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KINETIC MONTE CARLO SIMULATION OF GaAs GROWTH ON (001) SILICON

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SUMMARY

We studied antiphase boundaries (APB) suppression during the growth of GaAs on Si (001) substrates. The kinetics of anisotropic growth is described by Kinetic Monte-Carlo (KMC) simulations that reveal atomic details of the growth.

1. INTRODUCTION

The direct growth of III-V semiconductors on silicon substrates is of major interest for integrated photonics. However, it is plagued by various crystal defects. In particular, antiphase domains (APDs) are delineated by antiphase boundaries (APBs), 2D defects that act as shorts when they reach electrically active regions of devices [1]. Recently, Gilbert *et al.* demonstrated a growth strategy for APB suppression by APD burying during GaAs growth on (001) Si substrates [2]. In this work, we simulate the growth of GaAs on Si using the Kinetic Monte-Carlo (KMC) method, to better understand the APD burying mechanism.

2. KMC MODEL

We have developed an out-of-equilibrium model of GaAs growth on Si. KMC describes stochastic events such as adatom arrival and diffusion on a growing surface. The growth dynamics is analyzed via a Monte-Carlo solid-on-solid model where the process rates depend on nearest neighbor interactions and main crystallographic directions. First, the Si and GaAs surface energies are chosen to reproduce a 3D Volmer-Weber growth mode of GaAs on Si. Then, the anisotropy of the diffusion and incorporation events [3] is taken into account by considering different energetic barriers depending on the main crystallographic directions.

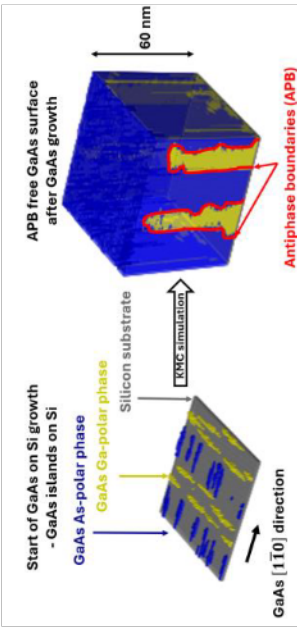


Figure 1 GaAs on Si APB burying by KMC simulation

3. RESULTS

Our simulations show that small differences between the diffusion energy barriers between [110] and $[1\bar{1}0]$ GaAs directions impact the domain growth. KMC simulations show that the As-polar phase slowly buries the Ga-polar phase during the growth, eventually resulting in an APB-free surface as shown in [2]. This work confirms that APD burying is due to the anisotropic diffusion and incorporation of Ga atoms on the GaAs surface, which leads to preferential growth directions depending on the GaAs phase.

4. ACKNOWLEDGMENTS

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5. REFERENCES

- [1] H. Kroemer, J. Cryst. Growth **81**, 193 (1987).
- [2] A. Gilbert, M. Ramonda, L. Cerutti, C. Cornet, G. Patriarche, É. Tournié, and J. Rodriguez, Adv. Opt. Mat. **11**, 2203050 (2023).
- [3] K. Ohta, T. Kojima, and T. Nakagawa, J. Cryst. Growth **95**, 71 (1989).