Discussion

Fig. 2 shows the back-gate voltage dependences of the PL peak energy and the drain current in 11-nm-thick lightly doped p-type GeOI . Here, the PL and I-V measurements were individually carried out, to avoid the temperature increase during PL measurement due to Joule heat generated by the drain current. Since the penetration depth of the excitation laser into GeOI was around 17 nm [9], the whole Ge film was considered to be characterized. As shown in Fig. 2, the red-shift of PL peak is clearly observed in the on-state of p-FET. Namely, the direct band gap becomes narrow by the hole accumulation. To our knowledge, this is the first and direct evidence of the free carrier effect on BGN. This fact has been definitely ignored in the conventional FET device modeling.

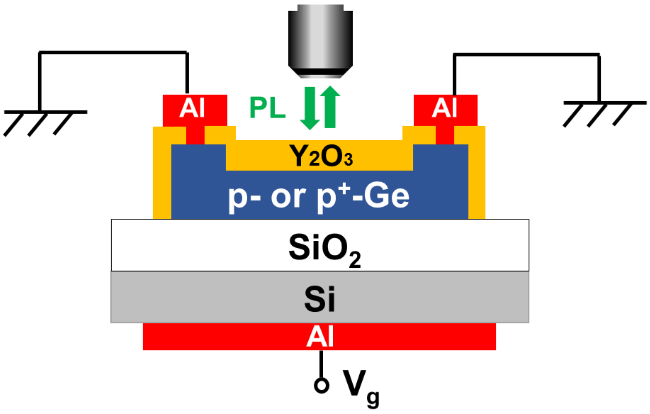

Fig. 1 The schematic image of the PL measurement with applying the back-gate bias. Only the free carrier density can be controlled during PL measurement, while the dopant atom density is constant.

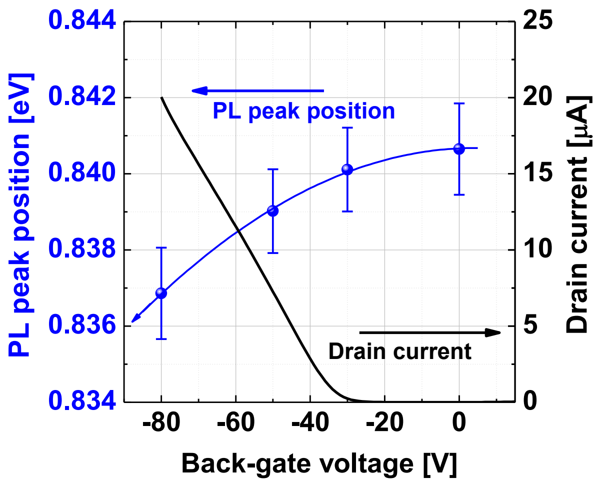

Fig. 2 The back-gate voltage dependences of the PL peak position and the drain current in 11-nm-thick lightly-doped p-type GeOI. The PL and I-V measurement were individually carried out, to avoid the temperature increase during PL measurement due to Joule heat.

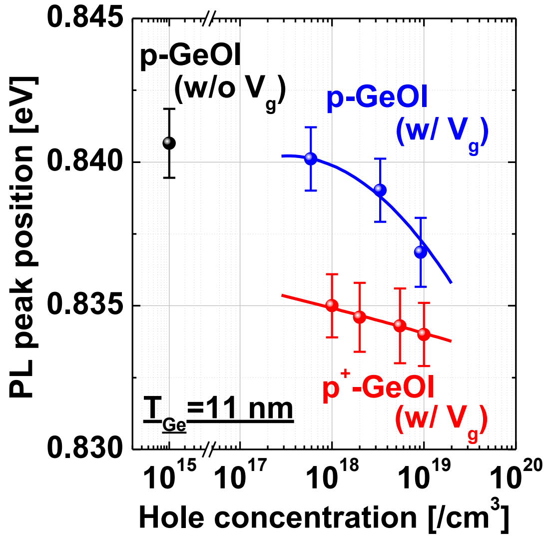

Fig. 3 The PL peak position of 11-nm-thick lightly- and heavily-doped p-type GeOI as a function of hole concentration, which was estimated by using eq. (1).

The free carrier effect on the direct band gap was also investigated in heavily-doped p-type GeOI. The results are shown in **Fig. 3**, in addition to lightly doped case. Here, the hole concentration (p) (cm^{-3}) was estimated from the transfer characteristics as follows.

$$p = \frac{C_{OX}\left(V_g - V_{th}\right)}{qT_{Ge}} \qquad (1)$$

C_{OX}, V_{th} and T_{Ge} are the oxide capacitance, the threshold voltage in FET and Ge thickness, respectively. Although the BGN was observed by hole accumulation in heavily-doped GeOI as well, the band gap of heavily-doped Ge seems to be narrower than that of lightly-doped one in the wide range of hole concentration. Therefore, it is inferred that the BGN in Ge is caused not only by the free carriers but also by the dopant atoms, although further quantitative study is needed. If it is the case, the impurity band formation and/or the random potential by impurities [5] should be taken into account together with the free carrier effect. This is now under investigation. In any case, it is definitely concluded that even only free carriers can modulate the energy band-gap of Ge.

To intuitively interpret free carrier effects on the BGN, we propose a model from the viewpoint of a modification of the covalent bonding by free carriers, as schematically shown in **Fig. 4**. Suppose the simple covalent bonding of two atoms with sp3 hybridized orbital in Ge. When an additional carrier is added in this system, there is still an energy gain in the covalent bonding. It is noted here that additional carriers are substantially quite small compared to actual number of bonding in Ge (in Fig. 4, an added hole is exaggerated very much). However, the hybridization gain should be decreased, because the overlap integral of the sp3 orbitals, which determines the energy gain by the covalent bond formation [10], can be altered by the additional carriers. In fact, since free carriers are 10^{-4}~10^{-6} of Ge atoms, we think it is more appropriate to describe the high carrier density region as the weakened covalent bonding system. Furthermore, we have already reported that the phonon softening (PS) by increasing free carriers in Ge [11]. The present model can explain both BGN and PS, simultaneously. Note that the present consideration will be more important in nano-scale devices, because the atomic nature will become more dominant.

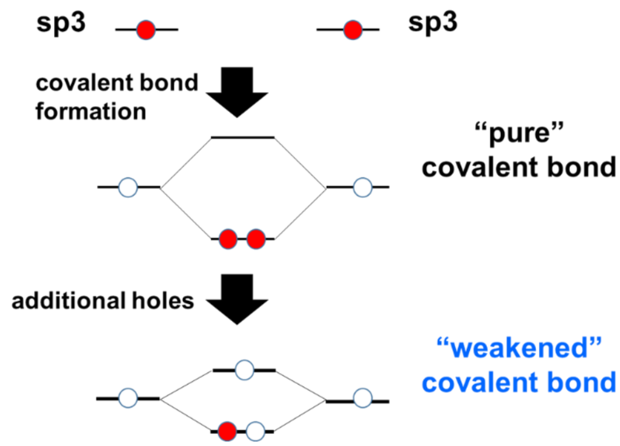

Fig. 4 . The schematic image of the energy level before and after the covalent bond formation in Ge, with low and high hole concentration. The hybridization energy gain should be altered by additional free carrier, resulting in the free carrier effect on BGN.

4. Conclusion

The free carrier effect on the BGN was experimentally demonstrated at a fixed dopant concentration for the first time. The carrier–induced BGN was observed in both lightly and heavily doped Ge. This effect is explainable by considering the model that the covalency in crystalline Ge is weakened by free carriers. Furthermore, the present consideration will be more important in the nano-scale FET such as Ge Fin-FET or ET-GeOI FET.

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