Modulation of 1.5 μm dislocation-related luminescence emitted from a direct silicon bonded interface by external bias

Xuegong Yu,[1] Lihui Song,[1] Deren Yang,[1,a)] Martin Kittler,[2] and George A. Rozgonyi[3]
[1]*State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou 310027, People's Republic of China*
[2]*IHP/BTU Joint Laboratory, Konrad-Wachsmann-Allee 1, 03046 Cottbus, Germany*
[3]*Department of Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina 27695, USA*

(Received 27 March 2010; accepted 27 April 2010; published online 27 May 2010)

Interfacial dislocation networks were formed in silicon by direct bonding technology. Cathodoluminescence and deep level transient spectroscopy measurements verified that the D1 luminescence at 1.5 μm is associated with carrier transitions via a dislocation-related deep level at 0.35 eV. Both the experiment and theoretical calculations demonstrate that application of an external bias voltage on the bonding interface increases the majority carrier density at this deep level, thereby enhancing the local dislocation-related luminescence. However, beyond a critical voltage, corresponding to saturation of the majority carrier occupancy, the luminescence intensity decreases, due to the reduction in minority carrier density. © *2010 American Institute of Physics*.
[doi:10.1063/1.3431580]

Light emission from silicon is an ongoing topic of strong interest since the far reaching silicon technology could benefit for the fabrication of an "on-board" light-emitting diodes (LEDs).[1] However, for silicon with indirect energy gap, intermediate energy levels have to be introduced for improving the radiative recombination efficiency.[2,3] Dislocation can induce the energy levels and therefore emit a band of luminescences, labeled D1–D4.[4] Of particular importance is the 1.5 μm D1 luminescence coupled with silica-based glass fiber. Thus, dislocations are potential strong candidate for silicon-based LED fabrication, with a 0.1% efficiency LED emitting 1.5 μm D1 luminescence being fabricated.[5]

Among these luminescences, the D1 and D3 lines are most probably phonon-assisted replicas of D2 and D4 lines, respectively.[6] The D3/D4 lines originated from the dislocation strain fields,[7] are attributed to the carrier transition between shallow levels at 70 meV.[8] However, the origin of D1/D2 lines is still less clear. Impurities decoration at dislocations can significantly enhance the D1 luminescence.[9,10] The spectral features of the D1 luminescence suggest that it should result from carrier transitions between two intermediate energy levels.[11] The temperature dependence of the D1 luminescence amplitude below 100 K indicates that one level must be very shallow, about 10 meV, and that the second one should be quite deep.[12] Even though a lot of efforts have been made to reveal the dislocation-related energy levels, a direct correlation of D1 luminescence with the deep level is still unconfirmed.

Three direct silicon bonded (DSB) wafers with a boron concentration of $1\times10^{15}/\mathrm{cm}^3$ were used for our experiments. The interstitial oxygen concentrations of all the wafers are $7-8\times10^{17}/\mathrm{cm}^3$ with a calibration coefficient of $3.14\times10^{17}/\mathrm{cm}^3$. The first two wafers were denoted homo-DSB1 and homo-DSB2, due to the (100)/(100) orientation of the DSB wafer pair. They contain interfacial dislocation networks with similar microstructures, formed under similar misorientations (tilt angle: 0.2°; twist angle: 8.2°–9°). For comparison, a third sample, called "hetero-DSB," was formed by directly bonding of (110)/(100) silicon, creating a large angle grain boundary (GB) interface without dislocations. Secondary ion mass spectroscopy (SIMS) revealed that the concentrations of oxygen at all GBs are 2~3 orders of magnitude higher than that in the substrate. Next, the bar-like samples cut from the wafers, were performed two ohmic contacts on both sides by scratching InGa eutectic solution, allowing an external voltage bias to be directly applied on the GBs. The CL measurements were performed on the cross-sections of the samples under different external voltage biases. In addition, a BioRad DLTS system (DL8000, 1 M Hz) was used to measure the energy levels of GB states by applying periodic voltage pulses across the GBs.

Figure 1(a) shows the CL spectra emitted from these three GBs with a beam current of 20 nA under an accelerating voltage of 30 kV at 77 K. Note that no dislocation-related luminescence is detected from the referenced hetero-DSB GB. The CL spectra emitted from the homo-DSB1 and homo-DSB2 GBs have different features, i.e., the D1-line is dominant at the homo-DSB1 GB, while the D3-line at the

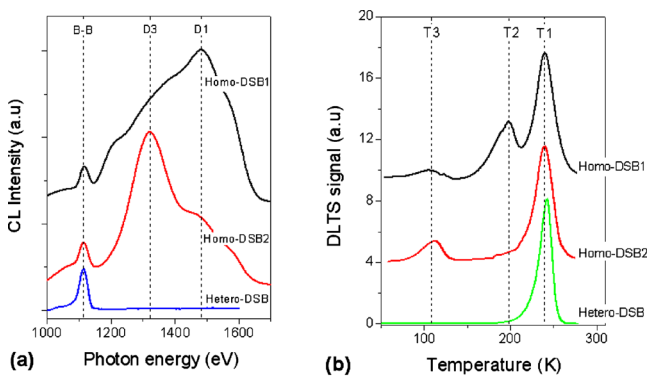

FIG. 1. (Color online) CL and DLTS spectra emitted from the DSB GBs. (a) The CL spectra; (b) The DLTS spectra.

a)Electronic mail: mseyang@zju.edu.cn.

homo-DSB2 GB. The deviation of CL spectra for these two GBs is not believed to originate from the microstructure of dislocation networks since they are quite similar. We suppose that the homo-DSB1 GB contains a proper concentration of oxygen or/and metal, which can interact with interfacial dislocations to benefit the enhancement of D1 luminescence.[9,10] Figure 1(b) shows the GB DLTS spectra following a filling pulse voltage of 7 V with a width of 100 ms. The reference hetero-DSB GB only exhibits a single trap, T1, while both of the homo-DSB GBs exhibit three traps, T1–T3. The T1 trap is located at around E_V+0.28 eV with hole capture cross-section of 10^{-17} cm^2. It is difficult to identify the exact nature of T1 trap. But, since the T1 trap can be yielded at the hetero-DSB GB, which belongs to the large-angle GB and should not contain any dislocations, we can rule out the correlation of T1 with dislocations. The T2 energy level is E_V +0.35 eV with hole capture cross-section of 10^{-14} cm^2, corresponding with the supposed D1 deep level, about E_g-hv. The T3 trap, at E_V+0.07 eV with hole capture cross-section of 10^{-15} cm^2, should be the shallow band caused by the strain field of dislocations, consistent with the result reported by Cavallini and co-workers.[8] More interestingly, the density of T2 traps at the homo-DSB1 GB is much larger than that at the homo-DSB2 GB, while it is contrary for the T3 traps. Considering that the homo-DSB1 GB contains a higher concentration of oxygen, as well as the possible metal contamination,[10] we believe that the T2 states might be a result of the metal or/and oxygen impurities coupling with the shallow band. A larger overlap between impurities and shallow band will increase the density of T2 states and meanwhile, reduce the density of T3 states. This DLTS result is in agreement with the luminescence spectra in Fig. 1(a), strongly supporting the proposal that the D1 luminescence is contributed to the carrier transition via the T2 deep level.

Figure 2 shows the CL scanning micrographs of the homo-DSB1 GB under different external bias voltages. It can be seen that the luminescence distribution extends in a wide region near the GB at zero voltage, determined by the minority carrier diffusion length. With the voltage increasing, the intensity of D1 luminescence first increases and then decreases after reaching a maximum value at a critical voltage. This indicates that the D1 luminescence intensity at the GB can be significantly modulated by the external bias voltage. Figure 3 shows the DLTS spectra of homo-DSB1 GB obtained by applying different filling pulse voltages with a width of 100 ms. One can see that both T1 and T2 trap intensities increase with the pulse voltage, due to the increase in the hole density on them. In the case of low filling pulse voltages, the T2 signal is dominant in the DLTS spectra, showing that the Fermi level is first pinned by the T2 states. Above a critical pulse voltage, the signal of T2 trap will be saturated but the hole density on T1 trap continually increases. This indicates that T1 states related to the distorted bonds exist in a wider energy range, pinning the Fermi level under higher bias voltages. So, the enhancement of D1 luminescence by applying an external bias voltage in Fig. 2 should be attributed to the increase in hole occupancy at T2 states. But, after the occupancy of deep level is saturated at a critical voltage, the reduction in minority carrier occupancy at the D1 shallow level will play an important role in the following decrease in D1 luminescence.

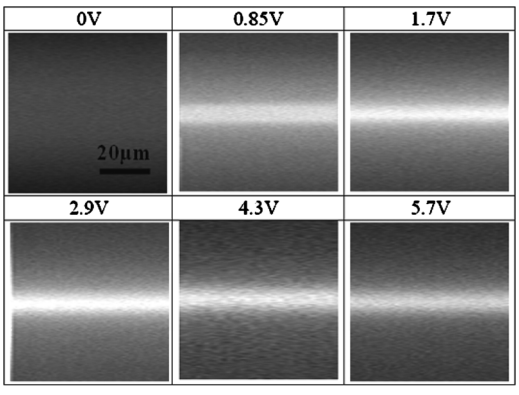

FIG. 2. CL scanning micrographs of the homo-DSB1 GB under different external bias voltages.

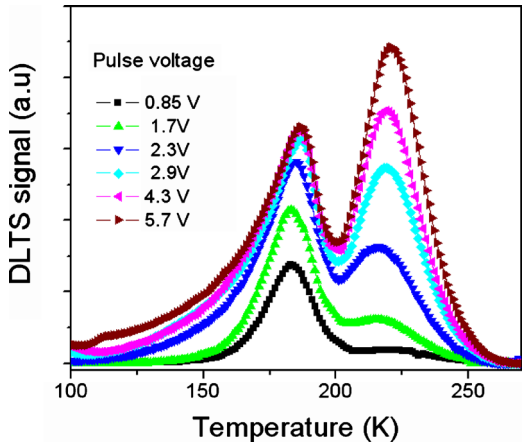

FIG. 3. (Color online) DLTS spectra of the homo-DSB1 GB obtained by applying different filling pulse voltages.

Figure 4(a) shows an energy band diagram near a p-type homo-DSB GB under an external voltage bias. The D1 radiative recombination occurs via two intermediate energy levels, i.e., one deep level at E_V+0.35 eV, named D1h, and one shallow level at E_C−0.01 eV, named D1e. The recombination rate, R, associated with the D1 luminescence intensity, is proportional to the product of hole density at the D1h level, p_t, and electron density at the D1e level, n_t, as follows:

$$R = rp_t n_t = rf_1 P_t f_2 N_t, \tag{1}$$

where r is the recombination coefficient; f_1 the hole occupancy of D1h level; f_2 the electron occupancy of D1e level; P_t the density of states for D1h level, and N_t the density of states for D1e level. Note that the hole and electron quasi-Fermi levels, E_{fp} and E_{fn} can be determined by the hole and electron concentrations at the GB, respectively. If assuming the GB as a double face-to-face Schottky diode, its equivalent circuit can be shown in Fig. 4(b). The V_L and V_R are the voltages distributed on the left and right diodes, respectively. In the case of low carrier injection level, the majority carrier (hole) concentration at the GB, p_{GB}, can be roughly expressed by,

$$p_{GB} = N_A e^{-(\phi_b - qV_L)/kT}, \tag{2}$$

where N_A is the dopant concentration; ϕ_b the built-in potential barrier; q the charge unit; k the Boltzmann constant, and T the absolute temperature. The minority carrier (electron) concentration in the conduction band at the GB, n_{GB}, can be calculated based on continuity equations as follows:

$$j_{GB} = j_{out} - j_{in} = q(r_{tot} p_{tot} n_{GB} - G)\Delta x, \tag{3}$$

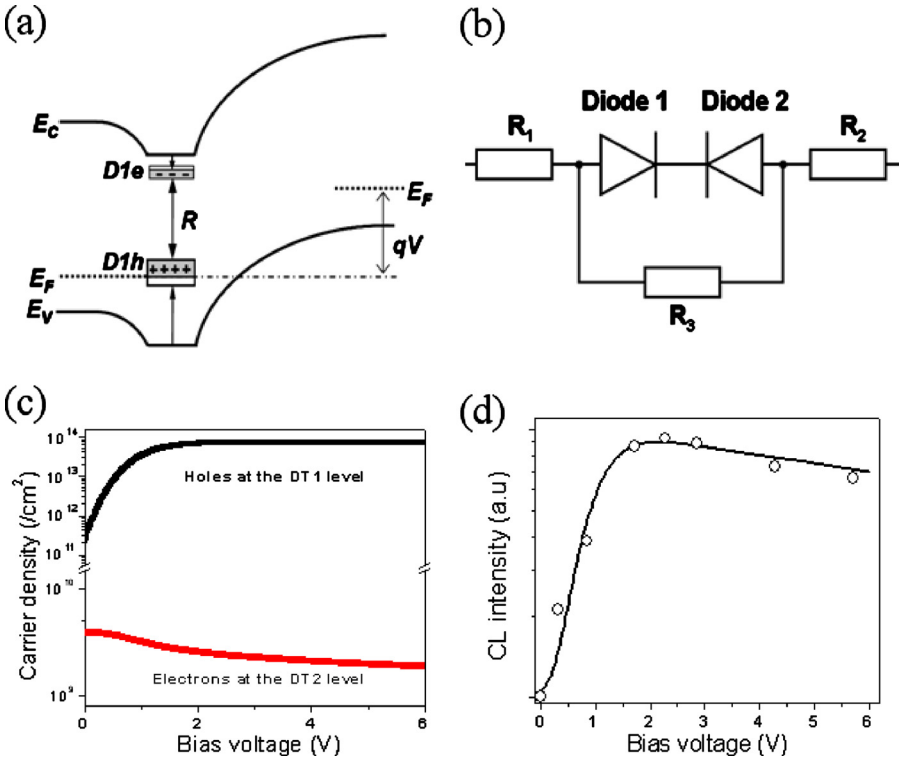

FIG. 4. (Color online) (a) Energy band diagram near the p-type homo-DSB GB under an external voltage bias; (b) the equivalent circuit of homo-DSB sample (R1, R2: series resistances; R3: shunt resistance); (c) The dependence of hole density at the D1h level and electron density at the D1e level on external bias voltage; (d) The experimental D1 luminescence (circle symbols) and the calculated radiative recombination rate (solid line) as a function of external bias voltage.

$$j_{\text{in}} = qD_n\lambda_1(\Delta n_L - G\tau_n) + q\mu_n\zeta_L\Delta n_L, \tag{4}$$

$$j_{\text{out}} = qD_n\lambda_2(\Delta n_R - G\tau_n) + q\mu_n\zeta_R\Delta n_R, \tag{5}$$

$$p_{\text{tot}} = N_A\left(\sqrt{\frac{2\varepsilon_{\text{Si}}(\phi_b - qV_L)}{qN_A}} + \sqrt{\frac{2\varepsilon_{\text{Si}}(\phi_b + qV_R)}{qN_A}}\right), \tag{6}$$

$$\Delta n_L \approx n_{\text{GB}}e^{(-\phi_b+qV_L)/kT}, \quad \Delta n_R \approx n_{\text{GB}}e^{[-\phi_b-q(V-V_L)]/kT}, \tag{7}$$

where j_{GB} is the electron recombination current density at the GB; j_{out} the electron current density out of the GB; j_{in} the electron current density into the GB; D_n the electron diffusion coefficient; $\lambda_{1,2}$ the eigenvalue of continuity equation; $\Delta n_{L,R}$ the excess electron concentration at the edge of depletion region; G the generation rate; τ_n the electron lifetime; μ_n the electron mobility; $\zeta_{L,R}$ the electric field; r_{tot} the total recombination probability; p_{tot} the whole hole density at the GB states; Δx the GB functional dimension, and ε_{Si} the silicon dielectric constant. Based on the equations above, the calculated hole density at the D1h level and the electron density at the D1e level as a function of bias voltages are shown in Fig. 4(c). Note that the hole density at the D1h level first rapidly increases with the bias voltage due to the down-shifting of GB hole quasi-Fermi level. It starts to be saturated at a critical voltage when the hole quasi-Fermi level moves below the energy position of D1h level. However, the electron density at the D1e level always decreases with the bias increasing, due to the GB electron quasi-Fermi level continually down-shifting with the bias voltage. The resultant D1 radiative recombination rate first increases due to the increase in majority carrier occupancy at D1h states, and then, decreases due to the reduction in minority carrier occupancy at the D1e states, see Fig. 4(d).

In summary, we have used DSB samples containing interfacial dislocation networks to establish the D1 deep level at the energy position of 0.35 eV in silicon band gap. Applying an external bias voltage enhances the majority carrier occupancy of this deep level, thereby significantly enhancing the D1 luminescence. However, this enhancement effect is limited to the reduction in minority carrier density at the D1 shallow level with the bias voltage increasing. Our simulations were in good agreement with the obtained experimental results. The present results are also very interesting for the fabrication of a higher efficiency dislocation-based LED.

This project is partly supported by National Natural Science Foundation of China (Grant Nos. 60906002 and 50832006) and "973 Program" (Grant No. 2007CB613403). The first author also thanks M. Reiche in MPI and M. Seacrist of MEMC for providing the DSB wafers.

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