

Interaction Between As_{Hg} and V_{Hg} in Arsenic-Doped $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$

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Arsenic-related defect complexes have been proven responsible for the charge-compensation effects in arsenic-doped $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, but the underlying mechanism is still unclear. In this study, we systematically investigated the interaction between arsenic donor (As_{Hg}) and mercury vacancy (V_{Hg}) versus the $\text{As}_{\text{Hg}}-V_{\text{Hg}}$ separation in arsenic-doped $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ using first-principles calculations. A new long-range interaction between As_{Hg} and V_{Hg} is found, and the related binding energies and electronic structures are calculated to reveal its coupling mechanism. Our results show that V_{Hg} can increase the distortion of the lattice collaboratively with As_{Hg} due to the different characteristics of As_{Hg} and V_{Hg} in distorting the lattice. The relaxational enhancement as well as the electrical compensation of the As_{Hg} donor is weakened as V_{Hg} moves away from As_{Hg} , and the underlying mechanism is revealed. In addition, a set of defect levels in the band gap generated from the donor-acceptor interaction are also shown, and the origin of these levels is explored. The results of this work are important for theoretically explaining the characteristics of complicated defect levels found in experiments.

Key words: Arsenic-doped $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, first-principles calculation, defects, long-range interaction

INTRODUCTION

$\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ layers grown by molecular beam epitaxy (MBE) are widely used for infrared focal-plane arrays. To fabricate p -on- n heterojunctions in infrared detectors, $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ materials are needed with both n -type and p -type doping. The group V element arsenic has been proven to be a good source for p -type doping of $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, as it shows low diffusivity and a relatively high sticking coefficient in low-temperature MBE growth.^{1,2} However, controlled p -type doping remains a critical problem in $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$ because of the amphoteric behavior of

arsenic.^{3,4} Arsenic can substitute at Hg sites or Te sites, and thus act as a donor or acceptor, respectively. The detailed configurations of arsenic-related substitutional defects (As_{Hg} or As_{Te}) depend on the material growth environment. Experiments have shown that arsenic is expected to substitute Hg in Te-rich epitaxial growth environments. To activate p -type conductivity, a two-stage annealing process is needed to transfer arsenic to Te sublattice sites.^{5,6}

In addition to arsenic-related point defects, native defects, especially mercury vacancies (V_{Hg}) with double acceptor levels, have been found to be abundant in as-grown arsenic-doped $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$. It is thought that intrinsic vacancy defects are important in controlling the electrical properties of materials.⁷⁻⁹ Furthermore, V_{Hg} has been considered

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