Comparison of Different Models for Arsenic Activation in HgCdTe

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***Abstract*—Arsenic doping of HgCdTe has proved problematic. Two-step anneals are usually required to activate the dopant. The model frequently used to explain p-type doping with arsenic requests an amphoteric nature of group V atoms in the II–VI lattice. This requires that group VI substitution with arsenic only occurs under mercury-rich conditions either during growth or the subsequent annealing, and includes site transferring of the As. However, there are inconsistencies in the amphoteric model and unexplained experimental observations. A new model, based on defect-mediated diffusion of the arsenic, is therefore proposed.**

I. INTRODUCTION

HgCdTe is the most commonly used material for infrared detection. For its band gap being tunable with cadmium composition, it can be used to fabricate infrared detectors over a wide infrared spectrum range, from short wave lengths of 1 μm to very long wave lengths of 20 μm [1]. Arsenic is the acceptor dopant of choice in molecular beam epitaxy (MBE) of HgCdTe. The advantages of arsenic include its low diffusivity and the fact that it is a shallow acceptor. A problem related to arsenic doping is caused by the manner of its incorporation in HgCdTe. As-grown MBE HgCdTe:As films typically show n-type conductivity. It was suggested that the reason for that is the amphoteric nature of As, which can occupy cation sites in HgCdTe as a donor As_{Hg} and tellurium sites as an acceptor As_{Te}. Under typical MBE conditions (Te-rich), arsenic is generally incorporated in HgCdTe as a donor. An activation of the arsenic acceptor is necessary to achieve p-type conductivity. This activation process is performed usually through a post-growth anneal that produces As_{Te} acceptors.

There are still many unknowns regarding arsenic p-doping [2]. One of the major puzzling is a knowledge of the As incorporation site before and after thermal activation. The proposed model by Berding *et al.* that arsenic is incorporated into mercury lattice sites during MBE growth under tellurium-rich conditions and that the high temperature annealing enables a site transfer of the arsenic atoms, i.e. from mercury lattice sites to tellurium sites was generally accepted [3]. However, in as-grown films, defects associated with arsenic incorporation are found; they also affect electrical and optical properties of HgCdTe [4-5]. In this work, we present a theoretical investigation of arsenic activation in HgCdTe considering different models. With help of the first principle calculations, we also proposed a new model to depict the corresponding diffusion mechanism.

II. RESULTS

There is no general consensus on the precise diffusion mechanism for arsenic in HgCdTe. To judge which model is rather reasonable, we need to get the magnitude of migration barrier. In the case of arsenic activation in HgCdTe, defect-mediated diffusion of arsenic is generally accepted. Firstly we require the creation of the relevant defects that represent different models, and then the migration of that defect. Fig.1 presents the migration barrier profile for arsenic in HgCdTe under different conditions. Comparing the height of barrier, we can find that Berding's model is prior to Shaw's and Schaake's ones. Note that tellurium antisite (Te_{Hg}) is always exits in as-grow MBE HgCdTe films, the model based on Te_{Hg} is proposed. The new model is more acceptable than the Berding's one for its low migration barrier. Also, it can explain the arsenic complexes found in recent experiments very well.

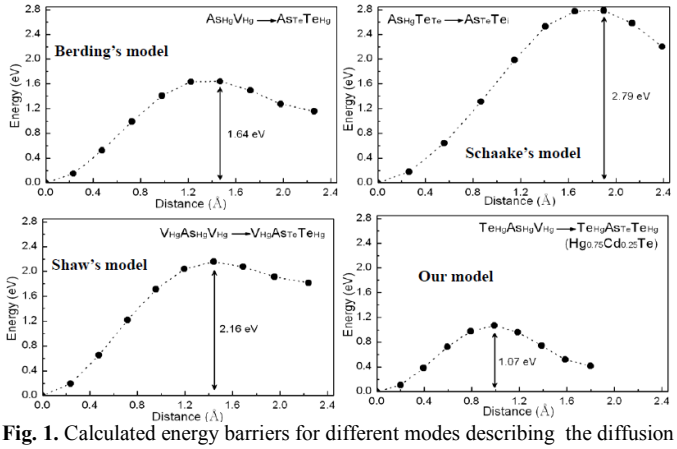

Fig. 1. Calculated energy barriers for different modes describing the diffusion of the arsenic in HgCdTe.

III. SUMMARY

In conclusion, a new model based on the tellurium antisite was introduced to account for arsenic activation in HgCdTe. The diffusion behavior of arsenic depends on Te_{Hg} and mercury vacancy. Reasonable agreement between experimental discoveries and model prediction was found. Moreover, a comparison between our model and other theoretical models has been made and their relationship was discussed.

REFERENCES

[1]. A Rogalski, "HgCdTe infrared detector material: history, status and outlook," *Rep. Prog. Phys.* Vol. 68, pp. 2267–2336, 2005.

[2]. J. W. Garland, C. Grein, and S. Sivananthan, "Arsenic p-doping of HgCdTe grown by Molecular Beam Epitaxy (MBE): A solved problem?" *J. Electron. Mater.,* vol. 42, pp. 3331-3336, 2013.

[3]. M.A. Berding, A. Sher, M.V. Schilfgaarde, A.C. Chen, and J. Arias, "Modeling of arsenic activation in HgCdTe,"*J. Electron. Mater.,* vol. 27, pp. 605-609, 1998.

[4]. F. Gemain, I. C. Robin, S. Brochen, P. Ballet, O. Gravrand, and G. Feuillet, "Arsenic complexes optical signatures in As-doped HgCdTe," *Appl. Phys. Lett.,* vol. 102, pp. 124104, 2013.

[5]. I.I. Izhnin, S.A. Dvoretsky, K.D. Mynbaev, O.I. Fitsych, N.N. Mikhailov, V.S. Varavin, M. Pociask-Bialy, A.V. Voitsekhovskii and E. Sheregii, "Defect study in molecular beam epitaxy-grown HgCdTe films with activated and unactivated arsenic," *J. Appl. Phys.*, vol. 115, pp. 163501, 2014.