As_{Ga}-Induced Dichroism in GaAs

In a recent Letter, Meyer, Spaeth, and Scheffler[1] reported a magnetic circular dichroism (MCD) study of the As_{Ga}-antisite defect in GaAs. The two observed MCD absorption bands were interpreted[1] as transitions from the ground state to *two* excited, resonant T_2 states of the singly ionized As_{Ga} double donor, D^+. On the basis of this model it was argued[1] that the ubiquitous $EL2$ level in GaAs[2] is *not* related to the As_{Ga} defect. It should be pointed out that there is no independent support for the existence of *two* excited T_2 states[3] of $As_{Ga}{}^+$ and that such a model predicts two symmetrical derivative-shaped MCD features, whereas the data indicate one derivative- and one bell-shaped MCD band.

In this Comment an alternative interpretation for the As_{Ga}-induced MCD bands is presented. The key is that the two bands have low energy thresholds close to 0.83 eV and 1.13 eV, respectively, the energy difference between the thresholds thus being close to the Γ_8-Γ_7 valence-band spin-orbit splitting, $\Delta_{s.o.} = 0.34$ eV, of GaAs. It is therefore suggested that the two MCD bands correspond to transitions of a hole from the first donor level (D^0/D^+) of As_{Ga} to the Γ_8 and Γ_7 valence bands, respectively: $D^+ + h\nu \rightarrow D^0 + h_v$. Electron-spin-resonance measurements have established[4] that the D^0/D^+ level of As_{Ga} is close to the low energy threshold of the MCD absorption curve of Meyer, Spaeth, and Scheffler.[1]

The MCD transition suggested here is basically an $E1$-allowed $s \rightarrow p$ transition since the As_{Ga} ground state has A_1 symmetry[3] and the uppermost valence band has T_2 orbital symmetry at Γ. Inclusion of spin-orbit coupling splits T_2 into the Γ_8 and Γ_7 valence bands. For nonzero k values, an additional, smaller splitting results from the heavy-hole–light-hole splitting of Γ_8.[5] Thus, the simplest analog is an alkali-atom-like level scheme with the excited Γ_8 level split into two Kramers doublets. This model predicts[6] a derivative-like MCD feature followed by a bell-shaped MCD band at higher energies with an intensity ratio of -3:1:2 in the sequence of increasing energy. Electron-phonon coupling and the dispersion of the three T_2 subbands in the vicinity of the Γ point serve to broaden the MCD transitions but broadening due to the latter effect is much less than might be expected.[7] The above simple intensity ratio may then no longer be strictly valid but the predicted MCD curve retains a shape consistent with the experimental curve.

It is thus seen that the original interpretation of the As_{Ga} antisite-induced MCD in undoped GaAs is neither unique nor free of deficiencies. Therefore the conclusion,[1] that the $EL2$ level[2] is not related to As_{Ga} appears very doubtful. In fact, the integrated MCD absorption curve of As_{Ga} is remarkably similar to the optical-hole ionization cross section, $\sigma_p^0(h\nu)$, of the $EL2$ level.[8].

Very fruitful discussions with J. Windscheif, R. Cox, R. Romestain, and J. Schneider are highly appreciated.

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Received 15 May 1984
PACS numbers: 71.55.Fr, 76.70.Hb, 78.20.Ls, 78.50.Ge

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