Photoluminescence and photoluminescence excitation of 0.635-eV *EL0* emission in oxygen-doped semi-insulating GaAs

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The 0.635-eV photoluminescence emission present in oxygen-doped semi-insulating GaAs was studied with respect to temperature variation and photoluminescence excitation. The photoluminescence characteristics of the 0.635-eV emission are distinctly different compared to those of 0.68-eV *EL2* emission. The radiative mechanism is explained well by the configuration coordinate model, which involves a complex center involving the deep oxygen donor on an arsenic site and a gallium vacancy as a nearest neighbor. The Frank-Condon shift and vibration energy of the excited state of the center were determined to be 0.16 and 0.025 eV, respectively.

I. INTRODUCTION

Recent studies[1-3] have shown that there are two deep donors near the mid-band-gap of both conducting and semi-insulating GaAs. The first is the well-known *EL2* (Ref. 4), which is related to an arsenic antisite As_{Ga}. The second, known as *EL0*, is believed to be associated with the presence of oxygen.[1,3] Deep-level transient spectroscopy showed[1] that GaAs grown in O-enriched ambients contains the *EL0* level with an activation energy for thermal emission of an electron at 0.825 eV below the conduction-band edge compared to 0.815 eV for *EL2*.

Work related to the electrical activity of O started quite early[5] after the O doping was found to render the material semi-insulating. However, the electrical activation was considered to be due to the indirect effect of O resulting from the reduction of Si donors. A photoconductivity experiment in *n*-type GaAs:O showed a level[6] at $E_c - 0.4$ eV. However, no photoluminescence (PL) work related to the 0.4-eV level was reported. A deep-level luminescence[3] at 0.635 eV appears in GaAs crystals grown by adding Ga_2O_3 to the melt or using wet B_2O_3 as an encapsulant in liquid-encapsulated Czochralski or horizontal Bridgman methods. The near 4-K PL intensity of this emission is much stronger than that of *EL2* emission[7,8] at 0.68 eV. The spark source mass spectrometry also showed an O content of $\sim(5-10)\times10^{15}$ cm^{-3} in the heavily O-doped crystals showing the 0.635-eV emission, whereas the O was not detectable in the samples not showing the 0.635-eV emission. Thus the 0.635-eV emission was attributed[3] to the presence of O. This assignment of the 0.635-eV emission to O is corroborated with the work of Kazuma, Sawada, and Yokoyama[9] and the earlier work of Turner, Pettit, and Ainsley.[10] However, others have suggested[11-13] that the emission near 0.64 eV is due to *EL2*. But, our recent photocurrent work[14] on the crystals showing the 0.635-eV emission showed that O produces a photoassisted thermal recovery effect with 1.1-eV light, which competes with the *EL2* photoquenching effect. This work is consistent with Parker and Bray's absorption work[15] on O-doped *n*-type GaAs. Thus it is clear that distinctly different levels compared to *EL2* are present in O-doped crystals. Furthermore, recent infrared works[16-18] directly showed that the local vibrational mode (LVM) absorption lines at 714, 729, and 845 cm^{-1} are associated with the vibrations of O impurities. So, it is evident that O is directly responsible for various optical signals. In the present work we report the details of the 0.635-eV emission in terms of temperature variation and photoluminescence excitation (PLE). The results show the distinct difference between the 0.635-eV O-related emission and 0.68-eV *EL2* emission. Finally, the characteristics of the 0.635-eV emission are discussed with a configuration coordinate model.

II. EXPERIMENT

Crystals used for the present experiment were grown by the horizontal Bridgman and liquid-encapsulated Czochralski methods. O doping was done by adding Ga_2O_3 to the melt and using wet B_2O_3 ($H_2O \gtrsim 1000$ ppm) as an encapsulant. A room-temperature carrier concentration of 15 samples showing the 0.635-eV emission ranged from $n = 5\times10^6$ to 1×10^{11} cm^{-3}. In addition to the O-doped crystals, undoped semi-insulating crystals were also examined to find any difference of PL characteristics compared to the O-doped crystals. An impurity analysis was made by spark source mass spectrometry. Liquid-helium cryopumping of the ion source region following the bakeout procedure was performed to reduce the residual background impurities such as O and CO. The results were recorded on photoplates and the impurity concentration was determined by an impurity and/or matrix ion intensity in conjunction with the disappearing-line method. It is known that this technique gives accuracies within a factor of 2–3 without specific calibration. The O content in samples showing the 0.635-eV emission was $(3-10)\times10^{15}$ cm^{-3}, whereas the O content in samples showing 0.68-eV emission was $<1\times10^{15}$ cm^{-3}—the approximate detection limit of our spark source mass spectrometer system.

The PL excitation was usually made with the 1.92-eV

line of a Kr-ion laser with a maximum intensity of 500 mW. The diameter of the laser beam spot was 1 mm. However, other excitation sources such as the 2.41-eV line of an Ar laser and the 1.77-eV line of a dye laser were also used in view of the work of Tajima, Iima, and Ishida,[19] and which showed that the peak energy of the 0.68-eV *EL2* emission can vary with excitation energy and can be shifted to 0.63 eV under proper excitation conditions. Spectral analysis of the PL spectrum was obtained with an $f=0.75$ m Spex monochromator using a liquid-nitrogen-cooled PbS detector. The PLE spectroscopy apparatus used monochromatic light from an iodine-tungsten lamp dispersed with an $f=0.25$ m monochromator and a liquid-nitrogen-cooled Ge detector. A lock-in amplifier was used for standard synchronous detection for all measurements.

III. RESULTS AND DISCUSSION

The wavelength dependence on the exciting lasers, described in Sec. II, was studied for the 0.635-eV emission. The peak energy remained at the same level regardless of the excitation energy. The PL intensity of the 0.635-eV emission was larger by more than ~50 times compared to that of the 0.68-eV band at $T=4.2$ K. Therefore, we are confident that our PL measurements are able to discriminate between *EL2* and *EL0*. Figure 1 shows the temperature dependence of the 0.635-eV emission at $T=2-300$ K. At $T=2-40$ K the PL spectrum is mainly due to the 0.635-eV emission, but at $T=40-110$ K the 0.635-eV PL is modified by the presence of a higher-energy transition than the 0.635-eV emission. At temperatures higher than ~110 K, the higher-energy emission disappears and the 0.635-eV emission becomes dominant again.

Figure 2 shows the temperature dependence of the 0.635-eV emission peak energy. The peak energy shifts to a higher energy with increasing temperature from 0.635 to 0.68 eV in the temperature range of 4–300 K. This contrasts with the temperature dependence of the *EL2* 0.68-eV emission. The peak energy of the 0.68-eV emission stays near 0.68 eV over the temperature range of 4–300 K.

Figure 3 shows the full width at half maximum W versus $T^{1/2}$ relation. The solid line is a theoretical fit to the measured data using the configuration coordinate model. The theoretical fit for the experimental 0.68-eV *EL2* emission[7] is presented with a solid line without experimental data. The fits were made by using the expression[20]

$$W=(8\ln 2)S(\hbar\omega)^2(2\bar{n}+1)^{1/2}\,, \tag{1}$$

where S is the Huang and Rhys constant, $\hbar\omega$ the vibrational phonon energy, and $\bar{n}=[\exp(\hbar\omega/kT)-1]^{-1}$. When the nonlinear electron-lattice interaction is assumed the vibrational energy $\hbar\omega$ obtained from Eq. (2) below is the excited-state vibrational energy in the configurate coordinate model. Lattice coupling strength is shown by the Huang and Rhys constant S. When the electron-lattice coupling is strong ($S>5$), luminescence emission shows the Gaussian form without discrete energy levels. The Frank-Condon shift is given by $\Delta_{FC}=S\hbar\omega$. Then the thermal energy E_{th} is given by

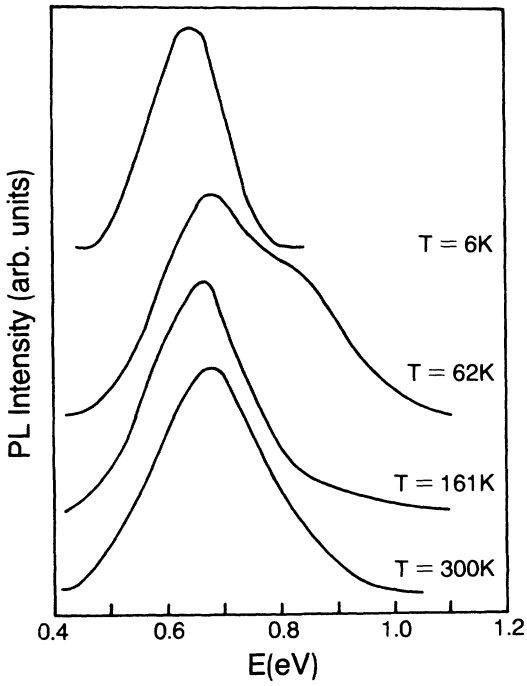

FIG. 1. Photoluminescence spectra of the 0.635-eV emission at various temperatures.

$$E_{th}=E_0+S\hbar\omega\,, \tag{2}$$

where E_0 is the luminescence transition energy. From the fit, we obtain $\hbar\omega=25\pm3$ meV, $S=6.5\pm0.5$, and $\Delta_{FC}=0.163$ eV. Thus a thermal energy of ~0.73 eV from the conduction-band edge is expected for the 0.635-eV emission. A similar thermal energy was observed[7] for the 0.68-eV *EL2* emission using the same method. The values obtained for the 0.68-eV emission were $S=5.5$ and

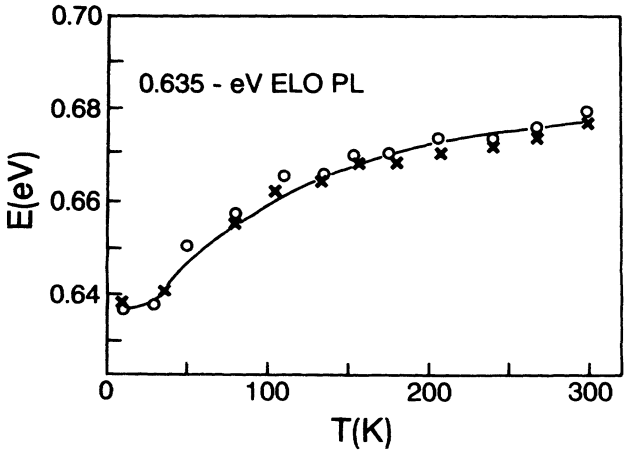

FIG. 2. Peak energy of the 0.635-eV emission vs T relationship for temperatures of 4–300 K for two samples. The solid line is a guide for the eye.

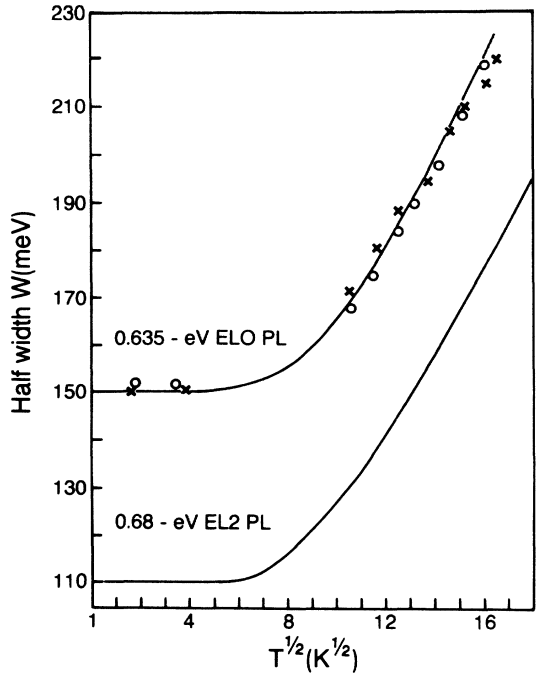

FIG. 3. Full width at half maximum W of the 0.635- and 0.68-eV $EL2$ emission vs $T^{1/2}$ for two samples. Solid lines are the theoretical fits. No experimental data are shown for the 0.68-eV emission.

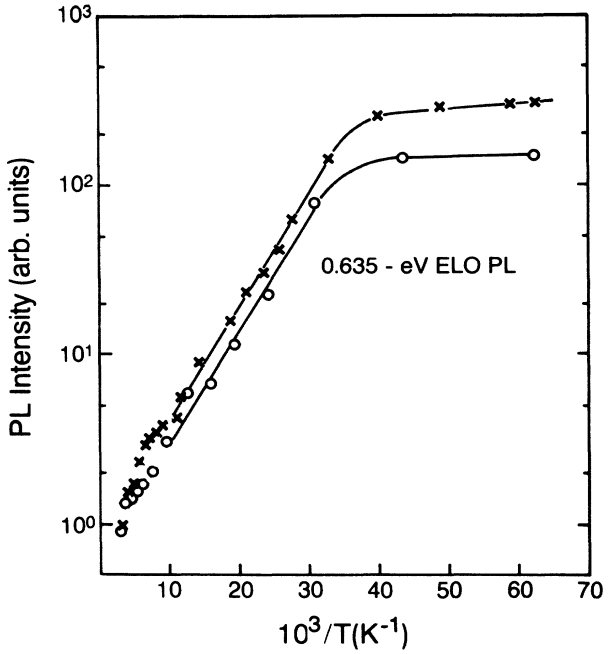

FIG. 4. Photoluminescence intensity of 0.635-eV emission versus $10^3/T$ relation for temperatures of 4–300 K for two samples.

$\hbar\omega = 20$ meV. The positive-energy shift of the 0.635-eV emission with increasing temperature can also be explained[21] by the configuration coordinate model. The shift is positive and opposite to the band-gap variation when the ground-state vibrational energy is larger than the excited-state vibrational energy, assuming the configuration coordinate modes do not change with temperature. Such positive PL peak energy shifts were observed from the Ga vacancy-donor complex[22] and As vacancy-acceptor complex,[23] respectively, present in n- and p-type GaAs.

Figure 4 shows the relation of the 0.635-eV emission intensity versus $10^3/T$ for two samples. The samples show a linear relation between the excitation and emission intensities over the excitation intensity variation of 1–3 decades depending on temperature. A strong decrease of the PL intensity can be represented by a slope of 13 ± 2 meV in the temperature range of 20–140 K. This is derived from the equation

$$I \propto \exp(\Delta E/kT) , \tag{3}$$

which is a form of $I \propto [1 + A \exp(-\Delta E/kT)]^{-1}$, where I is the PL intensity. Another decrease of the PL intensity at $T > 140$ K is represented by a slope of 55 ± 10 meV in the temperature range from ~ 160 to 300 K. At this stage, it is worthwhile to describe the thermal quenching behavior of the 0.68-eV $EL2$ emission. For the 0.68-eV $EL2$ emission we do not see any significant variation of the intensity in the temperature region where the activation energy of $\Delta E_1 = 13$ meV for the $EL0$ emission is observed. However, the $EL2$ PL intensity rapidly decreases in the temperature range from ~ 160 to 300 K. The relation of the PL intensity versus $10^3/T$ yields an activation energy of $\Delta E_2 = 55\pm10$ meV, which is the same as that observed for the $EL0$ emission in the same temperature range. So, we observe two activation energies of $\Delta E_1 = 13$ meV and $\Delta E_2 = 55$ meV and one activation energy $\Delta E_2 = 55$ meV, respectively, for the $EL0$ 0.635-eV and $EL2$ 0.68-eV emissions.

The thermal activation energy of $\Delta E_2 = 55$ meV obtained from both $EL2$ and $EL0$ emissions can be attributed to the presence of the nonradiative multiphonon capture process,[24] since the PL intensity varies with temperature as the inverse of the electron capture cross section when the nonradiative multiphonon process competes with radiative recombination. The capture cross section of an electron, n, for $EL2$ has been measured as the form[25] of $n = 5\times10^{-19}$ (cm^2)$+6\times10^{-15}$ (cm^2) exp[-56.6 (meV)$/kT$]. The electron-capture cross section of $EL0$ was shown[1] to follow the same temperature characteristics as that of $EL2$ in the temperature range of 260–450 K. So, we consider that the activation energy[1,25] obtained from the capacitance measurements is the same as ΔE_2 obtained from our temperature-dependent measurements. Thus the presence of ΔE_1 is unique for $EL0$ emission. The thermal activation energy ΔE_1 can be explained as follows.

(i) Other radiative centers compete with the 0.635-eV emission.

(ii) An energy state of the deep $EL0$ center is present at the energy level lower by 13 meV than the conduction-band edge.

(iii) The $EL0$ center is associated with a neighbor that has the same binding energy as ΔE_1.

However, we can rule out easily process (i) since we do not find any enhancement of PL intensity of other transi-

tions with increasing temperature. We will discuss processes (ii) and (iii) later.

Figure 5 shows the PLE spectra obtained from two samples. The PLE spectrum consists of a pronounced oscillation at energies larger than the band gap, at the below-band-gap peak at ~ 1.502 eV, and at the PLE onset near 1.49 eV. The pronounced oscillatory structures extend from the band-edge region to ~ 1.90 eV. The period of oscillation is 41.2 ± 0.5 meV. A similar oscillatory feature was previously observed for other GaAs emissions. The observation of the oscillation for a deep-center *EL*0 leads to a nature of the conduction electron-capture process into the deep center; namely, since a deep center is not expected to show any oscillatory change in the electron-capture process as a result of the different energy of the conduction-band electron, the oscillatory behavior must be attributed to indirect conduction-band electron capture into the deep center through a shallow donor state. In other words, the oscillatory structure of the 0.635-eV emission is due to the energy relaxation of the conduction-band electron through a successive longitudinal optical phonon with the energy-dependent capture of the conduction-band electron by a deeper donor via a shallow donor state. The energy relation for the PLE spectrum then can be represented as

$$E_n = E_g + (n\hbar\omega_{\mathrm{LO}} - E_d)(1 + m_e/m_{\mathrm{hh}}) , \tag{4}$$

where n is an integer and E_d is the shallow donor binding energy. The arrows in Fig. 5 show the calculated energy E_n. The parameters used are $E_g = 1.5196$ eV, $\hbar W_{\mathrm{LO}} = 36.7$ meV, $E_d = 5.8$ meV, and $m_e/m_{\mathrm{hh}} = 0.124$. ($m_e$ and m_{hh} are the effective electron and heavy-hole masses, respectively.)

Temperature was varied in order to study the 1.502-eV PLE peak. The PLE intensity of the 1.502-eV peak decreases with increasing temperature in the range 10–60 K. The PLE intensity versus $10^3/T$ relationship gives an activation energy of 7 ± 2 meV. The present value differs considerably from the 30 meV obtained with a deep-center emission by Shanabrook *et al.*[11] We attribute the activation of 7 meV as the thermal energy of the shallow donor. Then, the valence-band–to–donor transition is responsible for the 1.502-eV PLE peak. However, $E_g - E_d$ for the effective-mass donor is larger than 1.502 eV. This discrepancy can be attributed to the perturbed conduction- and valence-band edges due to the ionized donors and acceptors, which effectively deepen[26] the donor state compared to the usual unperturbed case. The 1.49-eV onset corresponds to the conduction-band–to–shallow-acceptor transition. C_{As} is present as the main shallow acceptor in Czochralski- and Bridgman-grown semi-insulating GaAs. Thus the 1.49-eV onset and subsequent PLE can be attributed to the increase of the conduction-band electron originating from the electron excitation of the C_{As}.

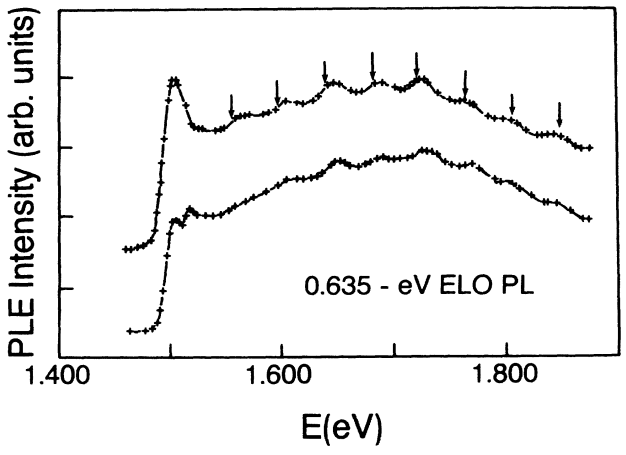

FIG. 5. Photoluminescence excitation spectra of the 0.635-eV emission from two samples. The arrows show E_n of Eq. (4).

Wager and Van Vechten[27] proposed an atomic model for the *EL*0 center and for *EL*2. *EL*0 consists of an O an As site donor as a nearest neighbor to a divacancy $V_{\mathrm{Ga}}V_{\mathrm{As}}$ for the normal state, V_{As}^{+}-O_{As}-V_{Ga}^{-} and an O and Ga site acceptor between two As vacancies, and V_{As}^{+}-O_{Ga}^{-2}-V_{As}^{+} for the metastable state. Recent LVM studies[16–18] show that O may exist in GaAs in two forms: interstitial O at 840 cm^{-1} of LVM absorption and V_{As}-O complexes with two LVM lines *A* and *B* at 735 and 714 cm^{-1}, respectively. The normal and metastable states of the two *A* and *B* LVM lines were tentatively explained by the different charge states of O (Ref. 18) or V_{As} (Ref. 17). Also, a deep donor at $E_c - 0.43$ eV was attributed[17] to the V_{As}-O center. However, it is not clear how the *EL*0 center responsible for the 0.635-eV PL emission fits into this explanation of LVM lines.

The positive shift of the 0.635-eV emission transition energy with increasing temperature and our fit to the configuration coordinate model indicate that the center responsible for the 0.635-eV emission is due to a nearest-neighbor associate of O with another element similar to the V_{Ga}-donor complex[22] in *n*-type materials and the V_{As}-Zn(Cd) complex[23] in *p*-type materials. Also, the cation vacancy-donor complexes are the well-known self-activated luminescence centers[28] in II-VI compounds. Paget and Klein earlier proposed[29] a model for a 0.64-eV band with a deep-donor–shallow acceptor pair with a well-defined separation between them. In our model we attribute the associate of O to an intrinsic acceptor V_{Ga}, namely, V_{Ga}-O_{As}, based on the nature of V_{Ga}. Also, an enhancement of the PL intensity of the usual neutral effective-mass donor-C_{As} acceptor-pair transition was observed in the below–band-gap energy of 0.9–1.4 eV after transforming the 0.635-eV emission to a metastable state. The enhancement is the same as the quenching spectrum of the 0.635-eV *EL*0 emission. The enhancement peak is at the same energy of the maximum quenching. The enhancement of the donor-C_{As} acceptor-pair emission intensity is due to the rearrangement of the photon flux arising from the competitive radiative process involved in the donor-acceptor pair and 0.635-eV emission after the transformation of the 0.635-eV emission center into the metastable configuration. (The above two transitions are the only radiative transitions in the energy region from the band edge to midband gap.) This shows that the C_{As}

is not involved in the formation of the 0.635-eV emission center. It is likely that the majority of C acts as an isolated shallow acceptor. Other shallow acceptors such as Mg, Si, and Zn are present in the bulk semi-insulating materials. However, the concentration is relatively small compared to C. The presence of stable isolated V_{Ga} in semi-insulating GaAs has never been established. However, it can be assumed that the V_{Ga} level lies near the valence band and acts as a multiple acceptor on the basis of theoretical[30,31] and experimental[32] works. When a defect complex, V_{Ga}-O_{As}, is formed, the energy levels of the individual constituents may change. However, Sankey *et al.*[33] find that the level spectrum of a complex is nearly the sum of the energy levels of the complex's constituents. This indicates that we can assume that the ground and excited states of the configuration coordinate diagram originate, respectively, from the V_{Ga} and O_{As} levels. The identification of O_{As} as a deep donor is supported by theoretical work[30] and experimental work[34] on GaP:O. The role of the effective-mass shallow donor, deduced from the 1.502-eV PLE peak, is not direct in the radiative recombination process of the 0.635-eV emission but only indirect since the donor state acts as an intermediary in the electron-capture process into the deep O_{As} donor. Now, we return to the possible identification of the thermal activation energy $\Delta E_1 = 13$ meV, which is present only for *EL*0 emission in the relation of PL intensity versus $10^3/T$. ΔE_1 can be a level of the complex center V_{Ga}-O_{As} or can originate from a neighbor associated with the V_{Ga}-O_{As} center. When we invoke V_{As} for the neighbor, which is known as a donor and is present[30] near the conduction-band edge, the center responsible for *EL*0 would be a defect consisting of O_{As}, V_{As}, and V_{Ga}. Basically, this is the model proposed[27] by Wager and van Vechten for *EL*0. This model also satisfactorily explains the metastability of the *EL*0 center by placing the different charge states, O_{Ga}^{-2} and O_{As}^{0}, for the metastable and normal states, respectively. However, we feel that further studies are needed for a better clarification of this issue. In general, the experimental data can be explained with a configuration coordinate model as described above. Figure 6 shows such a diagram for the 0.635-eV emission.

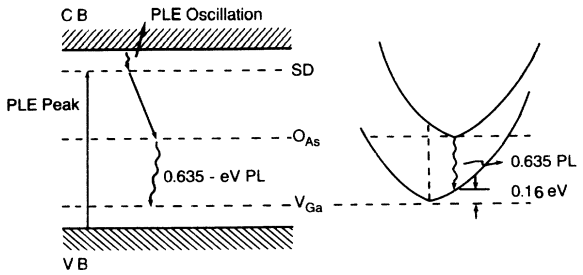

FIG. 6. (a) Schematic diagram of the 0.635-eV emission radiative process, the photoluminescence excitation peak due to the valence-band–to–effective-mass donor transition, and (b) the configuration coordinate diagram for the 0.635-eV emission.

IV. CONCLUSION

We have shown that the photoluminescence characteristics of the 0.635-eV *EL*0 emission differ from those of the 0.68-eV *EL*2 emission in terms of the transition energy, the full width at half maximum, low-temperature (2–20 K) photoluminescence intensity, and the temperature dependence of the transition energy (the 0.635-eV emission shifts to a higher energy with increasing temperature, whereas the 0.68-eV emission stays at the same energy). The configuration coordinate model is introduced to explain the observed configuration coordinate model; the ground and excited states are assumed to originate, respectively, from V_{Ga} and O_{As} levels. Thus, a complex nearest-neighbor center is introduced as the model for the *EL*0 center We find that the configuration coordinate model with the above complex explains the experiment very well.

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