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Effect of Oxidation-Induced Strain on Potential Profile in Si SETs Using Pattern-Dependent Oxidation (PADOX)

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1. Introduction

A method using pattern-dependent oxidation (PADOX) to fabricate a Si SET operable at relatively high temperatures is a reproducible and controllable one [1]. With this method, a Si wire on a SIMOX substrate is converted through mechanical stress during the oxidation into a small Si island sandwiched between two tunnel barriers. For this kind of SET, however, the origin of the potential profile responsible for SET operation has not yet been clarified completely. In this paper, we investigate the effect of an oxidation-induced strain during PADOX and describe a probable mechanism of the formation of this potential profile.

2. Effective Potential Taking into Account Only Structural Modification

Figure 1 shows a schematic diagram of a Si SET fabricated using PADOX and the coordinate system. The Si SET fabricated on a (001) SIMOX substrate still has a [110]-oriented wire region even after PADOX. A three-dimensional model image and the AFM-measured width and thickness along the Y axis of this wire region are shown in Figs. 2 and 3.

Here, we investigate an effective potential $U_{eff}(Y)$ which determines the electron motion along the wire region, using the data shown in Fig. 3 within the effective mass theory. The effective mass equation that includes $U_{eff}(Y)$ for an electron in three pairs of valleys along the [100], [010] and [001] axes (in this paper we denote these six valleys as [±a,0,0], [0,±a,0] and [0,0,±a] valleys) can be well approximated for the gentle structural modification shown in Fig. 3 as

$$\left\{-\frac{\hbar^2}{2m_Y}\frac{\partial^2}{\partial Y^2}+U_{eff}(Y)\right\}\phi(Y)=\varepsilon\phi(Y), \qquad (1)$$

where $\hbar$ is the reduced Planck constant, m_Y is $(m_t+m_l)/2$ for the [±a,0,0] and [0,±a,0] valleys (m_t =0.19 m_0 is the transverse mass, m_l =0.98 m_0 is the longitudinal mass and m_0 is electron rest mass), m_Y is m_t for the [0,0,±a] valleys [2], $\phi(Y)$ is an envelope function, and the effective potential $U_{eff}(Y)$ is given as the eigenvalue of the following two-dimensional eigenvalue equation in which Y is regarded as a parameter.

$$\left\{-\frac{\hbar^2}{2m_X}\frac{\partial^2}{\partial X^2}-\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}+V(X,Y,z)\right\}\chi(X,Y,z) = U_{eff}(Y)\chi(X,Y,z), \qquad (2)$$

where m_X =2 m_t m_l /(m_t+m_l), $m_z=m_t$ for the [±a,0,0] and [0,±a,0] valleys, $m_X=m_t$, $m_z=m_l$ for the [0,0,±a] valleys [2], $V(X,Y,z)$ is the cross-sectional potential, and $\chi(X,Y,z)$ is an eigenfunction.

The effective potential $U_{eff}(Y)$ calculated using eq. (2) and the data shown in Fig. 3 with the assumption of a rectangular cross-sectional shape is shown in Fig. 4. This figure shows that there is only one potential barrier without a potential well corresponding to an island for all valleys. Therefore, it is concluded that a potential profile responsible for SET operation cannot be produced only by structural modification.

3. Effect of Oxidation-Induced Strain

Oxidation of a Si nano-structure generates a huge amount of compressive stress, more than 20000 atm [3]. The compressive strain caused by this stress can exceed 1 % and this strain can reduce the bandgap more than 0.1 eV [4]. The bandgap change, obtained using the first-principles calculation, is shown in Fig. 5 as a function of the wire direction on the (001) plane. It can be seen that the bandgap reduction for the [0,0,±a] valleys does not depend on the wire direction so much. Therefore, it is possible that the compressive stress generated during PADOX reduces the bandgap and forms a potential well around the center of the wire stably for these valleys.

The reduction of the bandgap ΔE_G can be introduced to the effective potential as $U_{eff}(Y)$-0.75 ΔE_G for all valleys if we use the value of 75 % as the conduction band offset ratio [5]. This is because the effective masses and the positions of valley minima do not change appreciably regardless of the strain.

The modified effective potentials taking into account the bandgap reduction by compressive strain are shown in Fig. 6 with the assumption that the compressive strain appears only in the central part of the wire region. Figure 6 shows that it is possible that a SET operates reasonably under the modified effective potential for the [0,0,±a] valleys.

4. Conclusions

We have investigated the effect of an oxidation-induced strain in Si SETs fabricated using PADOX and have proposed a probable mechanism of the formation of the potential profile responsible for SET operation. The compressive strain generated during PADOX forms a potential well that corresponds to an island in a tunnel barrier produced by the reduction of width in a wire region.

References

[1] Y. Takahashi et al., IEEE Trans. Electron Devices, **43**, 1213 (1996).
[2] S. Horiguchi et al., Jpn. J. Appl. Phys. **34**, 5489 (1995).

[3] H. I. Liu et al., J. Vac. Sci. Technol. B **11**, 2532 (1993).
[4] K. Shiraishi et al., Mat. Res. Soc. Sym. Proc., **536**, (1999) in press.
[5] M. Murayama and T. Nakayama, J. Phys. Soc. Jpn., **61**, 2419 (1992).
[6] M. Nagase et al., Microelectron. Eng. **41/42**, 527 (1998).
[7] M. Nagase et al., Jpn. J. Appl. Phys. **35**, 4166 (1996).

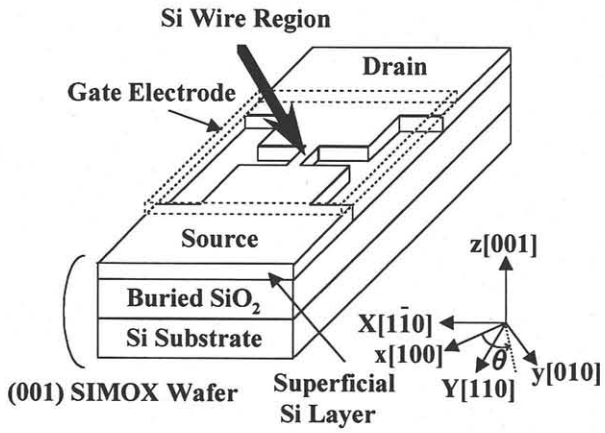

Fig. 1 Schematic diagram of a Si SET fabricated using PADOX and the coordinate system. θ is an angle from the x axis on the (001) plane.

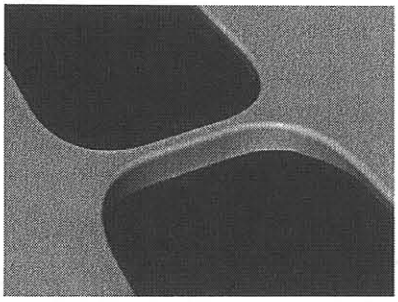

Fig. 2 Three-dimensional model image of the Si wire region after PADOX. The outline of this image was determined by the AFM-measured data shown in Fig. 3.

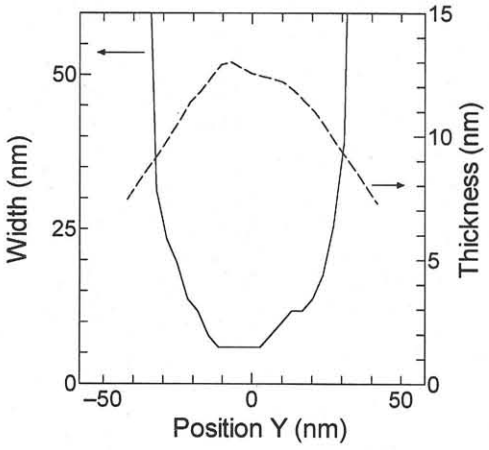

Fig. 3 AFM-measured width and thickness of the Si wire region along the Y axis. The width after removing the oxide layer was evaluated by means of the critical dimension method based on the image reconstruction [6]. The thickness of the buried Si was calculated from a height distribution of the oxide surface [7].

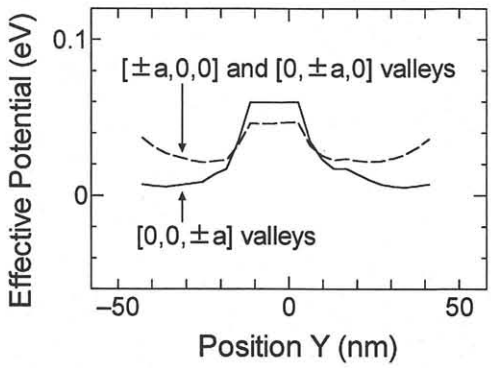

Fig. 4 Effective potential along the Y axis measured from the bottom of the conduction band in bulk Si.

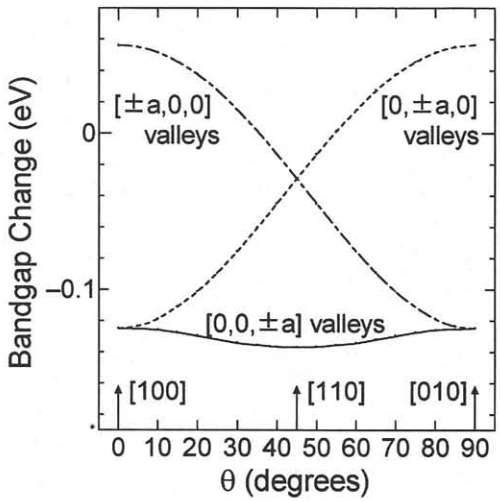

Fig. 5 Calculated bandgap change as a function of Si wire direction θ (see Fig. 1) when a two-dimensional compressive strain of 1 % is applied perpendicular to the Si wire direction.

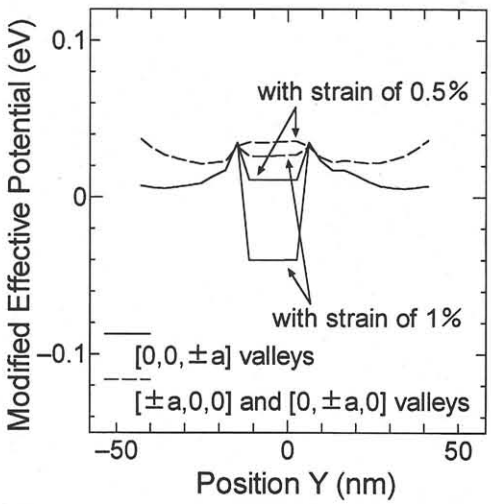

Fig. 6 Modified effective potential along the Y axis measured from the bottom of the conduction band in bulk Si, taking into account the bandgap reduction by compressive strain as a parameter.