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Comprehensive Study on Electron Mobility and Band Gap in Tensile Strained Ge

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Abstract

Calculations on the electron mobility and band-gap energy for all the surface orientations and the current directions under both biaxial and uniaxial tensile strain were carried out in order to clarify how strained Ge *n-type* transistors should be designed. It was revealed that the highest electron mobility is realized in (111) Ge with isotropic biaxial tensile strain with significant band-gap narrowing. A combination of [110] channel direction with uniaxial tensile strain parallel to the channel was found to provide technically the most preferable solution, considering the trade-off between the mobility and the band-gap energy.

1. Introduction

The trend toward miniaturization of CMOS devices has resulted in lowering power supply voltage, which is expected to be less than 1 V within a few years. In order to realize high current drivability with such low power supply voltage, devices having a high-mobility channel with strain and/or made of new materials such as Ge, SiGe, and III-V semiconductors are being intensively investigated [1, 2]. Among them, Ge is attracting much attention owing to high mobility of both electrons and holes [3]. However, whereas there have been many reports on pMOSFETs having a strained Ge channel, only a few nMOSFETs having a strained Ge channel have been reported [4]. Theoretical investigations predict that high electron mobility is realized in not compressively but tensile strained Ge [5, 6]. Although electron mobility in Ge with strain in (100), (110), and (111) planes has been investigated in detail [5, 6], systematic investigations of dependences of electron mobility on configuration of strain and channel direction have not been carried out. In this study, we comprehensively and quantitatively investigated electron mobility in arbitrarily oriented Ge channel with both isotropic/anisotropic biaxial and uniaxial tensile strain using a simple model as shown below. Dependences of band-gap energy on strain were also examined.

2. Model in Simulation

A mobility tensor at 300 K in bulk Ge was obtained by averaging mobility tensors of each energy valley with weights of the Boltzmann factors and DOS values of each energy valley. The reported value of 3,900 $cm^2V^{-1}s^{-1}$ in bulk Ge [3] was used for mobility in unstrained Ge. Dependences of energy of each valley on configuration of strain were calculated by means of deformation potentials [5]. In the calculation, isotropic/anisotropic biaxial and uniaxial tensile strain up to 1% was considered. Here, the surface orientation was defined as a plane parallel to the strain axes and the channel direction. In the cases of both biaxial and uniaxial strain, stress perpendicular to those axes was assumed to be zero. Under such strain, the lowest energy valleys are L valleys [5]. Hence, only L valleys were taken into consideration. Electron mobility of each energy valley was assumed to be inversely proportional to effective masses. Dependences of effective masses on strain were also calculated by using 2 equations containing 5 parameters, which were obtained by fitting to results of numerical calculations [7]. Dependences of relaxation times on strain were not taken into consideration. Band-gap energy was obtained by calculating a difference between the conduction band minimum and the valence band maximum, which was obtained by solving a secular equation at Γ point for deformation potential [8] and spin-orbit interaction.

3. Results and Discussion

Firstly, electron mobility was calculated for various strain configurations and channel directions. Even in the case of isotropic biaxial strain, mobility is anisotropic in the plane of strain. Only in the cases of (001) and (111) planes, mobility is isotropic owing to the symmetry of the crystal. It was shown that the highest mobility in the plane of strain is always higher than that in unstrained Ge. (Fig. 1) The highest mobility of 5,680 $cm^2V^{-1}s^{-1}$ was calculated for channels in the (111) plane. This is because most of the electrons populate the L valley along [111] direction with minimum conduction effective mass in the plane, owing to a decrease in energy of the valley. (Fig. 2)

In order to study the effects of more realistic strain configurations such as process-induced strain, mobility under anisotropic biaxial strain was calculated. The results showed that mobility decreases with relaxation of strain in the transverse direction in the (111) plane. (Fig. 3) This is due to an increase in electron population in the L valleys in [1-11] and [-111] directions whose conduction effective mass is not the minimum value along the channel direction. The influence of relaxation of strain in the transverse direction is small in the case that $\varphi = 0$. (Fig. 4) This is because dependences of energy of each valley on transverse strain are weak. Among planes having φ of 0, the (101) plane is the most preferable because of the highest mobility besides the robustness against relaxation of strain in the transverse direction. (Fig. 4)

Secondly, band-gap energy was calculated for various strain configurations. It was shown that the band gap is always narrower than that of unstrained Ge under 1% of isotropic biaxial strain. (Fig. 5) The band gap exhibits minimum value of 0.436 eV when the strain is applied in the (111) plane, because the energy of the L valley in [111] direction significantly decreases owing to the strain. (Fig. 2) A clear trade-off between high mobility and wide band gap is evident in Fig. 6, which plots the band-gap energy against the mobility for various planes of strain shown in Figs. 1 and 5. Fig. 6 also shows that [10-1] channel in (101) plane is the most preferable under the isotropic biaxial strain because band gap is wider than that of (111) plane by 76 meV while mobility is lower by only 1 %. Not only in the case of isotropic biaxial strain but also in the case of anisotropic biaxial strain, there is a trade-off between high mobility and wide band gap. (Figs. 7, 8) In the cases that both $\varphi = 0^o$ and 45°, band-gap energy corresponding to a particular value of mobility increases and mobility corresponding to a particular value of band-gap energy increases as transverse strain relaxes. Hence, higher strain relaxation in the direction perpendicular to the channel is more preferable considering the trade-off, with the result that the uniaxial strain parallel to the channel is the most preferable.

Preferable channel direction and corresponding mobility and band-gap energy values are summarized in Table I under both isotropic biaxial strain and

uniaxial strain parallel to the channel.

4. Conclusion

It has been shown that biaxial tensile strain on (111) surface results in the most significant band-gap narrowing, although the highest electron mobility is realized. On the other hand, uniaxial strain was found to relax the band-gap narrowing while keeping relatively high electron mobility for the channels along [110] direction.

Acknowledgement

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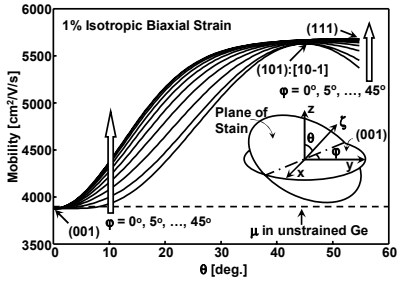

Fig. 1. Dependences of the highest mobility in the plane of strain of isotropic biaxial strain on orientation of the plane. Here, ζ is normal to the plane.

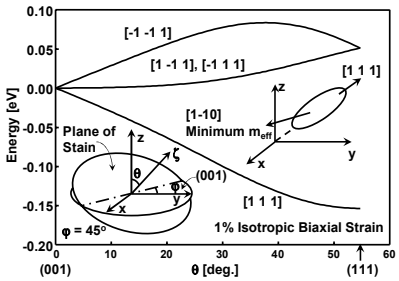

Fig. 2. Dependences of energy of each L valley on θ. Here, average energy is set equal to zero and φ = 45°.

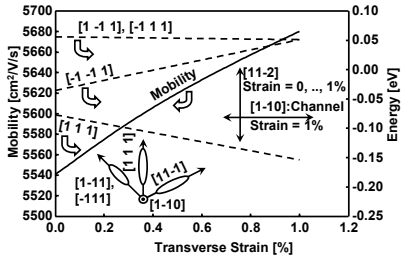

Fig. 3. Dependences of mobility and energy of each L valley on strain parallel to [11-2]. Here, the channel direction is fixed to [1-10] and strain parallel to [1-10] is 1%.

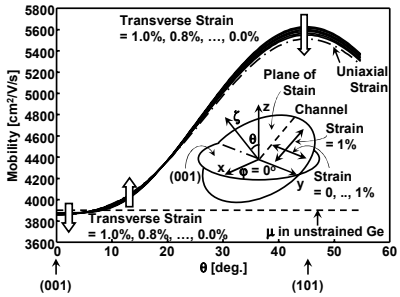

Fig. 4. Dependences of mobility on strain parallel to [010]. Here, the channel direction is perpendicular to [010] in the plane of strain and strain parallel to channel is 1%.

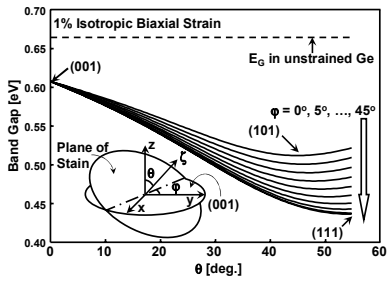

Fig. 5. Dependences of band-gap energy on orientation of the plane of isotropic biaxial strain.

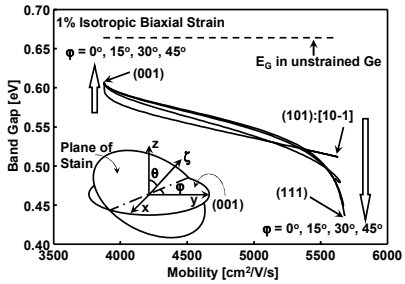

Fig. 6. Dependences of band-gap energy on the highest mobility in the plane of isotropic biaxial strain with various orientation of the plane.

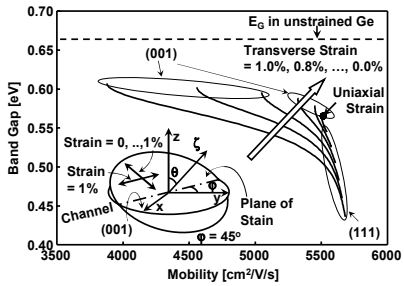

Fig. 7. Dependences of band-gap energy on mobility in [1-10] direction with various orientation of the plane of biaxial strain. Here, φ = 45°, strain parallel to [1-10] was 1%, and strain perpendicular to [1-10] in the plane was varied from 0 to 1%.

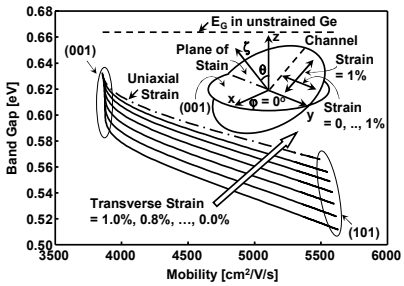

Fig. 8. Dependences of band-gap energy on mobility perpendicular to [010] in the plane of biaxial strain with various orientation of the plane. Here, φ = 0°, strain perpendicular to [010] in the plane was 1%, and strain parallel to [010] was varied from 0 to 1%.

Surface Orientation		(001)	(111)	(110)	(113)
Isotropic Biaxial	Channel	Arbitrary		[1-10]	
	μ(cm²V⁻¹s⁻¹) (x Ge/x Si)	3877 (0.99/2.58)	5680 (1.46/3.79)	5626 (1.44/3.75)	5415 (1.39/3.61)
	E_G(eV) (x Ge/x Si)	0.607 (0.91/0.54)	0.436 (0.66/0.39)	0.512 (0.77/0.46)	0.518 (0.78/0.46)
Uniaxial	Channel	[1-10] [110]	[1-10] [10-1] [01-1]	[1-10]	
	μ(cm²V⁻¹s⁻¹) (x Ge/x Si)	5512 (1.41/3.67)			
	E_G(eV) (x Ge/x Si)	0.565 (0.85/0.50)			

Table I. Preferable channel direction, mobility, and band-gap energy under both isotropic biaxial strain and uniaxial strain parallel to the channel direction. Here, values in parenthesis imply ratios of the values to those in unstrained Ge/Si.