Origin of Deep Localization in $GaAs_{1-x}Bi_x$ and its Consequences for Alloy Properties

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Introduction

The addition of Bi isoelectronic dopants to GaAs provides an attractive avenue for tailoring its electronic band structure, yet it also introduces less appealing and very strong hole localization. The origin of the localization is still not thoroughly understood, which has in part inhibited the practical use of $GaAs_{1-x}Bi_x$ alloys. In this study, the evolution of hole localization was evaluated as a function of composition. We find that spatial overlap of Bi-related bound states at concentrations >0.6% Bi effectively enables holes to be channeled to those at the lowest energies, thereby aiding localization of excitons >150 meV below the band gap. The large energy gap between these bound states and the GaAs valence-band edge combined with the slow upward movement of the valence band with composition causes deep localization to persist to high concentrations >6% Bi. The results provide important insight into the optical and transport behavior of $GaAs_{1-x}Bi_x$ and its implications for device applications.

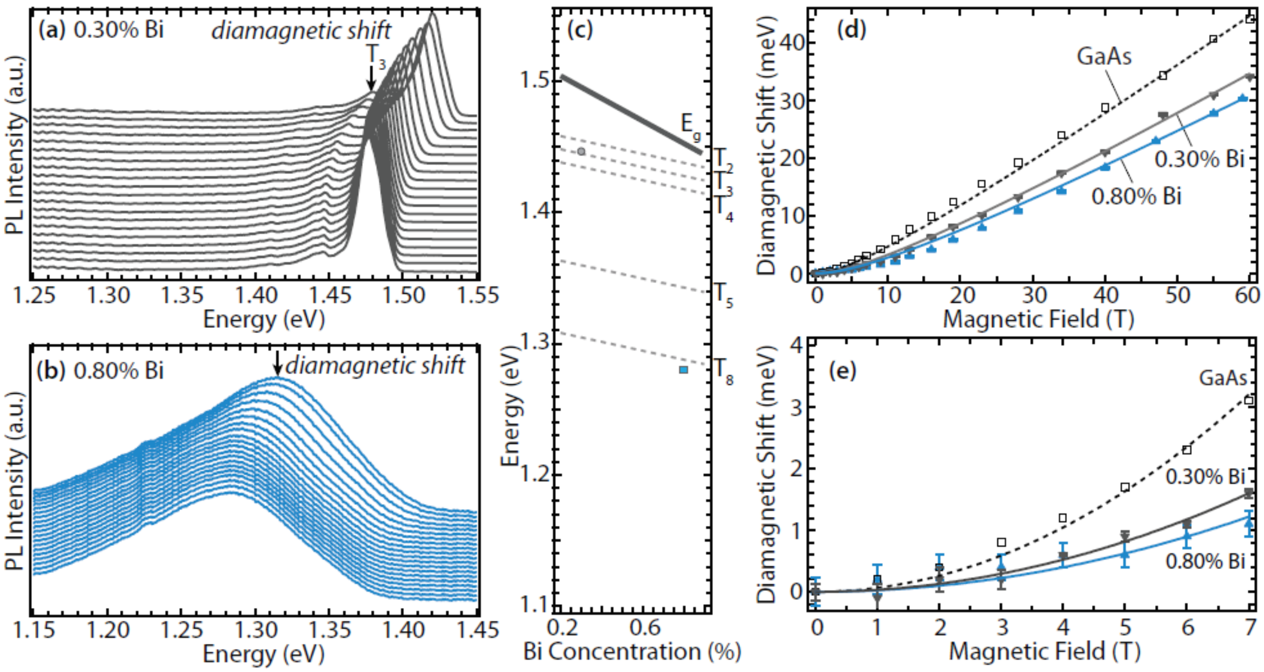

Figure: PL spectra measured at 1.5 K in magnetic fields up to 60 T for samples with Bi concentrations of (a) 0.30% and (b) 0.80%. (c) Zero-field PL peak energies for both samples. The diamagnetic shift of the PL peaks for both dilute bismide samples and the (A_0, X) peak of GaAs (spectra not shown) for the full range of magnetic fields (d) and the low-field region (e) are also displayed.

Results and Discussion

We study the evolution of localization in $GaAs_{1-x}Bi_x$ alloys as a function of composition in the range 0.26 to 1.75% Bi using a combination of variable temperature, time-resolved, and magneto-PL techniques to distinguish between localized and delocalized states. Alloys with Bi concentrations <0.4% Bi exhibit narrow emission signatures from bound Bi-related states near the VBE as well as lower-energy emission associated with deeper states. Alloys with Bi concentrations >0.6% Bi exhibit a single broad emission peak well below the band gap energy. By following the evolution between those two regimes in a detailed and systematic manner, we are able to determine that PL from samples with Bi concentrations >0.8% is pinned by a very deep Bi-related bound state. By identifying the fundamental origin of the deep localization in $GaAs_{1-x}Bi_x$ we are further able to predict that localization dominated by Bi-related bound states will transition to alloy-disorder-driven localization at concentrations >6%. This insight and high-level view of localization behavior in $GaAs_{1-x}Bi_x$ importantly suggest that optoelectronic devices fabricated with $GaAs_{1-x}Bi_x$ containing roughly >6% Bi will suffer less from strong localization than those containing <6%.

References

[1] Alberi, K. *et al.*, Physical Review Materials **2**, 114603 (2018).