Inert Gas bubble formation in sputtered CdTe thin film solar cells.

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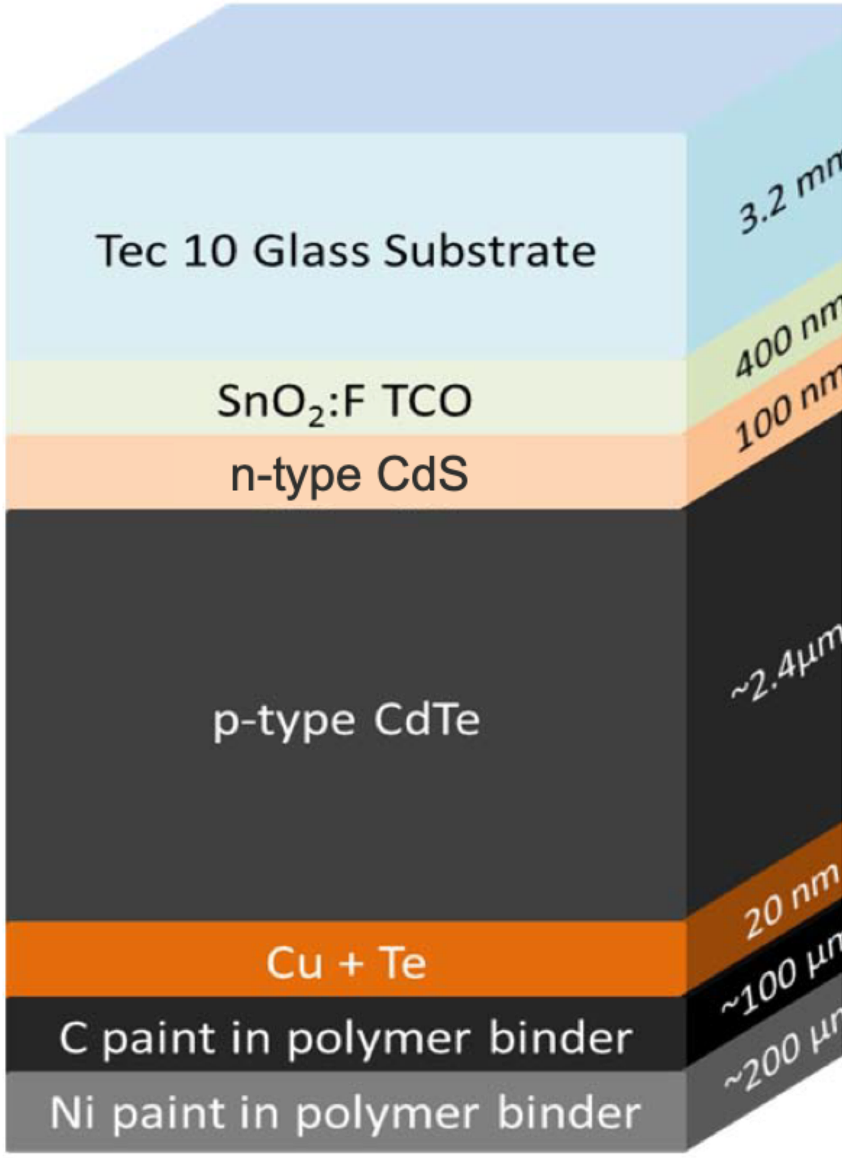
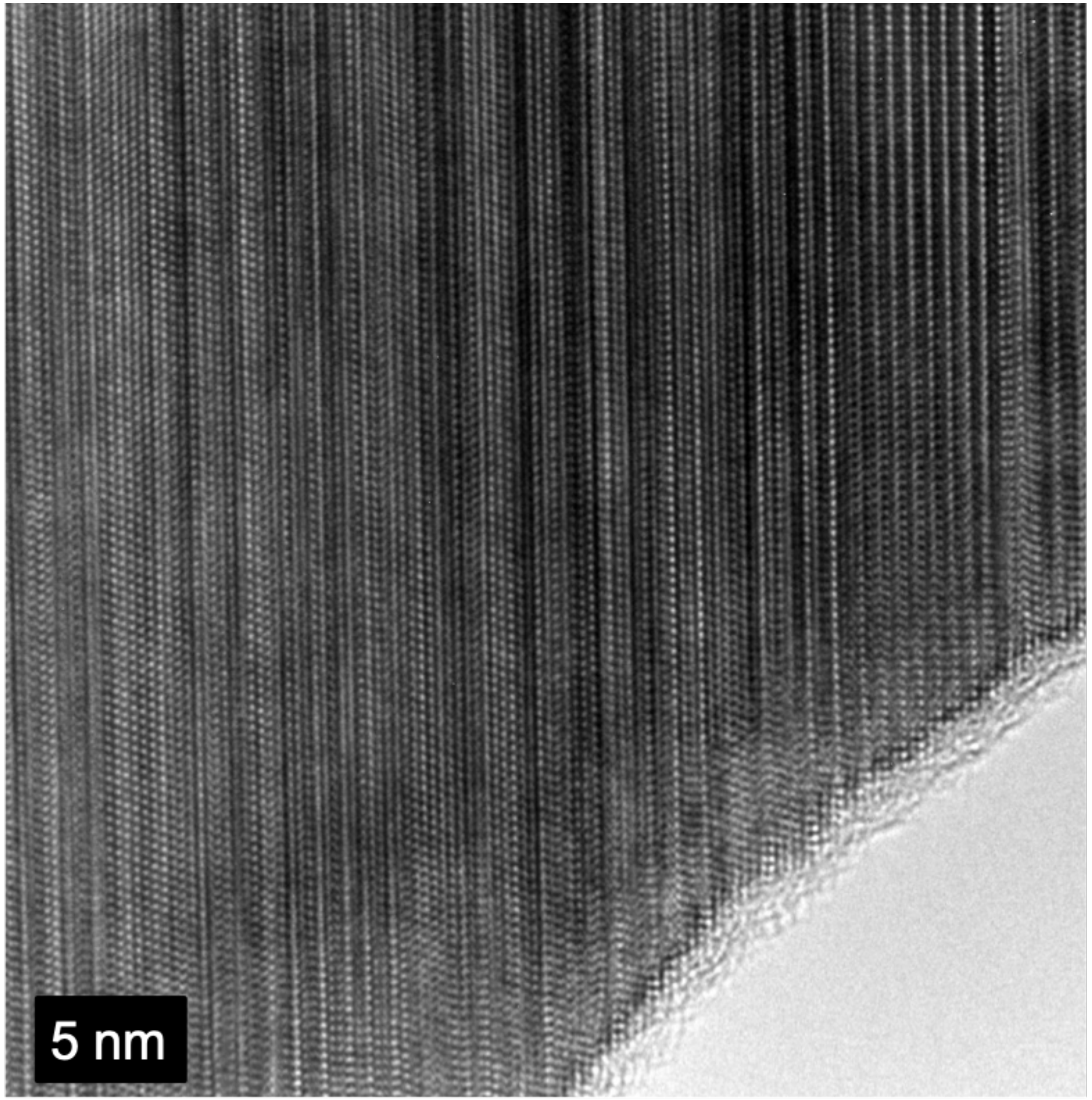
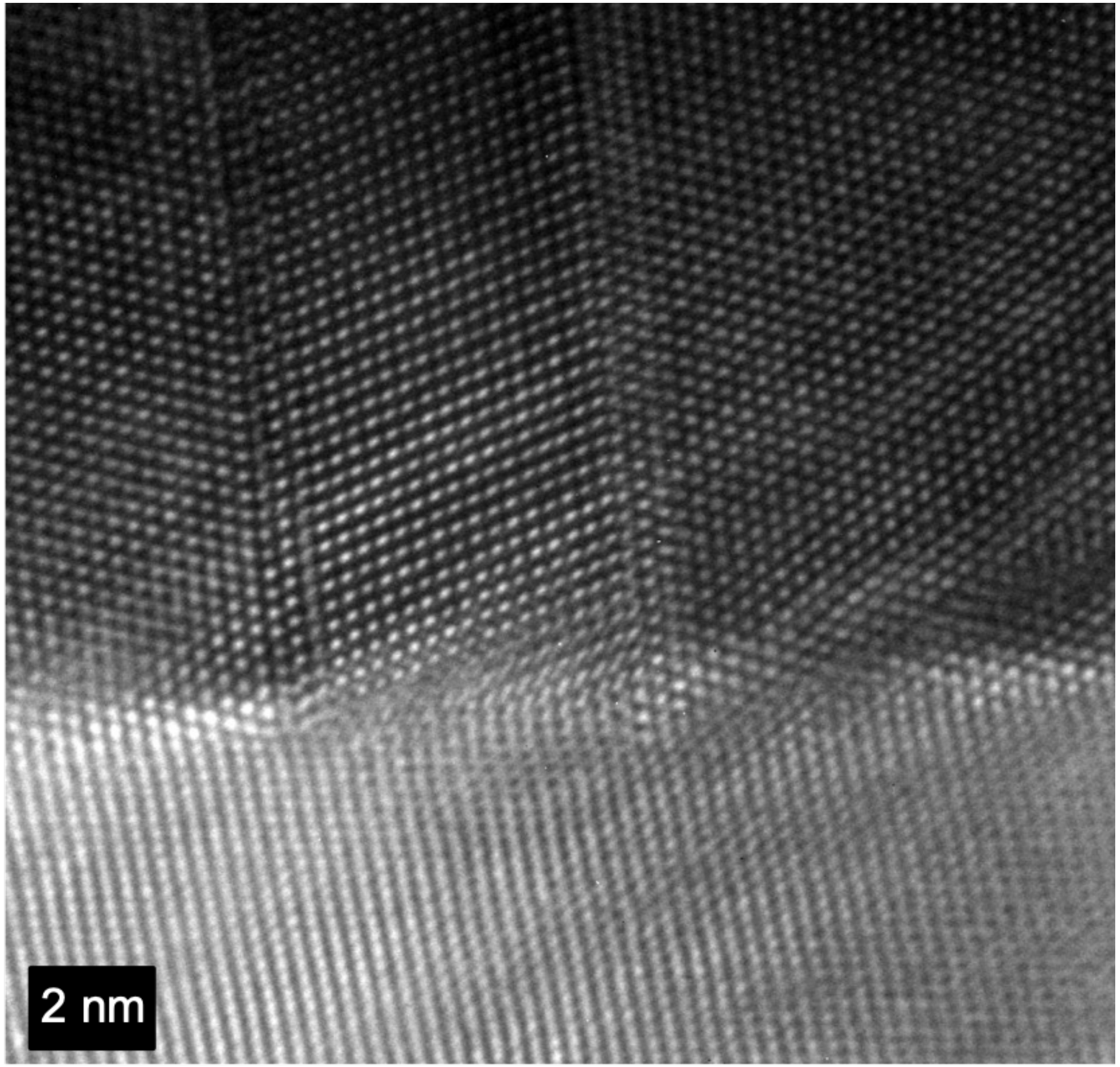
CdTe Solar Cells

- CdTe cells are competitive with silicon cells
- Current production method is closed space sublimation (First Solar).
- The current best research cell efficiency is 22.1% but the maximum efficiency is 33.7%.

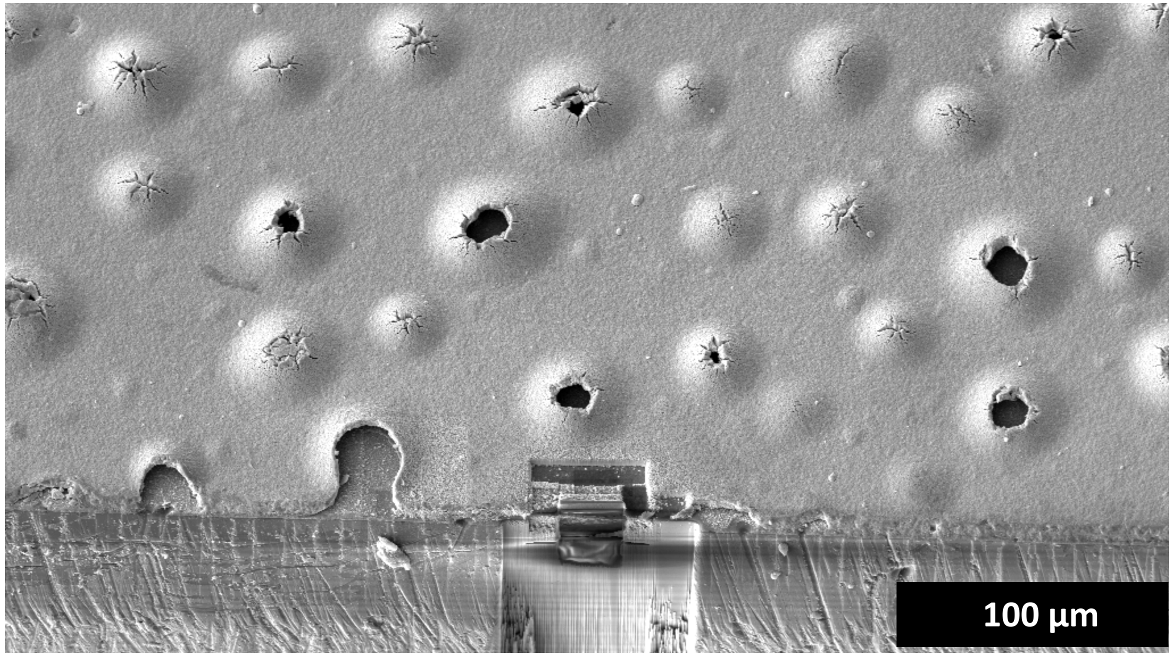


Removal of Stacking Faults

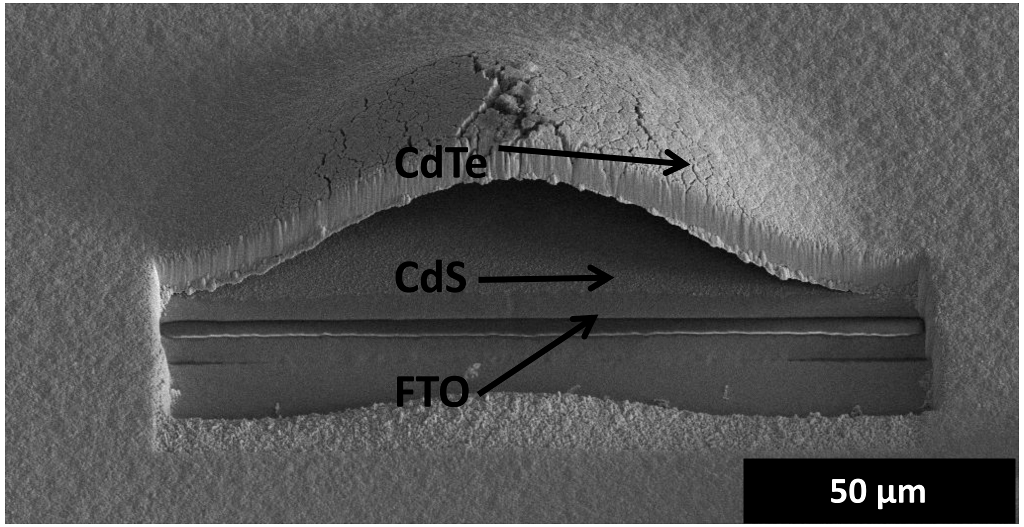




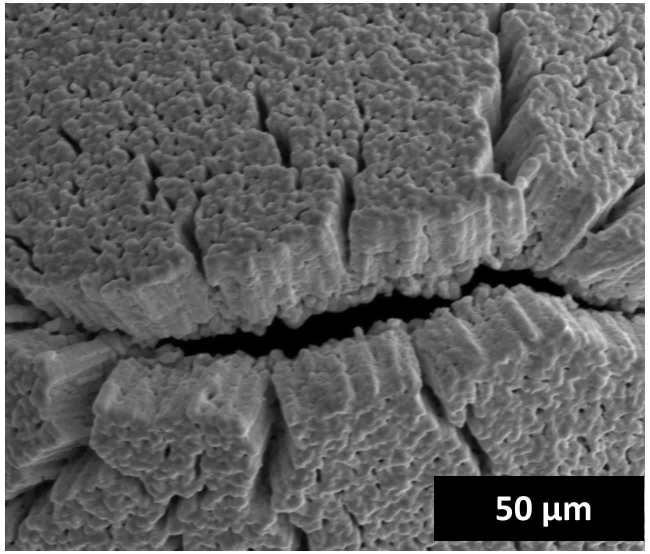
Pulsed DC sputtered CdTe after the cadmium chloride activation at 400^{o}C



- An SEM image of a sputtered device following activation with $CdCl_2$.
- Blisters appear on the surface.
- Blisters caused by working gas in magnetron

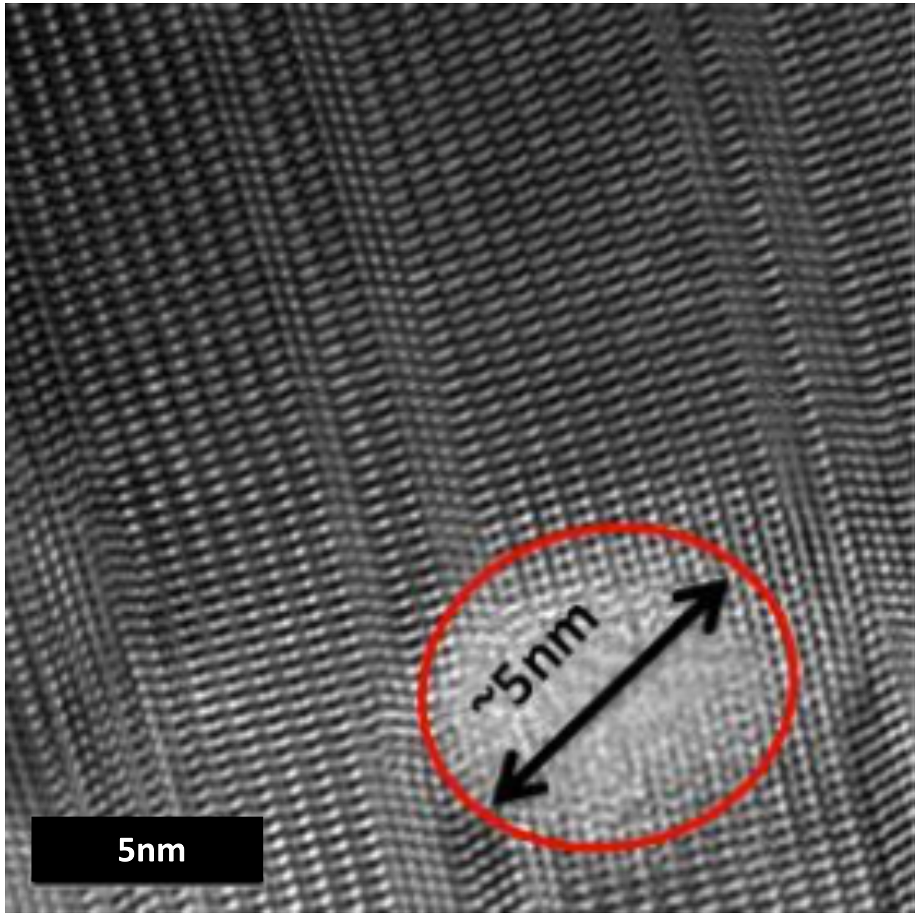


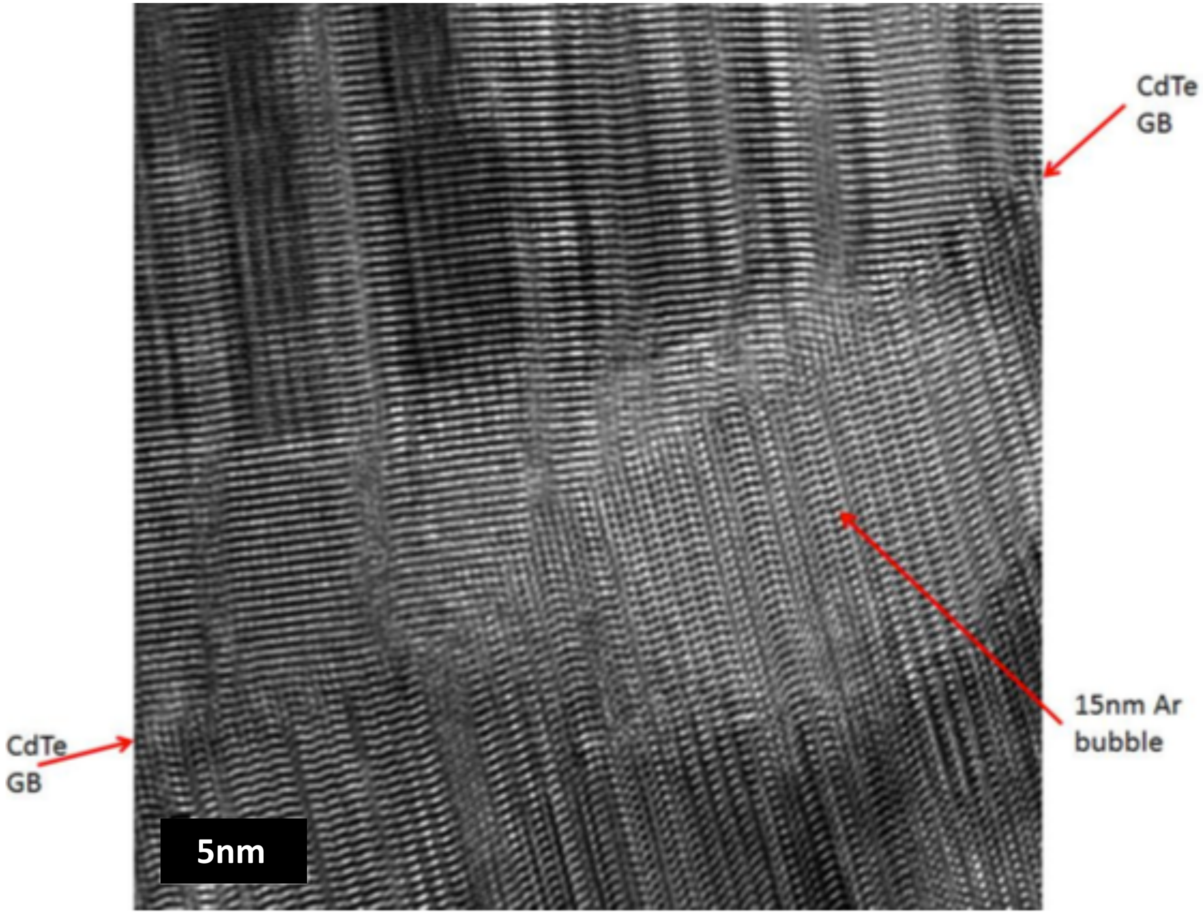
Delamination occurs at the CdS/CdTe junction.



- Exfoliation occurs at some surface blisters.

Argon in CdTe after RTP at 400 º C for 12 hours





- Argon incorporated during sputtering
- Argon agglomerates into ~5-15 nm clusters.

Methodology

- Atomistic Simulation using the Molecular Dynamics (MD) package LAMMPS with the force fields:
  - Stillinger-Weber for Bulk CdTe,
  - ZBL potential for Ar/Xe – CdTe interactions,
  - Lennard Jones potential for Ar-Ar and Xe-Xe interactions parameterised by Ashcroft and Mermin.

- Nudged Elastic Band (NEB) for diffusion pathways and energy barriers.

- Arrhenius' equation was linearised to estimate Arrhenius prefactors and hence determine transition time.

- ParSplice is also used to observe transitions at temperatures below 800 K in some cases.

Zinc-Blende CdTe

Normal Impact of Ar/Xe on Zinc-Blende CdTe

	5eV	10eV	15eV	20eV
Argon - (100)	0%	0%	4%	8%
Argon - (110)	0%	5%	7%	9%
Argon - (111)	0%	8%	13%	19%

	5eV	10eV	15eV	20eV
Xenon - (100)	0%	0%	0%	7%
Xenon - (110)	0%	0%	1%	4%
Xenon - (111)	0%	5%	11%	15%

Normal Impact of Ar/Xe on Zinc-Blende CdTe

↑ Incident Energy => ↑ Implanting

	5eV	10eV	15eV	20eV
Argon - (100)	0%	0%	4%	8%
Argon - (110)	0%	5%	7%	9%
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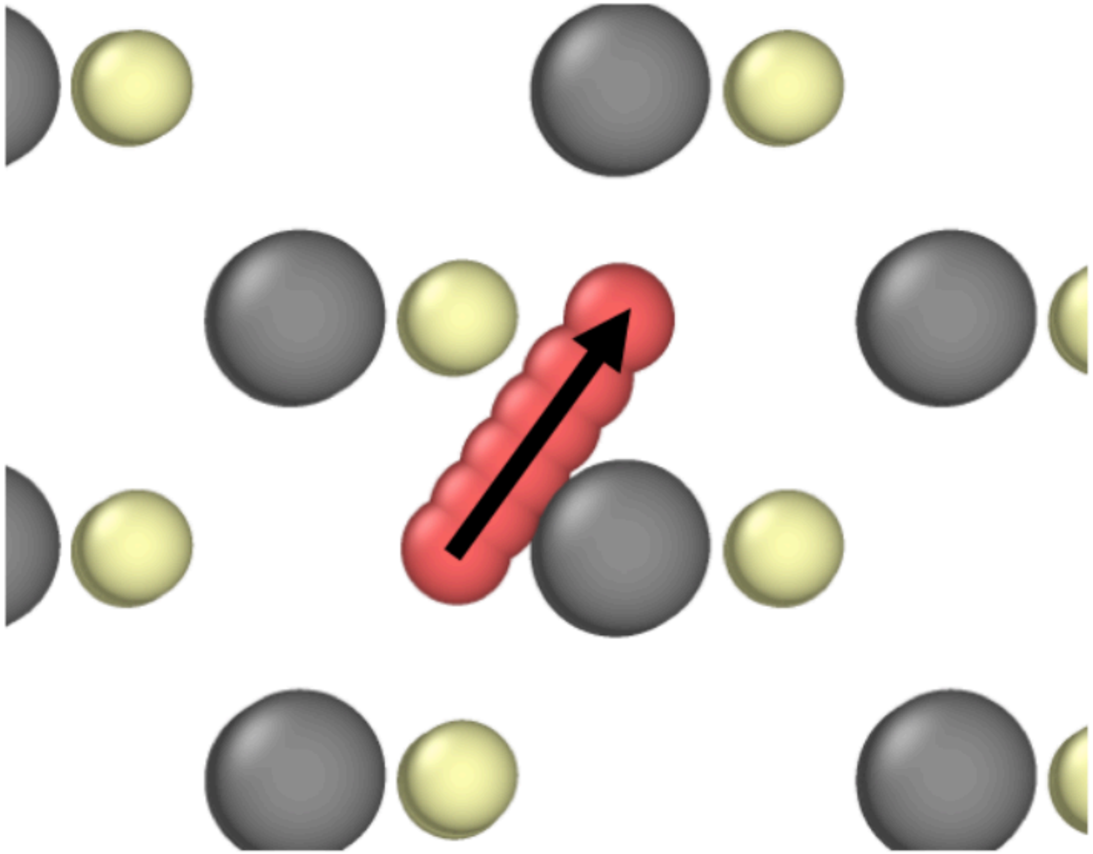
Argon Implanting > Xenon Implanting

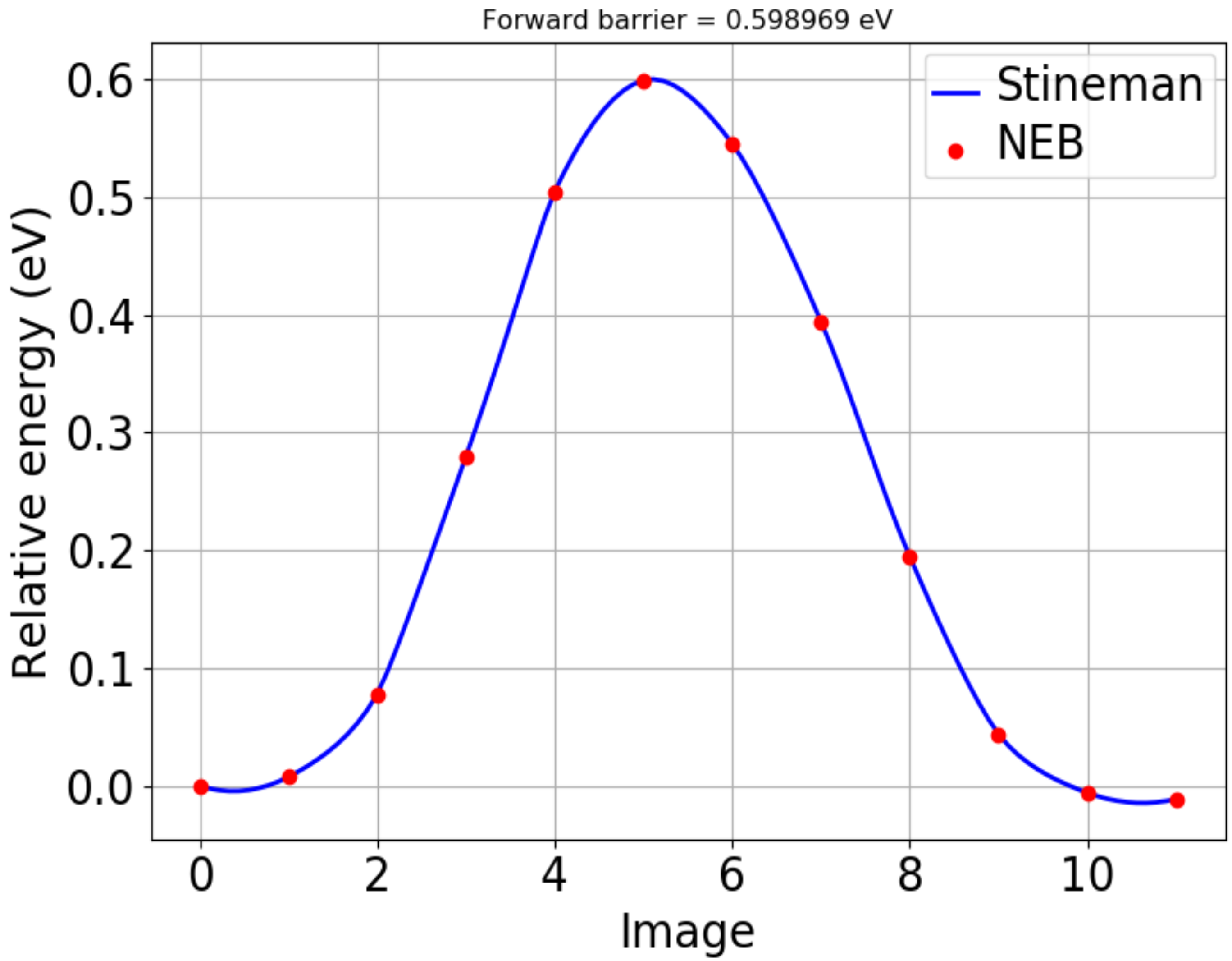
	5eV	10eV	15eV	20eV
Xenon - (100)	0%	0%	0%	7%
Xenon - (110)	0%	0%	1%	4%
Xenon - (111)	0%	5%	11%	15%

(100) Implanting < (110) Implanting < (111) Implanting

↑ Temperature => ↑ Implanting

Single Ar Diffusion in zinc blende CdTe Crystal

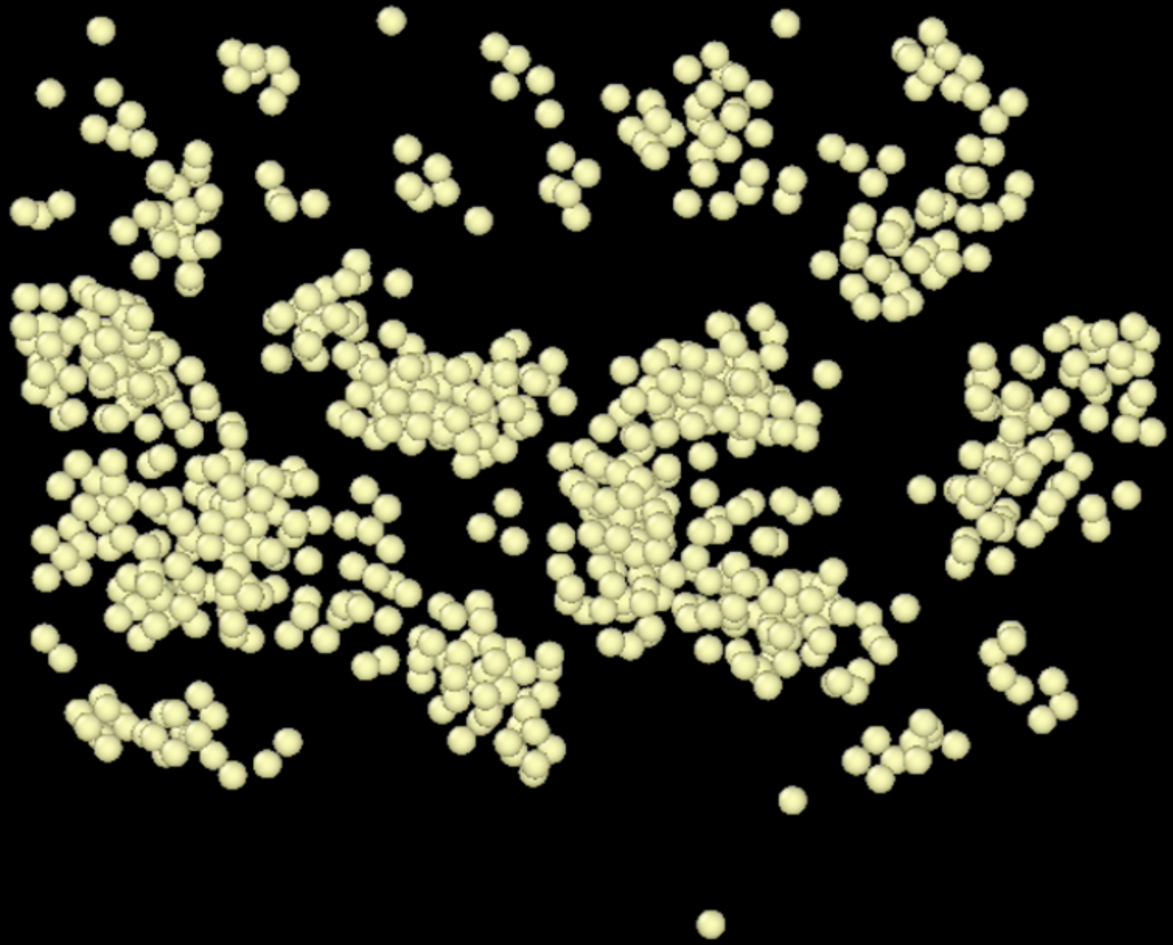




Energy Barrier for Single Argon Diffusing: 0.6eV

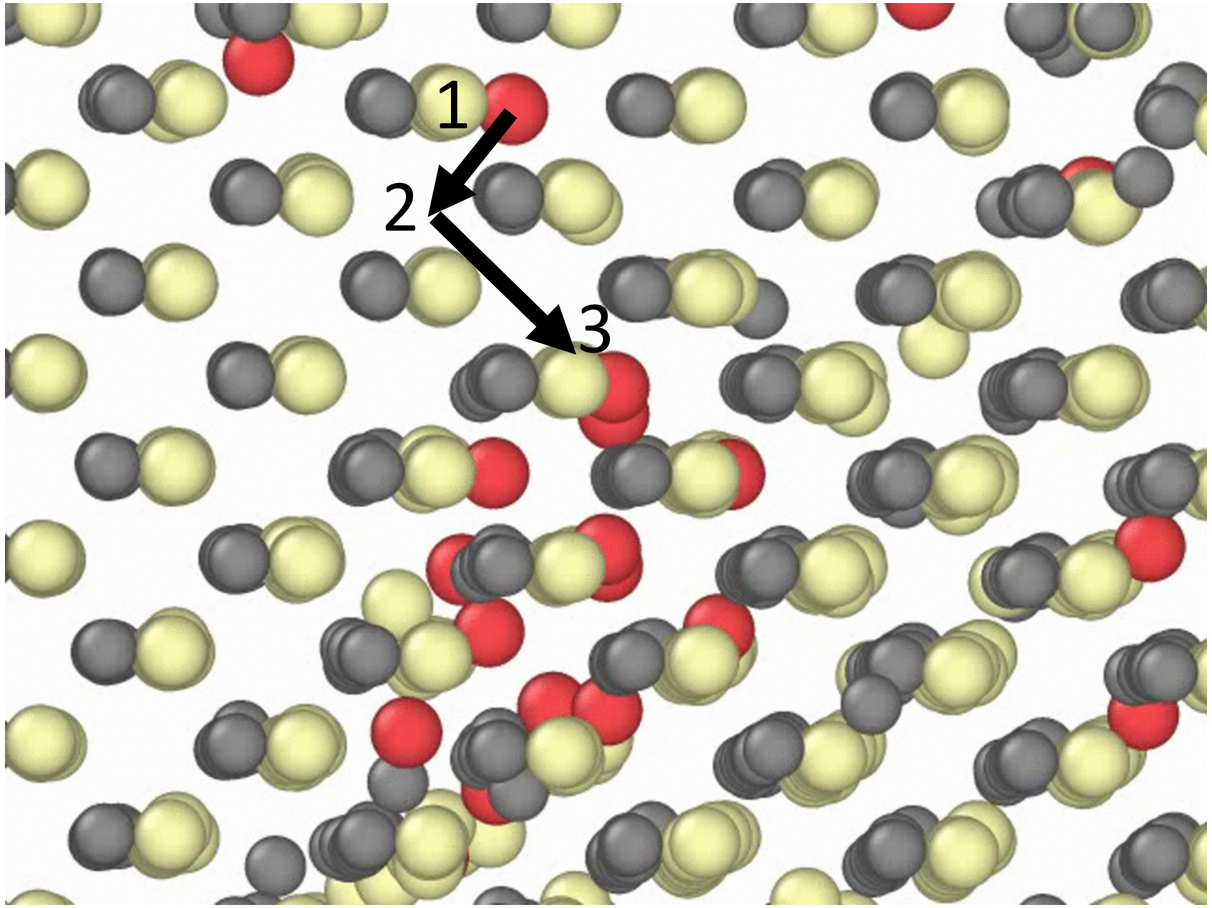
Energy Barrier for Single Xenon Diffusing: 0.74eV

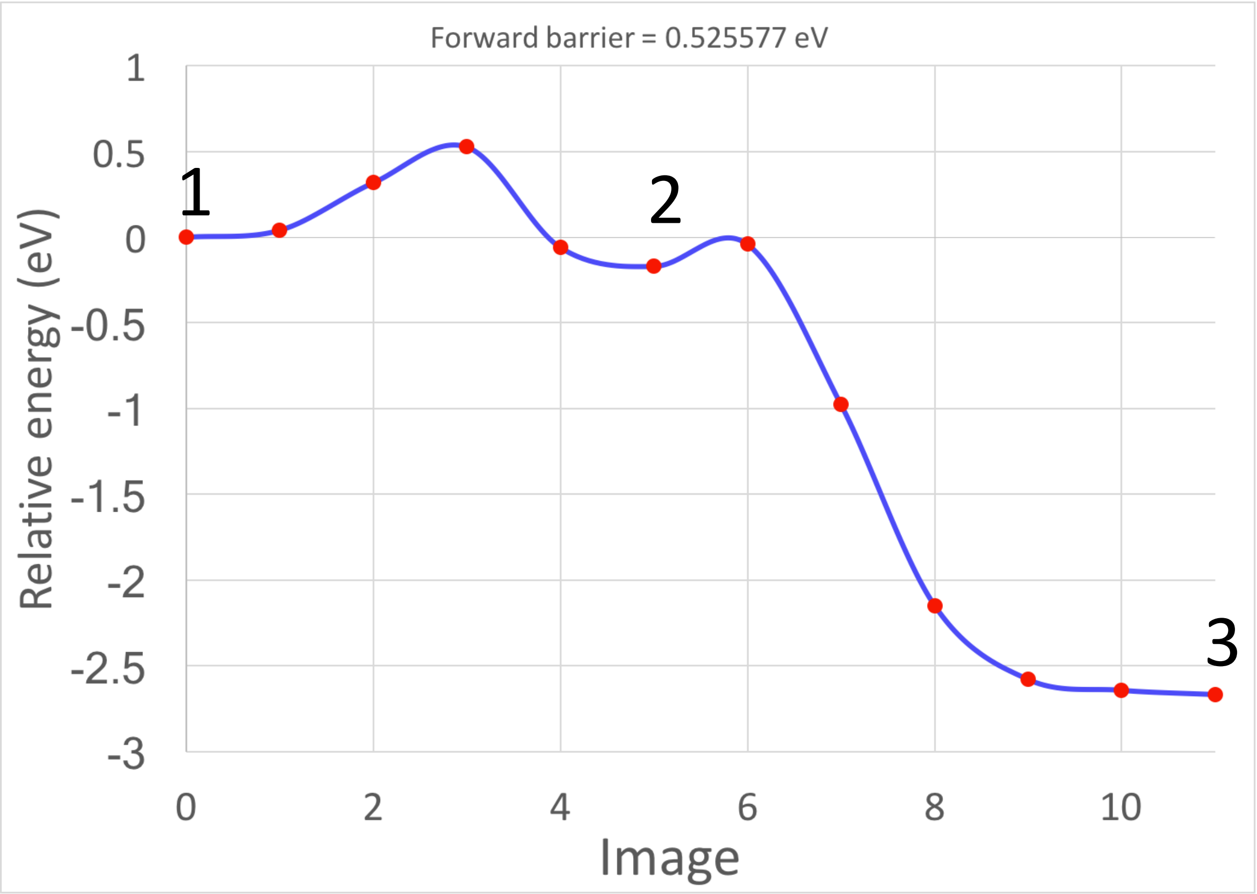
1ns simulation of 4% Argon in CdTe lattice at 723C (1000K) with CdTe removed for visibility (Final State)



- Ar clusters have begun to form even at this short time scale.
- Xenon clusters grow in a similarly in the same conditions.
- Xenon distributed and annealed at 1000 K for 3 ns has final distribution similar to Ar annealed for 750 ps.
- Xenon clusters will grow under experimental time scales

Ar Cluster Growth

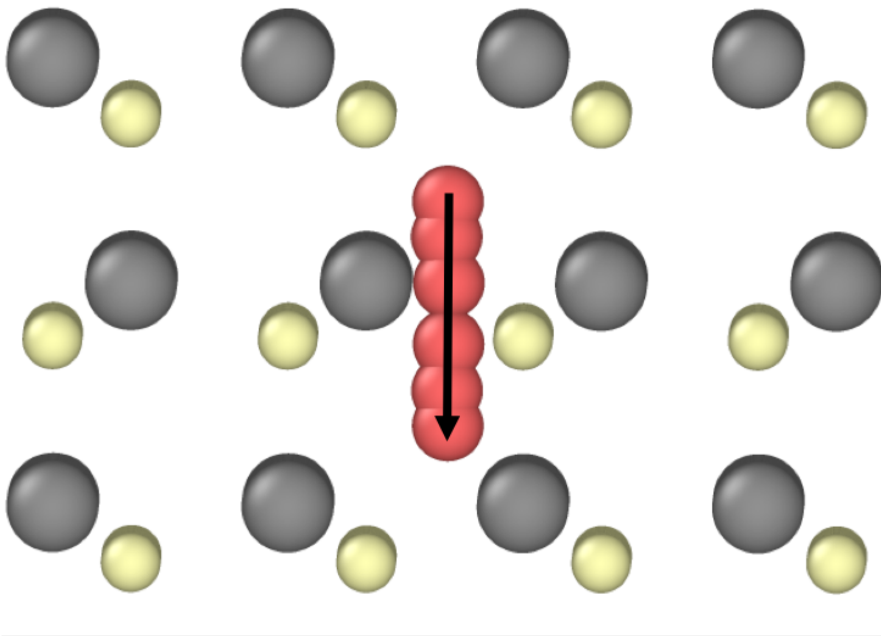


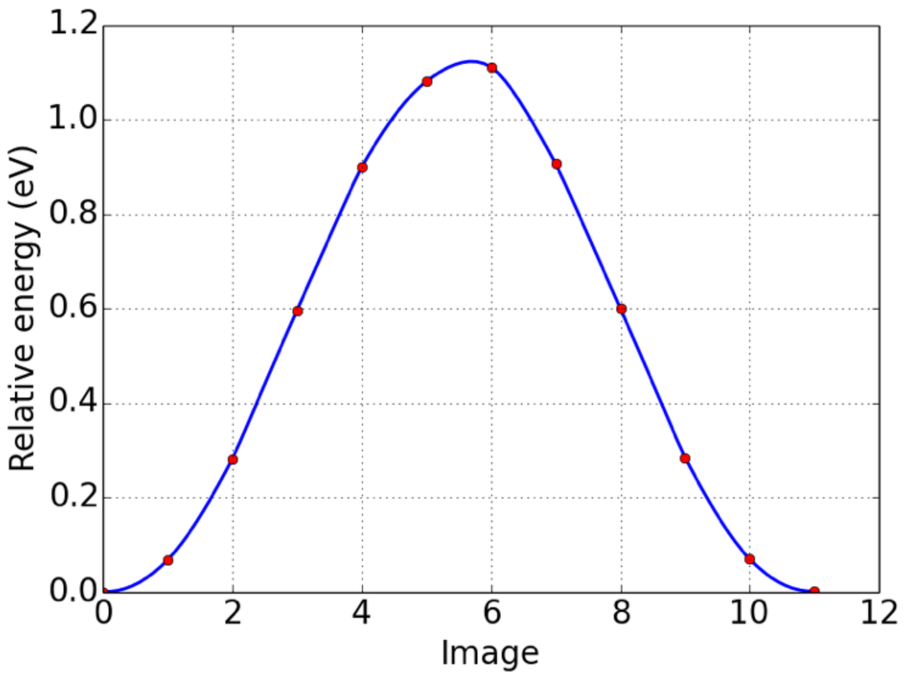


Low diffusion barriers (~0.53 eV and ~0.25 eV) for single Ar joining cluster.
High reverse barrier (~2.5 eV) for single Ar to leave cluster.

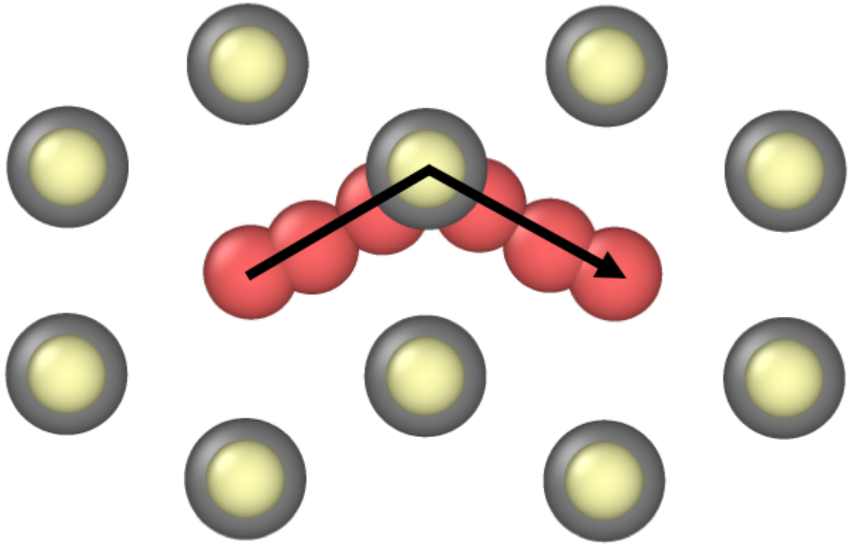
Wurtzite CdTe

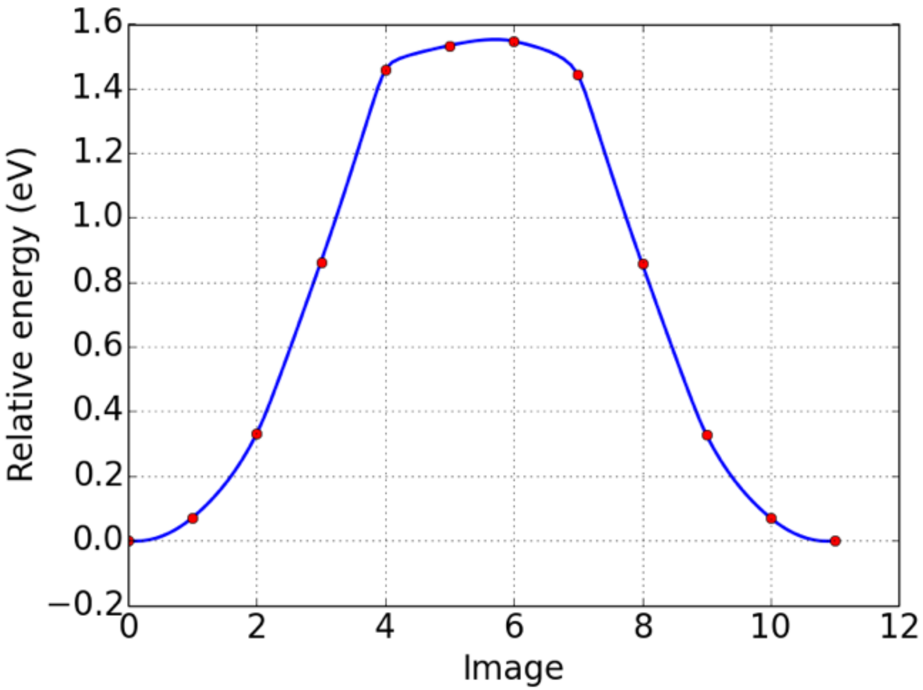
Wurtzite Diffusion





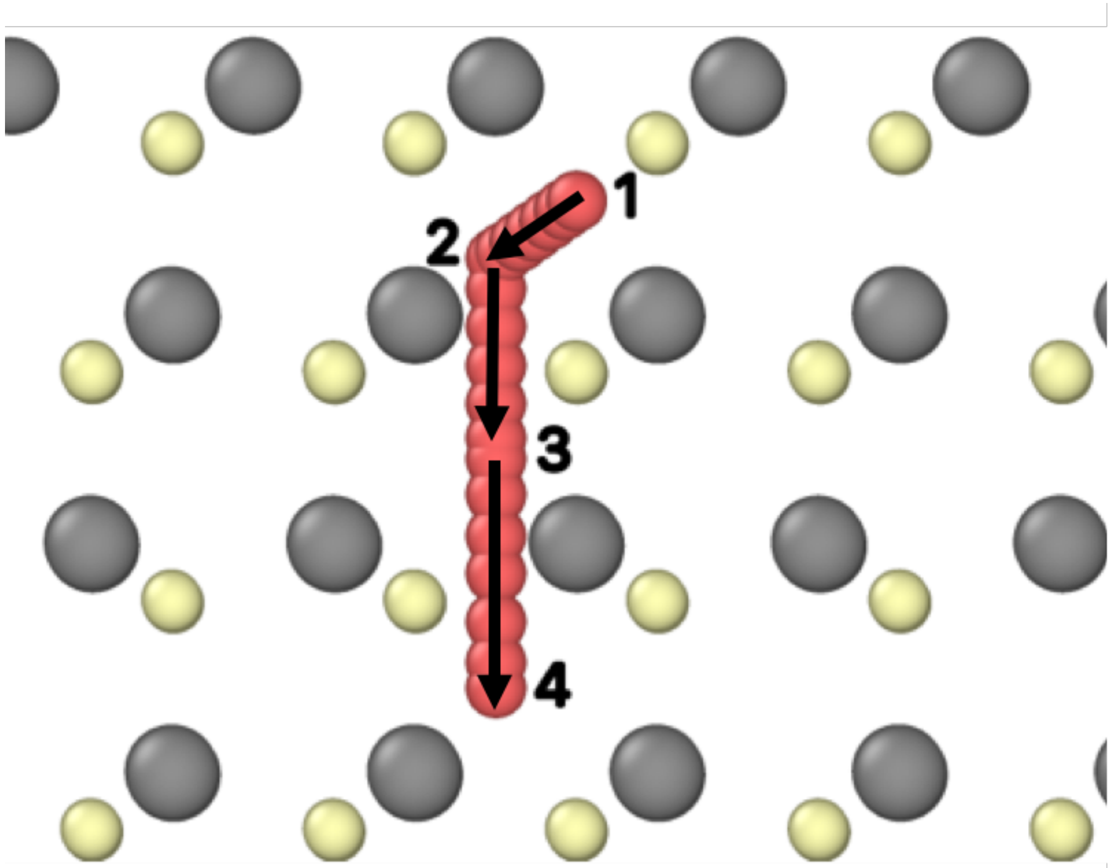
- Two non-equivalent pathways with energy barriers 1.12 eV and 1.54 eV.
- Above 800 K barrier is ~0.67 eV.
  Below 800 K barrier is ~1.4 eV.
- Xe pathways are the same but the barriers are 1.4 eV and 2 eV.

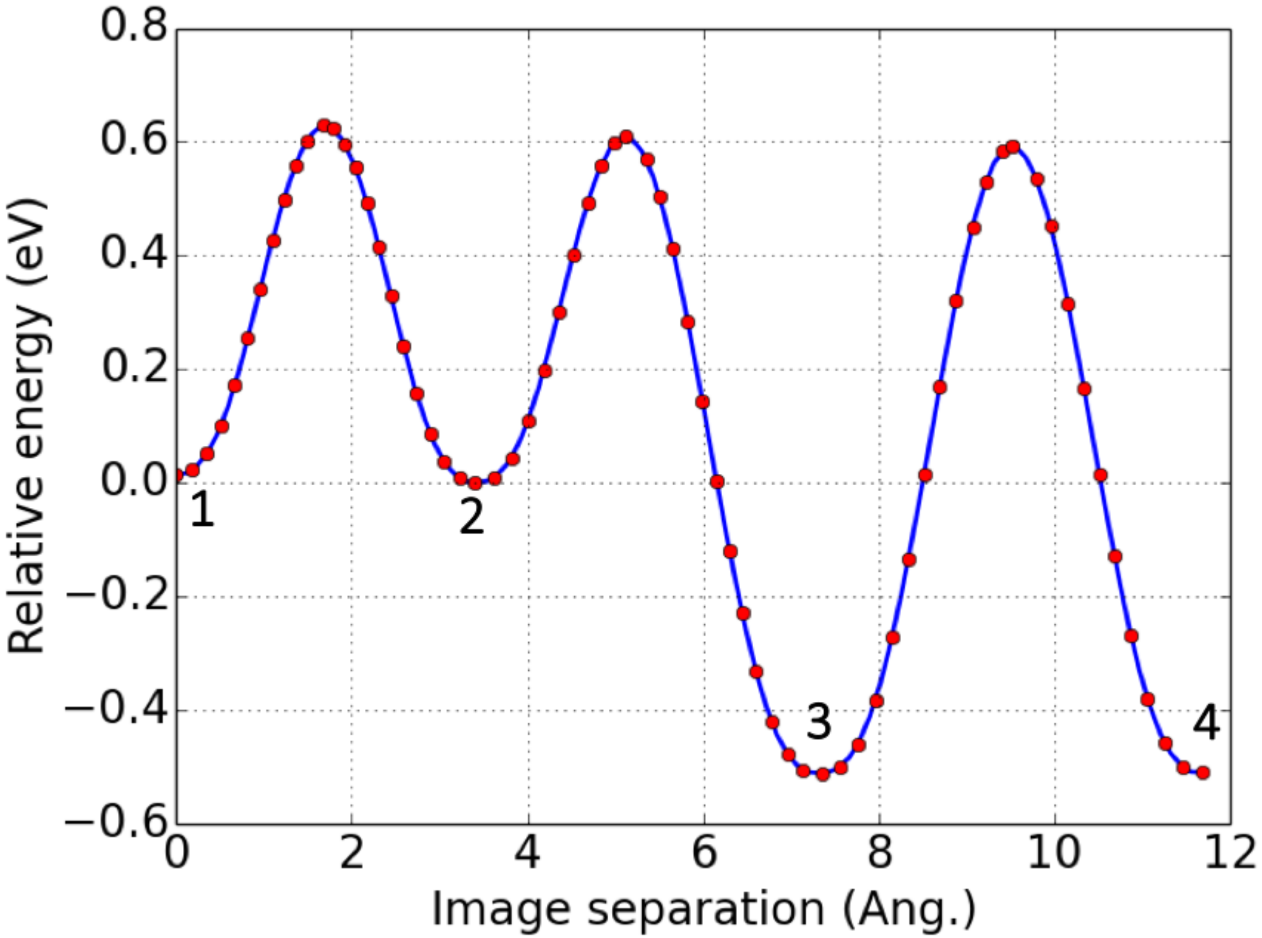




CdTe Stacking Faults

Transitions across stacking faults





Conclusions

Experimental:

- 5-15 nm Ar clusters form during in RTA of pulsed dc sputtered films
- $CdCl_2$ treatment causes μm sized blisters at the same temperature.

Simulation:

- Ar penetrates at <10 eV, threshold more with Xe -> Use Xe as working gas ?
- Diffusion barriers are lowered near clusters causing cluster growth.
- Clusters grow by diffusion of single atoms, minimising lattice distortion
- High barrier heights in wurzite mean that the bubble growth is inhibited by stacking faults; when they are removed (as after $CdCl_2$treatment) μm sized bubbles can form

Thank You!

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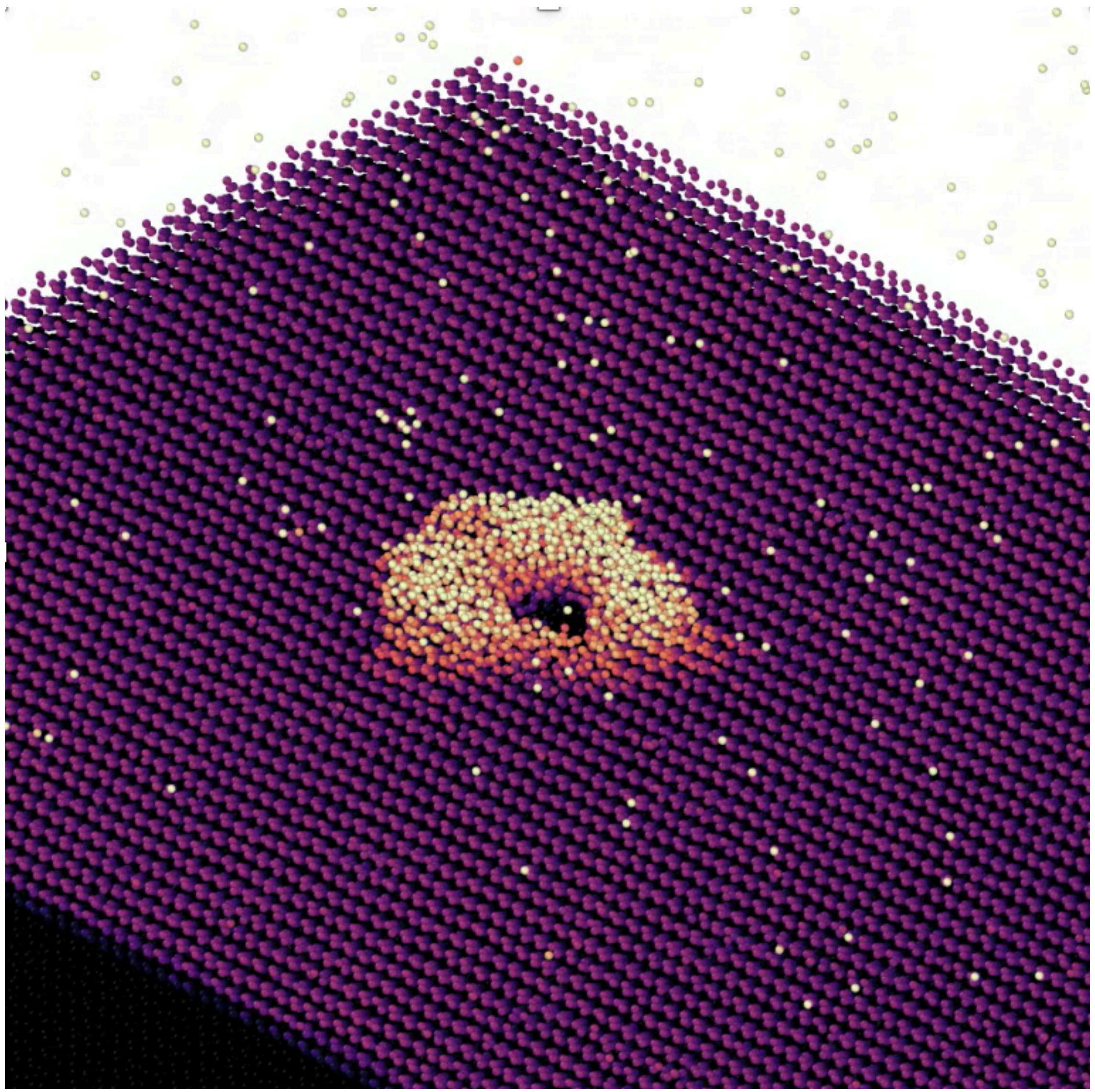

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