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Bandgap Control Using Strained Beam Structures for Si-Based Photonic Devices

Kohei Yoshimoto[1,2], Ryota Suzuki[1], Yasuhiko Ishikawa[1] and Kazumi Wada[1]

[1]Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo
7-3-1 Hongo, Bunkyo, Tokyo 113-8656, Japan
Phone: +81-3-5841-7141 E-mail: kwada@material.t.u-tokyo.ac.jp
[2]Institute of Industrial Science, The University of Tokyo
4-6-1 Komaba, Meguro, Tokyo 153-8505, Japan

1. Introduction

Lattice strain induces the changes in band edge/gap energies for semiconductors, being effective for high-performance photonic and electronic devices. Pseudomorphic heteroepitaxy is widely used to generate the strain, whose amount is determined by the mismatch of lattice constant between the heterolayer and the substrate. The mismatch of thermal expansion coefficient also induces the stain. The strain due to these mechanisms is generally below ~1%, while a larger strain is recently required to further improve the properties of Si-based materials such as high-mobility strained Si [1] and tensile-strained Ge [2], which is theoretically anticipated to be a direct bandgap material [3]. In order to induce a strain as large as several %, we have proposed the use of micro-beam structures [4]. The concept is to elastically deform the beam structure by externally applying a mechanical stress, inducing a bending strain as large as several %. The strain should be tunable depending on the applied stress, which cannot be realized in the previous methods. The beam structure should be applicable to Si and related materials such as Ge, which are formed on the beam structure of Si as an overlayer.

In this work, strain and bandgap energy for a Si micro-beam structure are theoretically investigated, and the bandgap change is experimentally studied using micro-photoluminescence (μ-PL) spectroscopy. As the proof of concept, it is experimentally shown that the application of mechanical stress to a Si beam leads to a large red shift (~200 nm) in the PL peak position, indicating a narrowing of bandgap due to the strain as large as 1.5%.

2. Uniaxial strain in mechanically stressed beam structure fabricated from Si-on-insulator (SOI)

The theoretical fracture stress for Si is more than 20 GPa [5], although the actual fracture stress is strongly dependent on the sample size and the crystalline quality. Namazu et al. reported that the fracture stress for submicron Si beams (17.5 GPa) is almost 40 times larger than that for millimeter-sized samples [6], and Alan et al. [7] achieved a higher stress of 18.2 GPa. These reports suggest that the micro-beam structure is promising to induce a strain as large as several %.

The strain distribution was theoretically examined using a finite element analysis for a simple straight beam structure of (001) Si in the [100] direction, which is fixed to a wide Si slab. Such a structure can be fabricated using a Si-on-insulator (SOI) wafer, as shown later.

Figure 1 shows a typical distribution of strain for a beam structure with the width of 5 μm, the length of 10 μm and the thickness of 1 μm. An external force is vertically applied to bend the beam by 3 μm at the edge. It is found that a large strain is generated near the opposite side of beam edge fixed to the slab. The maximum tensile strain of 2.1% is seen at the surface near the corners. A slightly smaller tensile strain of 1.8% is also seen at the center. Note that the compressive stain is generated on the backside with almost the same amount. A larger strain should be generated by increasing the bending.

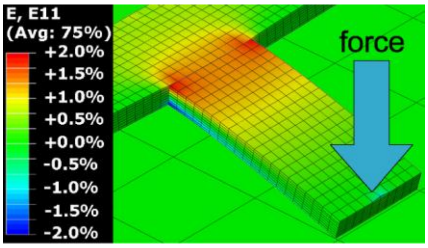

Fig. 1. A typical strain distribution for a Si micro-beam structure.

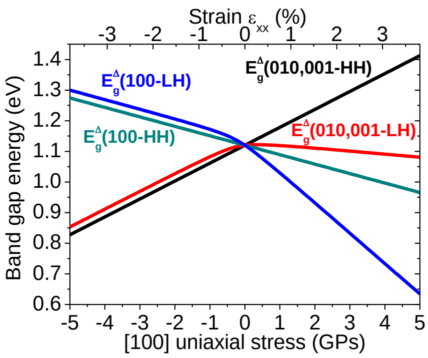

Fig. 2. Bandgap energies calculated for Si under [100] uniaxial stress.

A theoretical calculation was also performed on the strain-induced change in the bandgap energy for Si. The calculation was carried out for the [100] uniaxial stress using the deformation potentials reported in Ref. [8]. A splitting occurs for both of the conduction and valence bands. Under the compressive (tensile) stress in the [100] direction, the conduction band minima at the Δ points in the [±100] directions are higher (lower) in energy than those in the [0±10] and [00±1] directions, while the heavy-hole

(HH) valence band maximum is higher (lower) in energy than the light-hole (LH) valence band maximum.

Figure 2 shows indirect bandgap energies for Si under the [100] uniaxial stress. A bandgap narrowing occurs for both of the compressive and tensile stresses. This means that, independent of the location in the depth direction, the bandgap is reduced under a mechanical stress in Fig. 1. The largest narrowing is as large as 0.2 eV under a uniaxial stress of 2 GPa, corresponding to the strain more than 1%.

3. Experimental procedure

As the starting substrate, an SOI wafer was used with the top Si layer of 0.25 μm and the buried oxide (BOX) layer of 3 μm. Figure 3 shows the schematic illustration for the fabrication process. An electron-beam (EB) resist of ZEP520A was used. After the resist patterning using an EB lithography, the top Si layer was selectively etched with the resist masks using a reactive ion etching with Cl_2 and O_2 gases. In order to remove SiO_2 under the Si beams, the sample was dipped in a 1 HF (50wt%) : 1 H_2O solution for ~12min. By this wet etching, the SiO_2 layer under the Si beam was removed, forming a cantilever.

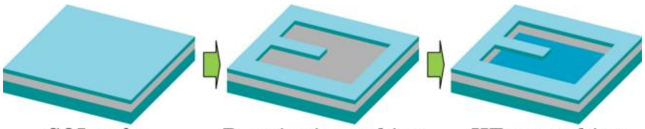

Fig. 3. Fabrication process of Si beams. Patterning of top Si layer and removal of BOX layer by HF were carried out.

In order to evaluate the bandgap energy for the fabricated Si micro-beams, μ-PL measurements were carried out. The size of measured beam is 3 μm in width, 15 μm in length and 0.25 μm in thickness. A microprobe needle was used to mechanically push the beam, or to provide an external stress, during the spectrum acquisition. An excitation laser with the wavelength of 457 nm and the power of ~ 4mW was used. It is noted that, due to the small spot size of ~1 μm, carriers are exited selectively near the edge of micro-beam fixed to the slab, where the large strain is induced.

4. Results and Discussion

Figure 4 shows typical μ-PL spectra obtained with and without the mechanical stress. In order to change the mechanical stress, three different points on the micro-beam were pushed. Several peaks were observed in each of the spectra due to the resonance in the beam along the width direction. It is more important that the spectrum is shifted towards lower photon energies by applying the stress. Taking into account that the amount of red shift increased with the applied stress, the red shift is ascribed to the bandgap narrowing induced by the bending of micro-beam structure. The amount of the shift is ~0.2 eV, corresponding to the uniaxial strain of 1.5%, according to Fig. 2. Therefore, the use of micro-beam structures is effective to induce a strain as large as several %.

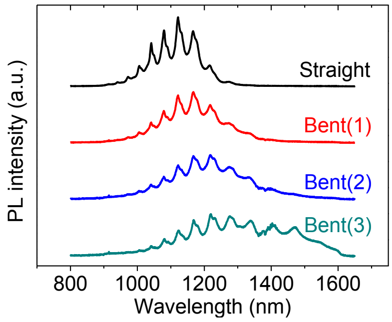

Fig. 4. Typical PL spectra from a Si micro-beam with and without external stresses. Straight and Bent(1)~(3) indicate spectrums of beam without being pushed and with different amount of strain respectively.

From the viewpoint of active photonic devices on Si, particularly light emitters, the beam structure should be applicable to other materials formed on Si. In the case of Ge on Si, a large tensile strain should lead to an indirect-direct transition in the band structure, as mentioned above. Since the direct bandgap is reduced to ~0.5 eV (λ ~ 2.5 μm) under ~2% biaxial tensile strain, mid-infrared light source is expected, which is useful for the detection of bio-molecules. GaAs on Si is expected to the near-infrared light source in the optical communication band (1.3 - 1.6 μm). The direct band gap is reduced from 1.42 eV to, e.g., 0.8 eV (λ = 1.55 μm) under 5% biaxial tensile strain. The results for Ge on Si and GaAs on Si will be presented near future.

5. Conclusions

Strain and bandgap energy for Si micro-beam structures were theoretically investigated, and the bandgap change was experimentally studied using μ-PL spectroscopy. It was experimentally shown that the application of mechanical stress to a Si beam leads to a large red shift (~200 nm) in the PL peak position, indicating that a narrowing of bandgap is realized due to the strain as large as 1.5%.

Acknowledgements

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