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Photoluminescence from triplet states of isoelectronic bound excitons at interstitial carbon-intersititial oxygen defects in silicon

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ABSTRACT

We report luminescence from spin triplet states of excitons bound to interstitial carbon-interstitial oxygen defects in silicon. The peak, which we call C_T-line, has an energy 2.64 meV lower than 790 meV (C-line), and splits into three peaks by application of magnetic field. Moreover, its peak position does not depend on the angle between the magnetic field direction and crystallographic orientation indicating the quenching of orbital angular momentum of the hole bound to the defect. These observations lead us to conclude that the C_T-line is the photoluminescence from a triplet state.

1. Introduction

Irradiated Czochralski-grown silicon (Cz-Si) exhibits photoluminescence via no-phonon (NP) transition of interstitial carbon-interstitial oxygen complexes (C_i–O_i) at 790 meV (C-line) [1–3]. This defect was observed and identified with the use of various experimental techniques such as infrared-absorption spectroscopy [4–6], photoluminescence (PL) [5,7–10], electron-spin resonance (Si-G15 spectrum) [11], Hall effect and DLTS [12], and local vibration mode spectroscopy [14,16], with strong support by density functional calculation [13–16]. The exciton bound to the C_i–O_i has been identified as a hole-attractive isoelectronic bound exciton (IBE) or pseudo-donor [10,19], where the formation of the exciton is initiated by capturing of a hole by the short-range defect potential followed by the capturing of an electron by the long-range Coulomb potential due to the hole [17,18]. When the short-range defect potential is much stronger than the spin-orbit interaction and/or the defect potential has low symmetry, the IBE becomes a spin singlet-triplet (ST) system composed by the electron and the hole [17]. The C_i–O_i defect has both the strong potential (hole binding energy E_h=341 meV) [10] and the low-symmetry potential (C_{1h} symmetry) [20] to compose the ST system. Actually, experiments to probe the decay kinetics suggested that the triplet state situated around 3.2 meV lower in energy than the singlet state corresponding to the C-line [21]. However, direct optical detection of the triplet state has never been reported before. The present paper reports direct-optical observation of the triplet states (C_T-line), whose peak position is 2.64 meV lower in energy than that of C-line. The temperature dependence of the relative intensity between the C_T-line and C-line and the PL measurements with externally applied magnetic field support our interpretation that the C_T-line is luminescence from the C_i–O_i having the triplet state.

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2. Experimental procedure

We used the *n*-type Cz-Si wafer, whose carbon concentration was approximately 10^{17} cm^{-3}. The electron irradiation to create C_i–O_i defects was performed with the acceleration energy of 1 MeV and a dose of 1×10^{18} cm^{-2} at room temperature.

The irradiated sample was mounted in a strain-free manner and immersed in a superfluid liquid helium bath. PL spectra were collected with BOMEM DA8 Fourier transform interferometer equipped with a liquid nitrogen-cooled germanium detector. The excitation was provided by the 1047 nm line of a Nd:YLF laser. A superconducting magnet was used to apply magnetic field parallel to the optical axis.

3. Results and discussion

Fig. 1 shows PL spectrum from C_i–O_i in Si at a helium-bath temperature of ~2.0 K without magnetic field. The sharp 789.67 meV line is the NP transition, which is often called either C-line or C_0-line [7]. The phonon replica (C_0^{LA}, C_0^{TA}) and the local vibration modes (C_0^{L1}, C_0^{L2}) due to the C_0-line are also shown in the Fig. 1. Moreover, the PL measurement shows not only the strong 789.67 meV line but also a 787.03 meV line, which we call C_T-line. The energy separation is 2.64 meV.

Fig. 2 shows the logarithm variation of the relative intensity between C_T-line and C_0-line against inverse kT, where k is the Boltzmann constant and T is the temperature. I_{C_T} and I_{C_0} indicate the intensity of C_T-line and C_0-line, respectively. The temperature

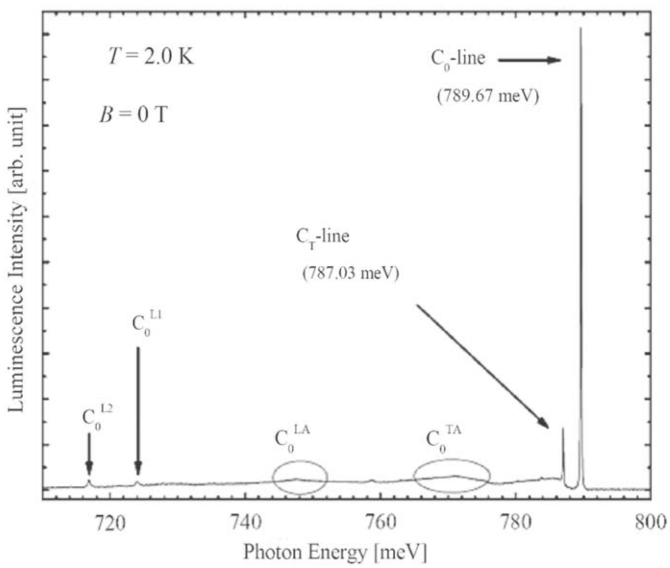

Fig. 1. Photoluminescence spectrum from C_i–O_i defects in Si.

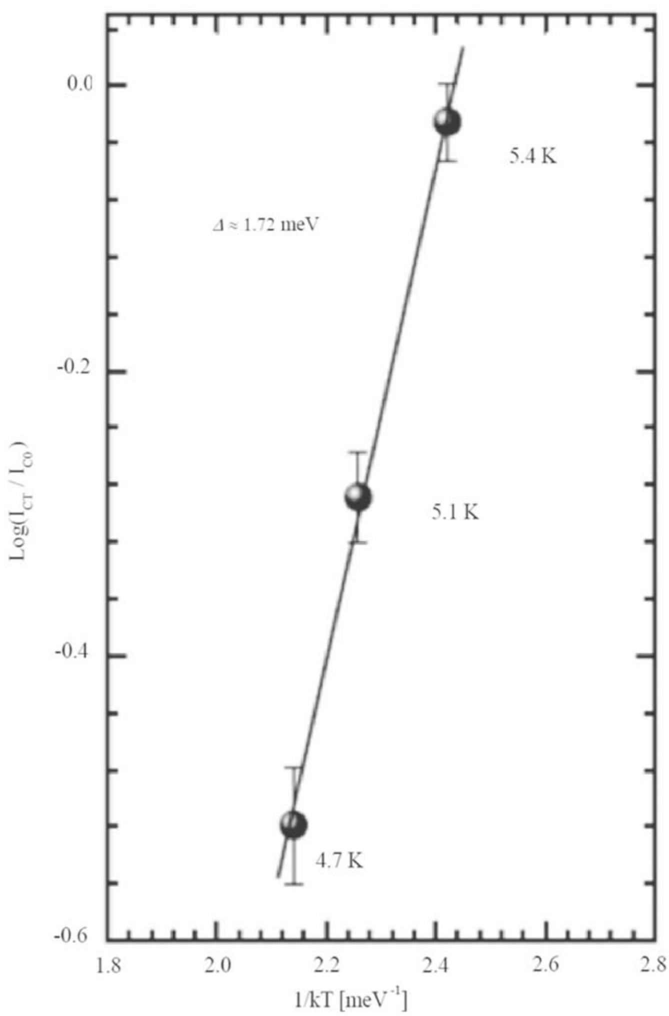

Fig. 2. Temperature dependence of the relative intensity between the C_T- and C_0-lines.

here was estimated from the linewidth of free excitons [3,22] from commercial float-zone *n*-type silicon substrate placed right next to the sample under the measurement.

Since both C_T- and C_0-lines are excitonic luminescence arising from the same defect, the relative intensity is expected to follow the Boltzmann distribution. Indeed a straight line fitting to the data is obtained, assuming that the relative intensity of the two levels in thermal equilibrium is expressed as [23].

$$\frac{I_{C_0}}{I_{C_T}}(T) = \frac{g_{C_0} f_{C_0}}{g_{C_T} f_{C_T}} \exp\left(-\frac{\Delta E}{kT}\right)$$

where g_i and f_i (i=C_0, C_T) are the degeneracy factors and transition probabilities, respectively. The good fit shown in Fig. 2 was obtained with $\Delta E \approx 1.7$ meV agree fairly well with experimentally observed line separation of 2.64 meV suggesting that the C_T-line is the luminescence from the C_i–O_i luminescence centers.

The behavior of the C_T-line with the externally applied magnetic field of 3 T is shown in Fig. 3. The bottom spectrum in the Fig. 3 is the C_T-line without magnetic field, the one in the middle was recorded with 3 T magnetic field applied in the direction parallel to [1 0 0] crystal axis (θ=0°), the one on the top was recorded with 3 T magnetic field applied in the direction 10 degrees away from [1 0 0] to [1 1 1] crystal axis (θ=10°). The middle spectrum shows that the C_T-line is separated into 3 lines under the magnetic field. This splitting indicates clearly that the C_T-line is composed of the 3-degenerate bound-excitonic state associated with C_i–O_i. A comparison of the top and middle spectrum shows that the peak position remains the same even after some rotation of the crystallographic orientation. Therefore, we reach the conclusion that the C_T-line is the photoluminescence

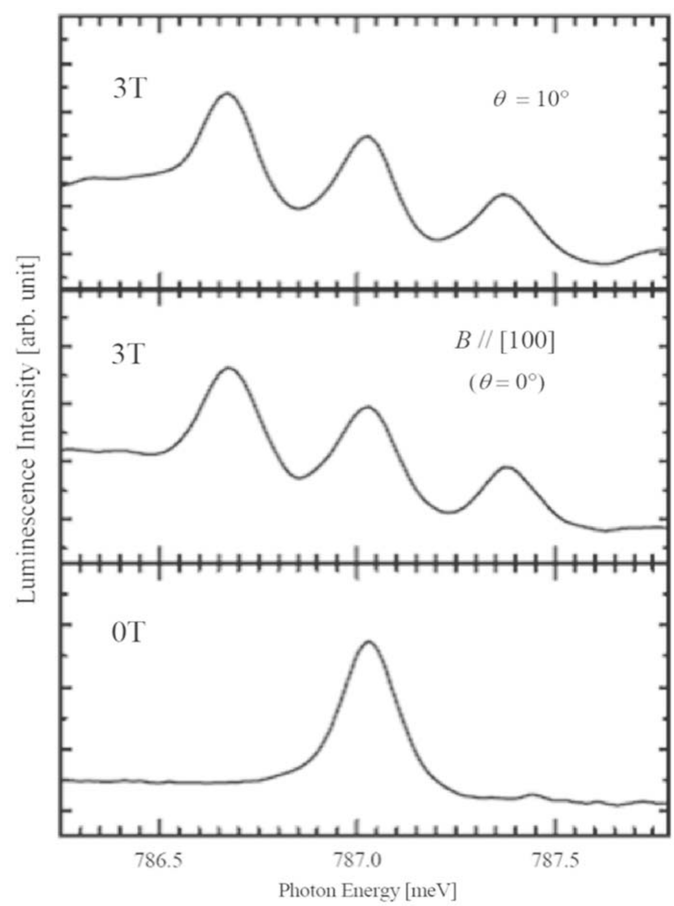

Fig. 3. Zeeman spectra of the C_T-line. The bottom spectrum is the C_T-line without magnetic field, the one in the middle was recorded with 3 T magnetic field applied in the direction parallel to [1 0 0] crystal axis (θ=0°), the one on the top was recorded with 3 T magnetic field applied in the direction 10° away from [1 0 0] to [1 1 1] crystal axis (θ=10°).

from the 3-degenerate state of the excitons bound to the C_i–O_i in Si. Moreover, the C_T-line does not depend on the direction of the magnetic field. Therefore, we conclude that the C_T-line is the transition from the isotropic spin triplet state.

The previous works show that the low-symmetry strain field in the C_i–O_i defects lifts the degeneracy of the hole state (Γ_8) [17], and therefore the ST system is created because the hole's orbital-angular momentum is quenched. Thus, the quenched angular momentum also influences that the peak positions of the C_T-line have the independence of the applied magnetic-field direction. Moreover, it has also been reported that the energy difference between the spin singlet state and the triplet state is around 3.2 meV by the previous work [21]. This value is in good agreement with our 2.64 meV obtained from the difference between the C_T-line and C_0-line. In addition, the intercept at $T \rightarrow \infty$ in the Fig. 2 is nearly equal to -4.2, which indicates the logarithm of $g_{C_T} f_{C_T}/g_{C_0} f_{C_0}$. With g_{C_T}=3 and g_{C_0}=1, $\log_{10}(f_{C_T}/f_{C_0}) \approx -2.3$. The previous work predicted $\log_{10}(f_{C_T}/f_{C_0}) \approx -2.8$ for the C-line [24]. Therefore, our experimental results obtained from the intercept at $T \rightarrow \infty$ in the Fig. 2 are also consistent with the previous work.

4. Conclusion

We have found a new PL line appearing at energy 2.64 meV lower than the large peak appearing at 790 meV for the complex of interstitial carbon-interstitial oxygen complexes and attributed this to the emission from the triplet states of the same defect.

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References

[1] A.V. Yukhnevich, Sov. Phys.–Solid State 7 (1965) 259.
[2] A.V. Yukhnevich, V.D. Tkachev, Sov. Phys.–Solid State 8 (1966) 1004.
[3] G. Davies, Phys. Rep. 176 (1989) 83.
[4] R.C. Newman, A.R. Bean, Radiat. Eff. 8 (1971) 189.
[5] G. Davies, A.S. Oates, R.C. Newman, R. Woolley, E.C. Lightowlers, M.J. Binns, J.C. Wilkes, J. Phys. C 19 (1986) 841.
[6] L.I. Murin, V.P. Markevich, J.L. Lindström, M. Kleverman, J. Hermansson, T. Hallberg, B.G. Svensson, Solid State Phenom. 82–84 (2002) 57.
[7] J. Wagner, K. Thonke, R. Sauer, Phys. Rev. B 29 (1984) 7051.
[8] W. Kürner, R. Sauer, A. Dörnen, K. Thonke, Phys. Rev. B 39 (1989) 13327.
[9] S. Hayama, G. Davies, J. Tan, J. Coutinho, R. Jones, K.M. Itoh, Phys. Rev. B 70 (2004) 035202.
[10] K. Thonke, A. Hangleiter, J. Wagner, R. Sauer, J. Phys. C Solid State Phys. 18 (1985) L795.
[11] J.M. Trombetta, G.D. Watkins, Appl. Phys. Lett. 51 (1987) 1103.
[12] P.M. Mooney, L.J. Cheng, M. Suli, J.D. Gerson, J.W. Corbett, Phys. Rev. B 15 (1977) 3836.
[13] S. Hao, L. Kantorovich, G. Davies, J. Phys. Condens. Matter 16 (2004) 8545.
[14] L.I. Khirunenko, M.G. Sosnin, Yu.V. Pomozov, L.I. Murin, V.P. Markevich, A.R. Peaker, L.M. Almeida, J. Coutinho, V.J.B. Torres, Phys. Rev. B 78 (2008) 155203.
[15] D.J. Backlund, S.K. Estreicher, Phys. Rev. B 77 (2008) 205205.
[16] J. Couthinho, R. Jones, P.R. Briddon, S. Öberg, L.I. Murin, V.P. Markevich, J.L. Lindström, Phys. Rev. B 65 (2001) 014109.
[17] B. Monemar, U. Lindefelt, W.M. Chen, Physica 146B (1987) 256.
[18] J.J. Hopfield, D.G. Thomas, R.T. Lynch, Phys. Rev. Lett. 17 (1966) 312.
[19] J.H. Svensson, B. Monemar, E. Janzén, Phys. Rev. Lett. 65 (1990) 1796.
[20] C.P. Foy, J. Phys. C Solid State Phys. 15 (1982) 2059.
[21] G. Bohnert, K. Weronek, A. Hangleiter, Phys. Rev. B 48 (1993) 14973.
[22] G. Davies, J. Phys. Chem. Solids 32 (1970) 883.
[23] M. Singh, D.C. Lightowlers, G. Davies, C. Jeynes, K.J. Reeson, Mater. Sci. Eng. B 4 (1989) 303.
[24] G. Davies, Phys. Rev. B 51 (1995) 13783.