Electrical Activity of Frank Partial Dislocations and the Influence of Metallic Impurities in Czochralski-Grown Silicon

SHEN Bo(沈波), YANG Kai(杨凯), CHEN Peng(陈鹏), ZHANG Rong(张荣), SHI Yi(施毅), ZHENG You-dou(郑有炓)
Department of Physics, Institute of Solid State Physics, Nanjing University, Nanjing 210093

T. Sekiguchi, K. Sumino
Institute for Materials Research, Tohoku University, Sendai 980, Japan

(Received 15 November 1996)

Electrical activity of Frank partial dislocations bounding stacking faults and the influence of Fe impurities in Czochralski-grown silicon are investigated by means of the electron-beam-induced-current(EBIC) technique. Frank partials free from metallic impurities exhibit EBIC contrast at low temperatures but not at room temperature, indicating that they are only accompanied with shallow energy levels in the band gap. The energy level related to a Frank partial is determined to be about $E_c - 0.08$ eV in n-type Si. Frank partials decorated by Fe impurities become EBIC active at room temperature.

PACS: 61.72.−y, 72.20.−i, 71.55.Eq

Extended defects such as dislocations and stacking faults are common microdefects induced in Si crystals during thermal processes of device fabrication. The electrical properties of dislocations and stacking faults in Si have been widely investigated by means of deep level transient spectroscopy, electron spin resonance, Photoluminescence (PL), and the electron-beam-induced-current (EBIC) technique.[1,2] It is thought intensively that dislocations are accompanied with deep energy levels in the band gap and affect the electrical properties of Si crystals.

However, dislocations in Si are very easy to be unconsciously decorated by metallic impurities due to the strain field around them. The weak decoration of metallic impurities on dislocations cannot be detected by using conventional transmission electron microscopy. Therefore, it is questioned that deep levels related to dislocations originated from dislocations themselves or caused by the decoration of metallic impurities on them. Recently, Higgs *et al.* reported that *D*-band PL of dislocations in Si was due to the decoration of metallic impurities on them.[3] Wilshaw *et al.* found that stacking faults did not exhibit EBIC contrast at room temperature in a "clean" Si crystal.[4]

The EBIC technique has high spatial resolution and is very sensitive to the metallic decoration on extended defects. In this study, we apply EBIC technique to investigate the electrical activity of Frank partial dislocations bounding stacking faults and the influence of Fe impurities in Czochralski-grown silicon (CZ-Si). The energy level related to a Frank partial is determined semi-quantitatively on the basis of the Shockley-Read-Hall (SRH) recombination theory.

The CZ-Si crystal was n-type, P-doped, resistively of 10 Ω·cm, grown along the [111] direction, in which the initial oxygen concentration was about 9.0×10^{17} atoms/cm^3. Specimens were cut from the above Si ingot into a shape of parallelepiped with the size of $1.5 \times 6.0 \times 10.0$ mm with surfaces parallel to the (111), $(1\bar{1}0)$, and $(11\bar{2})$ planes. Frank partial dislocation loops bounding bulk stacking faults were introduced into specimens through a two-step annealing (750°C, 15 h + 1100°C, 20 h) in Ar. They were several tens of micron in diameter with a density of about 8.5×10^{8} cm^{-3}. Then, some of specimens were contaminated with Fe by annealing them together with high purity Fe wire at 1100°C in a vacuum. According to the literature,[5] the concentration of Fe impurities in the specimens is about 2.0×10^{15} atoms/cm^3.

EBIC measurements were performed with a TOPCON DS-130 scanning electron microscope in an EBIC mode controlled by a computer with an electron beam of 20 kV and 1.0 nA. The temperature range for EBIC measurements was between 40 K and room temperature (290 K). The surface of EBIC samples was parallel to the (111) plane. The Schottky contact on the surface was made by means of Au evaporation. The EBIC contrast C of a defect is defined as $C = (I_b - I_d)/I_b$, where I_b is the EBIC intensity of the background, and I_d the EBIC intensity at the location of a defect.

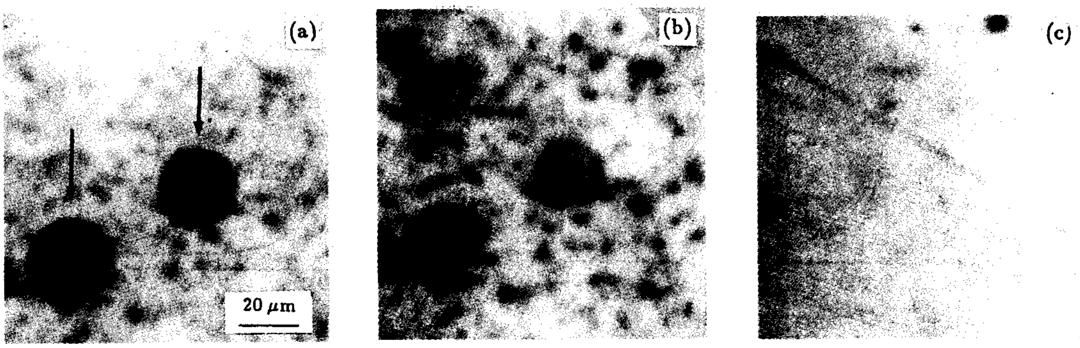

Fig. 1. EBIC images of Frank partial dislocations bounding stacking faults at (a) 50 K, (b) 110 K, and (c) 290 K in a noncontaminated specimen.

Figure 1 shows the EBIC images of bulk stacking faults in a specimen free from metallic impurities at various temperatures. Dark circles shown by arrows are the EBIC contrast from Frank partials and stacking faults bounded by them on the (111) plane parallel to the specimen surface. Both Frank partials and stacking fault planes exhibit EBIC contrast only at low temperatures. About the EBIC activity of stacking fault planes, we will discuss in a separate paper. The contrast of Frank partials is very strong at 50 K, becomes weak at 110 K, and disappears at room temperature.

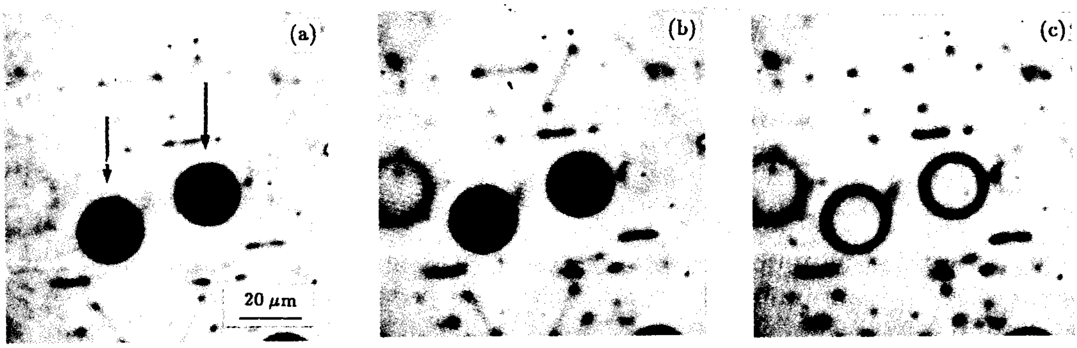

Fig. 2. EBIC images of Frank partial dislocations bounding stacking faults at (a) 50 K, (b) 110 K, and (c) 290 K in a Fe-contaminated specimen.

Figure 2 shows the EBIC image of Frank partials bounding bulk stacking faults in a Fe-contaminated specimen at various temperatures. The EBIC contrast of Frank partials is observed not only at low temperatures but also at room temperature.

Figure 3 compares the temperature dependencies of the EBIC contrasts of Frank partials in noncontaminated and Fe-contaminated specimens. The contrast in noncontaminated specimen decreases with increasing temperature and disappears at temperature around 210 K. The contrast in Fe-contaminated one also decreases with increasing temperature between 40 and 120 K. However, it becomes to increase with increasing temperature above 120 K, and is very strong at room temperature.

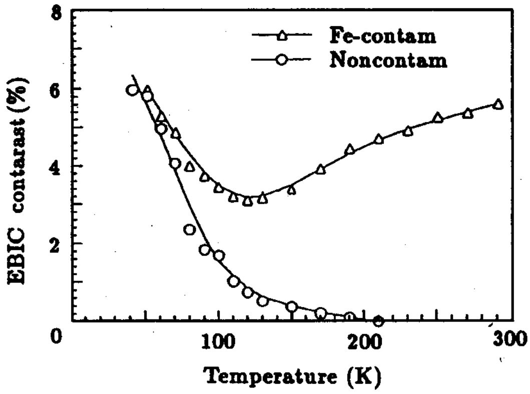

Fig. 3. Temperature dependencies of EBIC contrasts of Frank partial dislocations bounding stacking faults in noncontaminated and Fe-contaminated specimens.

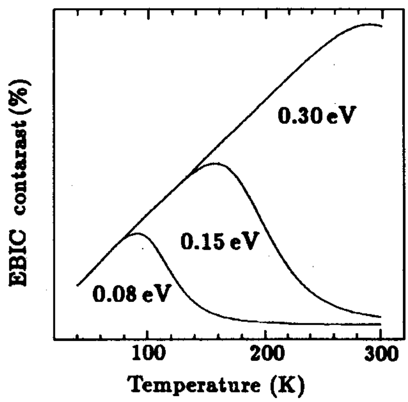

Fig. 4. Simulated temperature dependencies of EBIC contrasts of a dislocation accompanied by different energy levels in n-type Si on the basis of the SRH recombination theory. The level of the dislocation is assumed as 0.08, 0.15, and 0.30 eV, respectively, under the conduction band.

Above results indicate that Frank partials free from metallic impurities are electrically active at temperatures lower than 210 K and electrically inactive at room temperature. It is that the contamination of Fe induces that Frank partials become electrically active at room temperature. This means that a Frank partial is only accompanied by a shallow level in the energy gap. We can apply SRH recombination theory to determine the position of the energy level related to it semi-quantitatively.[6,7]

The EBIC contrast of a defect in Si is related to the lifetime τ of excess carriers and the diffusion constant D of carriers by[8]

$$C \propto \frac{1}{D\tau}\,. \tag{1}$$

According to the Einstein relation, $D = (k_B T/e)\mu$, where k_B is Boltzmann constant, τ the observing temperature, e the electric charge of the electron, and μ the carrier mobility. Since the lattice scattering to carriers is the predominant component of μ at temperatures above 60 K,[9] we assume simply that μ is proportional to $T^{-3/2}$ approximately. Therefore, D is related to T by $D \propto T^{-1/2}$.

According to the SRH theory, if excess carriers in Si recombine at the energy level E_t induced by the defect in the gap through the mechanism of indirect recombination, the lifetime τ for n-type Si is described as

$$\tau = \frac{(n_0 + n_1 + \Delta n)\tau_{p0} + (p_1 + \Delta n)\tau_{n0}}{n_0 + \Delta n}\,, \tag{2}$$

where

$$\tau_{p0} = \frac{1}{N_t \sigma_p \langle v_{th} \rangle_p}\,, \tag{3}$$

$$\tau_{n0} = \frac{1}{N_t \sigma_n \langle v_{th} \rangle_n}\,, \tag{4}$$

$$n_1 = N_c \exp\left(\frac{E_t - E_c}{k_B T}\right)\,, \tag{5}$$

$$p_1 = N_v \exp\left(\frac{E_v - E_t}{k_B T}\right), \tag{6}$$

n_0 is the equilibrium concentrations of electrons, n the concentrations of excess carriers, τ_{n0}, σ_n, and $\langle v_{th}\rangle_n$ are minority carrier lifetime, capture cross section, and average thermal velocity for electron, respectively, τ_{p0}, σ_p, and $\langle v_{th}\rangle_p$ the corresponding values for holes. N_t is the concentration of recombination centers, E_t is the position of the defect level, E_c and E_v are the positions of the conduction and valence band edges, N_c and N_v the equivalent density of states in the conduction and valence band, respectively.

Then, we obtain

$$C \propto T^{1/2} \frac{n_0 + \Delta n}{(n_0 + n_1 + \Delta n)\tau_{p0} + (p_1 + \Delta p)\tau_{n0}}. \tag{7}$$

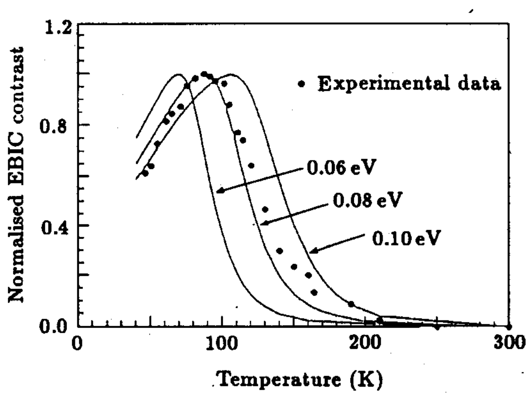

Fig. 5. Temperature dependencies of EBIC contrasts of a Frank partial dislocation in a noncontaminated specimen and simulated dependencies on the basis of the SRH recombination theory.

From Eq. 7, we find that the EBIC contrast of a defect is determined by the E_t in the gap and the temperature T of observation. The temperature dependence of the EBIC contrast of a dislocation in respect to different energy levels calculated from Eq. 7 is shown in Fig. 4. Here, we assume that the N_t is $10^{13}\,\mathrm{cm}^{-3}$, the n is $10^{15}\,\mathrm{cm}^{-3}$, and $\sigma_n = \sigma_p = 10^{-14}\,\mathrm{cm}^2$.[10] We find that a dislocation accompanied by a shallow level only exhibits EBIC contrast at low temperatures. This is due to the change of the occupation of carriers at the shallow center, caused by the shift of the Fermi level with temperature. The maximum contrast of the dislocation shifts toward higher temperature if the energy level becomes deeper in the gap. The contrast becomes to increase with increasing temperature until room temperature (290 K) if the level is deeper than $E_c - 0.30\,\mathrm{eV}$ in the gap.

Fitting the temperature dependence of the EBIC contrast of the Frank partial free from metallic impurities, as shown in Fig. 5, we obtain that the energy level related to the Frank partial itself is about $E_c - 0.08\,\mathrm{eV}$ in the gap in n-type Si.

In conclusion, electrical activity of Frank partial dislocations bounding stacking faults and the influence of Fe impurities in CZ-Si are investigated by means of the EBIC technique. Frank partials free from metallic impurities exhibit EBIC activity at low temperatures but not at room temperature, indicating that they are only accompanied with shallow energy levels in the band gap. The energy level related to a Frank partial is determined to be about $E_c - 0.08\,\mathrm{eV}$ in n-type Si. Frank partials decorated by Fe impurities become EBIC active at room temperature.

REFERENCES

[1] L. C. Kimerling, H. J. Leany and J. K. Patel, Appl. Phys. Lett. 30 (1977) 217.
[2] J. Kanewski, M. Kanewska and A. R. Peaker, Appl. Phys. Lett. 60 (1992) 359.
[3] V. Higgs, M. Loulding, A. Brinklew and P. Kinghtley, Appl. Phys. Lett. 60 (1992) 1369.
[4] P. R. Wilshaw, T. S. Fell and M. D. de Coleau, J. Phys. IV (Paris) (1991) C6-3.
[5] E. R. Weber, Appl. Phys. A 30 (1983) 1.
[6] W. Shockley and W. T. Read, Phys. Rev. 87. (1952) 835.
[7] M. Kittle and W. Seifert, Mat. Sci. Eng. B 24 (1994) 28.
[8] C. Donolato, Optik, 52 (1978) 19.
[9] S. M. Sze, *Physics of Semiconductor Devices* (John Wiley and Sons, Inc., 1981).
[10] A. Ourmazd, Crys. Res. Technol. 16 (1981) 137.