

Ge Self-Diffusion in Compressively Strained Ge Grown on Relaxed Si_{0.2}Ge_{0.8}

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1. Introduction

Recently, there has been an increased interest in the use of compressively strained germanium (s-Ge) in channel regions of p-type metal-oxide-semiconductor (MOS) field-effect-transistors because of their ability to enhance hole mobility. Compressively s-Ge is fabricated on relaxed silicon germanium (SiGe), which has a smaller lattice constant than that of Ge, and strain is controlled by varying the Ge content in the relaxed SiGe. A thorough understanding of Ge self-diffusion in s-Ge leads to clarify the properties of point defects and their associated dopant diffusion mechanisms, which is crucial for the technical innovation of s-Ge channel MOS devices. In recent years, there have been several interesting reports on Si and Ge self-diffusion in relaxed SiGe [1-3]. To the best of our knowledge, there is no report on self-diffusion in s-Ge. It is difficult to observe and quantitatively evaluate diffusion in s-Ge because the strain is easily relaxed during annealing. In order to maintain the strain, s-Ge needs to be a thin layer, where dislocation density is low. In this work, we successfully fabricated relaxed Si_{0.2}Ge_{0.8}/compressively s-Ge isotope superlattice (SL)/relaxed Si_{0.2}Ge_{0.8} heterostructures. Furthermore, we present the first measurements of Ge self-diffusion in compressively s-Ge.

2. Experiment

Figure 1 shows the schematic illustration of relaxed Si_{0.2}Ge_{0.8}(50nm) / s-GeSL(60nm) / relaxed Si_{0.2}Ge_{0.8}(50nm) heterostructures fabricated in this study. In order to smooth the sample surface and avoid contaminating the s-Ge layer, a 50-nm-thick Si_{0.2}Ge_{0.8} buffer layer was grown by molecular beam epitaxy on Si_{0.2}Ge_{0.8} virtual substrates, which in turn was grown by chemical vapor deposition. The GeSL, composed of alternating layers of isotopically enriched ⁷⁰Ge and natural Ge (^{nat}Ge), was grown on the buffer layer. Finally, a 50-nm-thick relaxed Si_{0.2}Ge_{0.8} cap layer was grown on the top as a stressor. The GeSL was sandwiched by two ^{nat}Ge (10nm) layers which act as barrier layers for Si interdiffusion into GeSL (40nm). These samples were annealed at temperatures between 475 and 600 °C for 0.5 – 61 h in a resistively heated furnace under a flow of 99.999 % pure Ar. The strains in the s-Ge were measured by X-ray diffraction (XRD). The depth profiles of ⁷⁴Ge in the heterostructures were measured by secondary ion mass spectroscopy (SIMS). Ge self-diffusivities in s-Ge were determined by using a partial differential equation

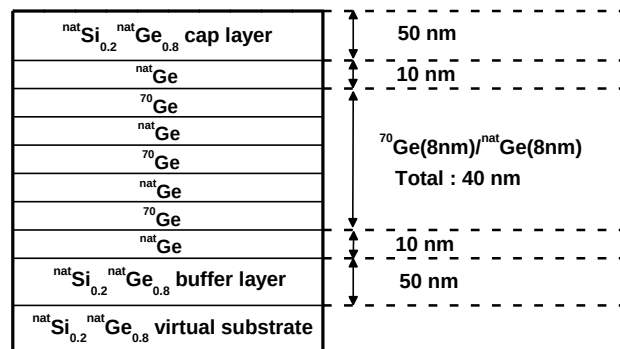


Fig. 1 Schematic illustration of relaxed Si_{0.2}Ge_{0.8}(50nm)/s-Ge isotope SL(60nm)/relaxed Si_{0.2}Ge_{0.8}(50nm) heterostructure.

solver ZOMBIE. By using cross-sectional transmission electron microscopy, we saw that the effects of strain relaxation due to the creation of dislocations are negligible.

3. Result and discussion

Figure 2 shows the intensity peaks of asymmetrical (224) reciprocal space mapping (RSM) before and after annealing at 550 °C for 6 h, where the Q_x corresponds to horizontal lattice constant. The Q_x of s-Ge agreed well with that of relaxed Si_{0.2}Ge_{0.8}, both before and after annealing. The strains in s-Ge calculated from these peak values were – 0.71%, which corresponds to an in-plane stress of – 0.96 GPa, in the sample before annealing with the minus sign for compressive strain, and – 0.66% after annealing. We obtained similar results of – 0.71 % after annealing at 550 °C for 1 h and – 0.66% for 3 h, respectively. These results show that the compressive biaxial strain of approximately – 0.7% was maintained during the annealing process. Figure 3 shows the depth profiles of ⁷⁴Ge in the heterostructures measured by SIMS before and after annealing at 550 °C for 1 – 6 h and the simulation results. The SIMS depth profiles were fitted using a single value of Ge self-diffusivity for each temperature. We obtained a Ge self-diffusivity value of 6.40×10⁻¹⁸ cm² at 550 °C under compressive strain of approximately – 0.7%. Figure 4 compares the temperature dependencies of Ge self-diffusivities in the strained and relaxed Ge obtained in this work, and the diffusivities in relaxed Ge previously reported in [4]. The values for relaxed Ge show an agreement with the previously reported values. However, we found that the Ge self-diffusivities in s-Ge were about 3.5 times larger than those in relaxed Ge at a diffusion

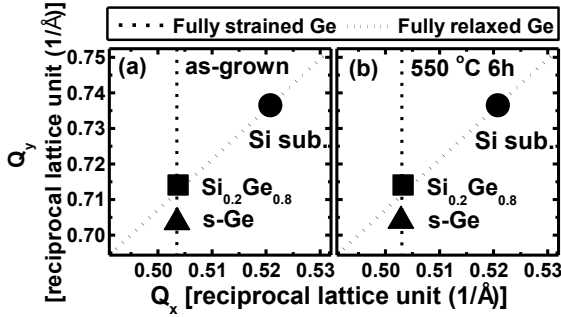


Fig. 2 Intensity peaks of asymmetrical (224) RSM (a) before and (b) after annealing at 550 °C for 6 h.

temperature within the range of 475 – 600 °C. The activation enthalpies of Ge self-diffusion were estimated to be 3.07 eV in s-Ge and 3.11 eV in relaxed Ge. It is known that Ge diffuses by a vacancy in relaxed Ge [4]. The closeness of the values indicates that Ge self-diffusion in compressively s-Ge also proceeds by the vacancy mechanism. Furthermore, we discuss the increase of the diffusivities in s-Ge in terms of the activation volume (V^{SD}) of self-diffusion.

$$V^{SD} = -kT \left(\frac{\partial \ln D}{\partial p} \right)_T, \quad (1)$$

where k is Boltzmann constant, T is absolute temperature and D is self-diffusivity at constant temperature [4,5]. V^{SD} can be either positive or negative, depending upon whether D decreases or increases with p , respectively. The activation volume characterizes the effect of pressure (p) on self-diffusivity and is an important property of the defects responsible for the diffusion. The activation enthalpy of self-diffusion under pressure changes by the work pV^{SD} of the system. In the case of the vacancy mechanism, V^{SD} is the volume change of the system upon the formation (V^F) and migration (V^M) of a vacancy, according to $V^{SD} = V^F + V^M$. (2)

When a vacancy is created in crystalline Ge, one Ge atom leaves a lattice site and migrates to the surface. The volume of the crystal increases by one Ge atomic volume (Ω_{Ge}) at standard T and p at the surface. V^F , however, depends on the degree to which the atoms surrounding the vacancy relax into it. Specifically, V^F is decreased by the relaxation

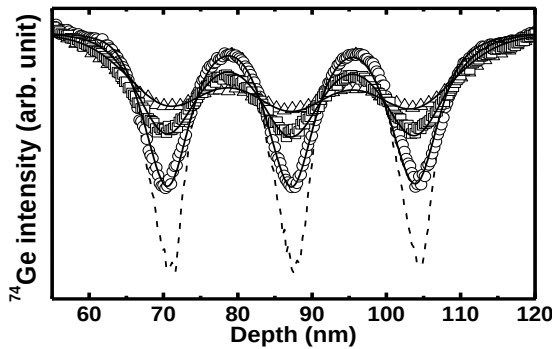


Fig. 3 SIMS and simulated depth profiles of ^{74}Ge in the $\text{Si}_{0.2}\text{Ge}_{0.8}/\text{GeSL}/\text{Si}_{0.2}\text{Ge}_{0.8}$ heterostructures. Dashed line, open circles ($\circ$), open squares ($\square$), and open triangles (Δ) represent the SIMS profiles before and after annealing at 550 °C for 1, 3 and 6 h, respectively. Solid curves are the simulation results.

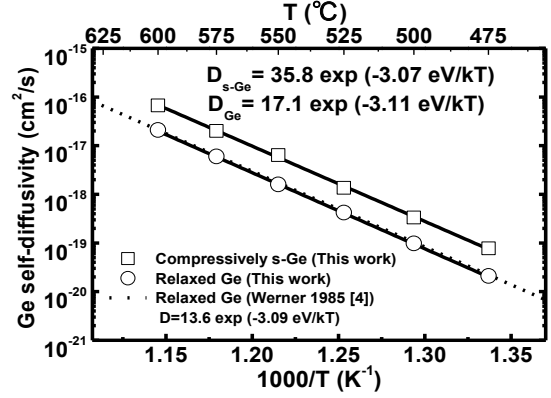


Fig. 4 Temperature dependences of Ge self-diffusivities

volume (V^R) which is negative and, as a result, less than Ω_{Ge} . Therefore, V^{SD} is given by

$$V^{SD} = \Omega_{Ge} + V^R + V^M \quad (3)$$

Here, V^M is also negative due to the fact that the diffusing atom via a vacancy is expanding a constriction at the saddle point in its migration path [4]. Moreover, Aziz et al. [5] have reported that, if we have biaxial stress (σ_{biax}), V^F is dominated by the relaxation and migration terms because there is no force on the surface and the work to create a lattice site at the surface should be zero. According to these models, the activation volume (V_{biax}^{SD}) of Ge self-diffusion under compressive biaxial stress should be negative. In this work, the decrease of the activation enthalpy of Ge self-diffusion in s-Ge compared to that of relaxed Ge by the magnitude of the work $|\sigma_{biax} V_{biax}^{SD}|$ resulted in the increase of self-diffusivities, which allows us to obtain $V_{biax}^{SD} = -0.66 \pm 0.06 \Omega_{Ge}$. This result is consistent with previous work stating that relaxation in Ge is strong [4].

4. Conclusion

In conclusion, by means of $\text{Si}_{0.2}\text{Ge}_{0.8}/\text{GeSL}/\text{Si}_{0.2}\text{Ge}_{0.8}$ heterostructures, the first measurements of Ge self-diffusion under compressive biaxial strain were performed. We found that Ge self-diffusivities in compressively s-Ge are larger compared to those in relaxed Ge. Moreover, we obtained $V_{biax}^{SD} = -0.66 \pm 0.06 \Omega_{Ge}$.

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References

- [1] P. Laitinen, A. Strohm, J. Huikari, A. Voss, C. Grodon, I. Riihimaki, M. Kummer, J. Aysto, P. Dendooven, J. Raisanen, W. Frank, and the ISOLDE Collaboration, Phys. Rev. Lett. **89** (2002) 085902,
- [2] N. R. Zangenberg, J. L. Hansen, J. Fage-Pedersen, and A. N. Larsen, Phys. Rev. Lett. **87** (2001) 125901.
- [3] R. Kube, H. Bracht, J. L. Hansen, A. N. Larsen, E. E. Haller, S. Paul, W. Lerch, Mater. Sci. Semicond. Process. **11** (2008) 378.
- [4] M. Werner, H. Mehrer, and H. D. Hochheimer, Phys. Rev. B **32** (1985) 3930.
- [5] M. J. Aziz, Appl. Phys. Lett. **70** (1997) 2810.