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Model of V_{Hg} Incorporation in Arsenic-Doped HgCdTe: First-Principles Calculations

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Following the suggestion that the As_{Hg}–V_{Hg} and As_{Hg}–$2V_{Hg}$ defect complexes are potential sources of carrier compensation observed in As-doped HgCdTe, we have studied the electronic properties and formation energies of these complexes. We find that these complexes are electrically active acceptors but have exceedingly high formation energies, meaning that they play no role in carrier compensation except at low temperatures. V_{Hg} will thus likely remain as an isolated defect. Such a model of V_{Hg} incorporation allows us to further predict the postgrowth As activation. Our prediction emphasizes the As_{Hg}–$2V_{Hg}$ complex as the starting defect for As activation, rather than the As_{Hg}–V_{Hg} pair as previously suggested.

Key words: Arsenic-doped HgCdTe, first-principles calculations, Hg vacancies

INTRODUCTION

There has been considerable interest in the use of arsenic (As) as a *p*-type dopant in epitaxial HgCdTe.[1–3] Unfortunately, the doping process lacks good control because of the amphoteric nature of As in HgCdTe—arsenic in as-grown materials behaves as a compensated donor and can be activated as a desired acceptor through postgrowth annealing.[4,5] Major efforts in the last few years have been made to search for effective activation schemes experimentally; nevertheless, the nature and origin of the defects that lead to the carrier compensation in as-grown materials remain the least understood issue, being a crucial step towards controlling the conversion of As from a donor to an acceptor.

Since the growth of high-quality HgCdTe is confined to the Te-rich region, the materials are considered to contain a large number of Hg vacancies (V_{Hg}), which are available for the As dopants to be incorporated as substitutional As_{Hg} donors. Electrical measurements have shown that the as-grown materials are weakly *n*-type,[6] indicating that the native defects strongly affect the electronic properties of As_{Hg} donors. Its shallow acceptor character and exceedingly high concentration lead to the accepted wisdom that the V_{Hg} defect is responsible for the reduced electrical activity of As_{Hg} donors. In view of HgCdTe with narrow gap and compensating conductivity, it is difficult to provide direct experimental evidence for such wisdom. So far, the As_{Hg}-to-V_{Hg} transition has been detected by Shao et al.[7–11] through specific photoluminescence (PL) measurements, confirming that the presence of V_{Hg} is one cause for the compensation. It seems that the coexistence of As_{Hg} and V_{Hg} would offer a possibility for the combination of As_{Hg} donors and V_{Hg} acceptors, but the optical signals related to As_{Hg} + V_{Hg} defect complexes were not observed. These experiments thus cast doubt on the most widely invoked argument of the defect complexes associated with As_{Hg} and V_{Hg} as a potential source of the compensation.[5,11–18]

Prior to the PL studies, *ab initio* calculations by Berding et al.[6,13–18] predicted that the As_{Hg}–V_{Hg} pair is the starting defect for the activation of As_{Hg} donors. They explained the critical reliance of the

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