Ion Irradiation Simulations to Study Quantum Dot Formation in III-V Semiconductors

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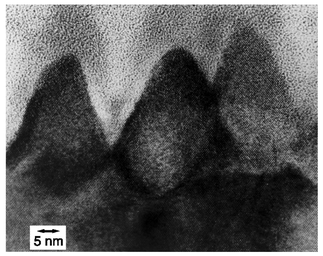
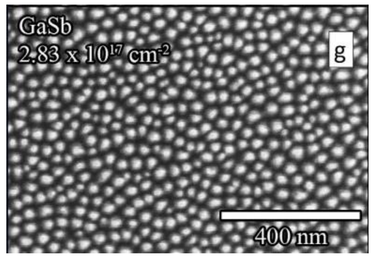
Background

- Ion irradiation is a scalable technique to fabricate unique nanostructures on surfaces of semiconductors.
- Irradiation-induced **quantum dot** formation was first observed on gallium antimonide (GaSb) [1].



Cross-sectional TEM image of nanostructures on a GaSb surface [1].

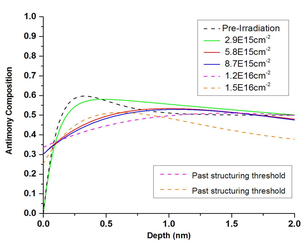


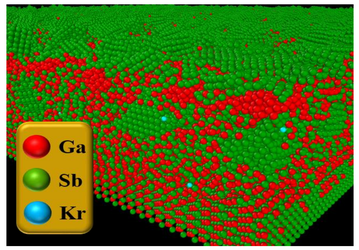
SEM micrograph of irradiated GaSb under 500 eV Kr+ ions [2].

- Theoretical model of quantum dot emergence on GaSb is not well developed.

Motivation

- Recent experiments suggest that nanopatterning is a **composition-driven mechanism**.



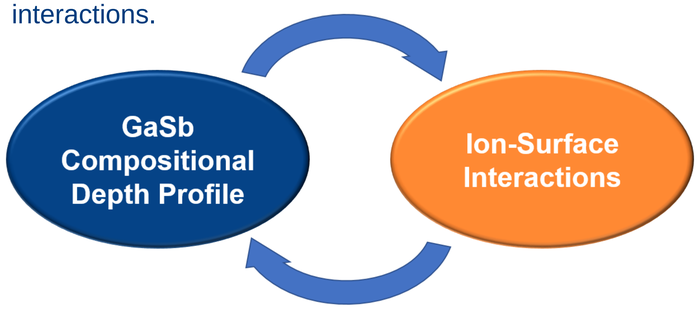


(Left) ARAES data on the depth-dependent Sb composition under 500 eV Kr+ ion. (Right) Molecular Dynamics simulation output showing phase separation of GaSb.

- The formation of such metastable phase separation is evident in **atomistic Molecular Dynamics (MD) simulations**.

Key Focuses:

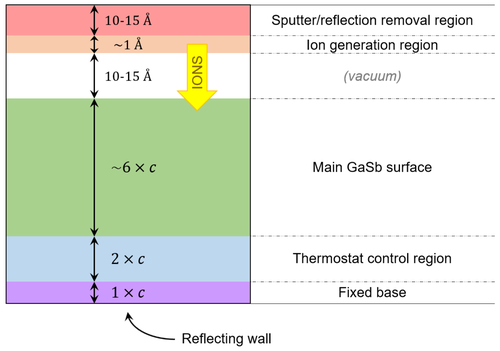
1. Understand how the GaSb compositional depth profile responds to prompt interactions with incident ions.
2. Analyze how the compositional profile governs ion-surface interactions.



Methodology

Types of Simulations

1. Crystalline GaSb response to ion irradiation.
2. Single ion implantation in four GaSb compositional depth profiles.



Schematic of the simulation environment.

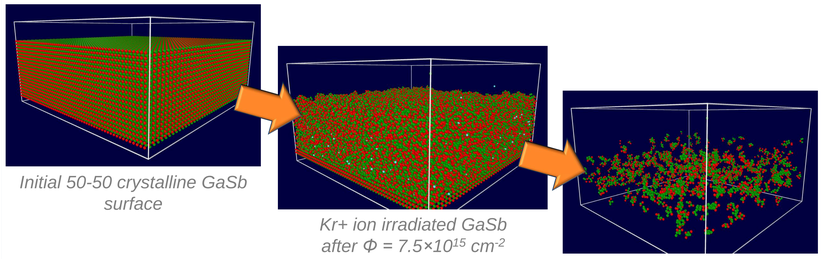
Simulation Constraints

- MD simulations are carried out using LAMMPS [3].
- Lateral periodic boundary conditions, fixed boundary on bottom, free top boundary.
- Reflecting wall or second removal zone at bottom prevents loss-of-atom errors.

Results

Crystalline GaSb Irradiation

Goal: Understand how the compositional depth profile emerges from prompt ion-surface interactions.



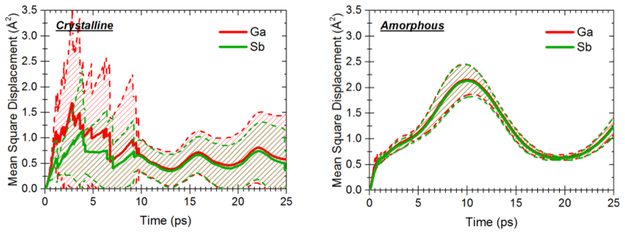
Initial 50-50 crystalline GaSb surface

Kr+ ion irradiated GaSb after Φ = 7.5×10^15 cm^-2

Clusters of Sb in GaSb after irradiation

- Phase separation is not observed.
- Crystalline Sb clusters nucleate, despite the lack of a global compositional depth profile.

Contrast the mobilities of Ga and Sb



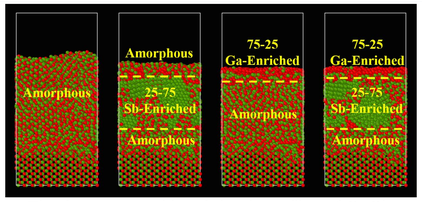
Mean square displacements of Ga and Sb in crystalline and amorphous GaSb. Dotted lines show standard deviations.

Ga and Sb have similar mobilities, implying that Sb cluster formation is thermodynamically-driven as opposed to being governed by kinetics.

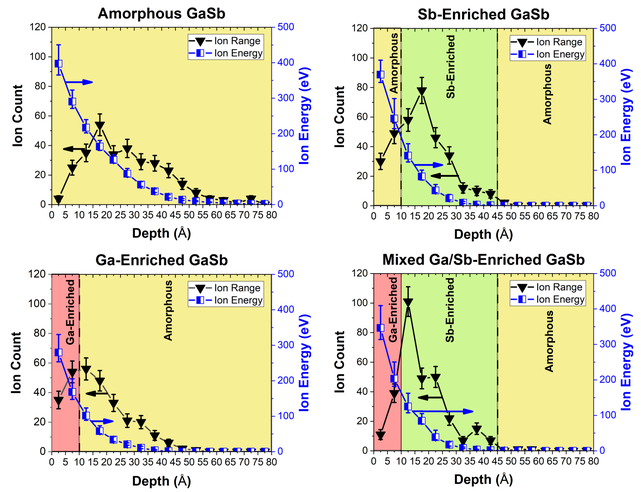
Results

Single Ion Simulations

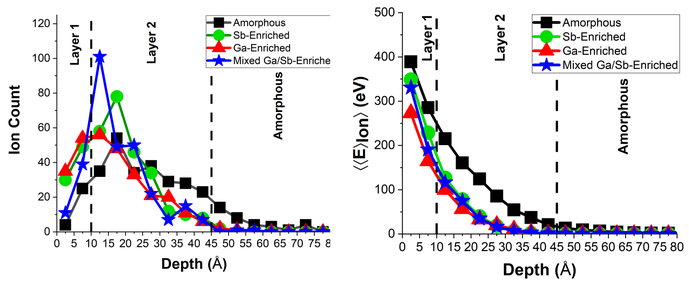
Goal: Analyze how ion-surface interactions depend on the GaSb compositional depth profile.



The four compositional depth profiles of GaSb.



Ion range and energy deposition profiles for each of the four GaSb compositional depth profiles.



Ion range (left) and energy loss (right) distributions of 360 single ion impacts into each compositional depth profile of GaSb.

- The ion range peak is narrower in profiles with altering compositions than the amorphous profile (uniform composition).
- Ions lose more energy in profiles with altering compositions than in the amorphous GaSb.

These suggest possible **interface effects** induced by the compositional depth profile on fundamental ion-surface interactions.

Conclusions

- Sb clusters form despite the lack of a global compositional depth profile. This is not driven by the contrasting kinetics of Ga and Sb.
- Interfaces between layers of distinct composition affect the ion range and energy loss distribution.

References

[1] S. Facsko, T. Dekorsy, C. Koerdt, C. Trappe, H. Kurz, A. Vogt, and H. Hartnagel, *Science* **285**, 1551-1553 (1999).
[2] El-Atwani, O., Norris, S.A., Ludwig, K., Gonderman, S., and Allain, J.P., *Sci. Rep.* **5**, 18207 (2015)
[3] S. Plimpton, *J. Comp. Phys.* **117**, 1-19 (1995).