Comments

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Comment on "Atomic model for the *EL*2 defect in GaAs"

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The excited state of the intracenter transition associated with *EL*2 centers in GaAs is found to be degenerate with the conduction band. This is in disagreement with the atomic model proposed by Wager and Van Vechten.

The atomic model for *EL*2 centers in semi-insulating GaAs proposed by Wager and Van Vechten[1] (WV) seems to account partially for what is known experimentally. Their model shows that the stable state of *EL*2 consists of a divacancy on one side of an As_{Ga} antisite and the metastable state corresponds to the As_{Ga} antisite which separates the two vacancies. The intracenter transition responsible for the energy band 1.03–1.27 eV is interpreted by this model as the excitation of V_{Ga} to a final state which is not resonant with the conduction band until the photon energy exceeds 1.35 eV.

In this comment, we show that the intracenter transition may not be related to V_{Ga} but it is related to another component of *EL*2. In addition, the zero-phonon line (ZPL) associated with this intracenter transition has been observed for photon energies larger than 1.35 eV.

A typical optical absorption[2] of the *EL*2 center in GaAs shows three distinguishable threshold regions, at 0.82, 1.03, and 1.27 eV. These regions were related to transitions from *EL*2 to the conduction band,[3,4] an intracenter transition[5] within *EL*2 that leaves the electrons localized, and a transition from the valence band to an acceptor level associated with the *EL*2 center,[6] respectively. The intracenter transition was interpreted as an A_1 to T_2 transition[4] and an A to E transition.[2,7] Both intrepretations relate this transition to an As_{Ga} antisite with the excited state degenerating low in the conduction band. These interpretations are in excellent agreement with the theoretical predictions[7–10] and in disagreement with the WV model.

According to the WV model, the excited state of the intracenter transition is resonant with the conduction band only for photon energies larger than 1.35 eV. In addition, this model predicts that the ZPL is not observed at all for the intracenter transition when the excited state becomes resonant. These interpretations are in disagreement with the Fourier-transform infrared-absorption measurements.[2] We have used various filters to control the photon energy. The results show that the ZPL is observed for photon energies both smaller and larger than 1.35 eV. This leads to the assertion that the intracenter transition cannot be related to V_{Ga} with a ground state $E_{-/0}(V_{Ga})=E_v+0.01$ eV.

To support this claim we tested the WV model against the experimental results of Samuelson and Omling.[11] Samuelson and Omling made attempts to trace *EL*2 from GaAs to GaP and found that the metastable state disappears for $x>0.3$ where x is the index in $GaAs_{1-x}P_x$. At this value of x, the excited state of the intracenter transition emerges out of the conduction band. This is under the assumption that the intracenter transition is related to the *EL*2 ground state. The mechanism of the disappearance of the metastable state is not known. However, Samuelson and Omling speculated that it may be necessary for the final state to be degenerate with the conduction band in order for it to populate or transform to the metastable state. This is in excellent agreement with the assertion that the metastable state is finalized via the resonant state.[12]

Although the reasons for the degeneracy of the final state of the intracenter transition with the conduction band are now known, the WV model is unable to explain such behavior. Also it is difficult to understand the association of vacancies that annealed out at temperatures of approximately 670 K with *EL*2, which is stable up to 1070 K.[13,14]

In conclusion, the intracenter transition observed in the optical-absorption measurements may not be related to V_{Ga}, but it is related to another component of *EL*2, most likely the As_{Ga} antisite.

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