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Applications of Molecular Dynamics (MD) in Semiconductor Materials Research

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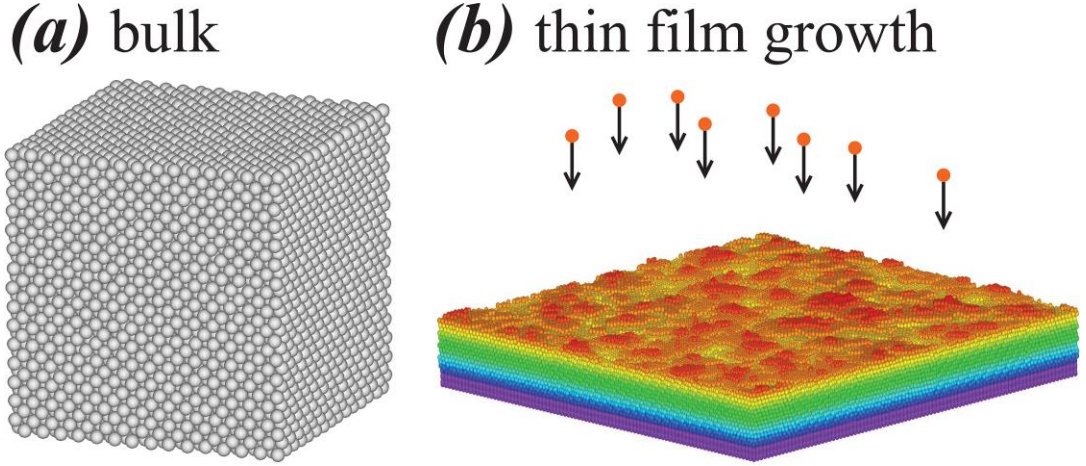
Outline

- Molecular dynamics simulation methods
- Graphene growth
- Photovoltaic CdTe/CdS research
- MD guided misfit dislocation theory
- Solid state lighting $In_xGa_{1-x}N$/GaN research
- Microfabrication of semiconductors
- Summary

Molecular Dynamics (MD) Methods

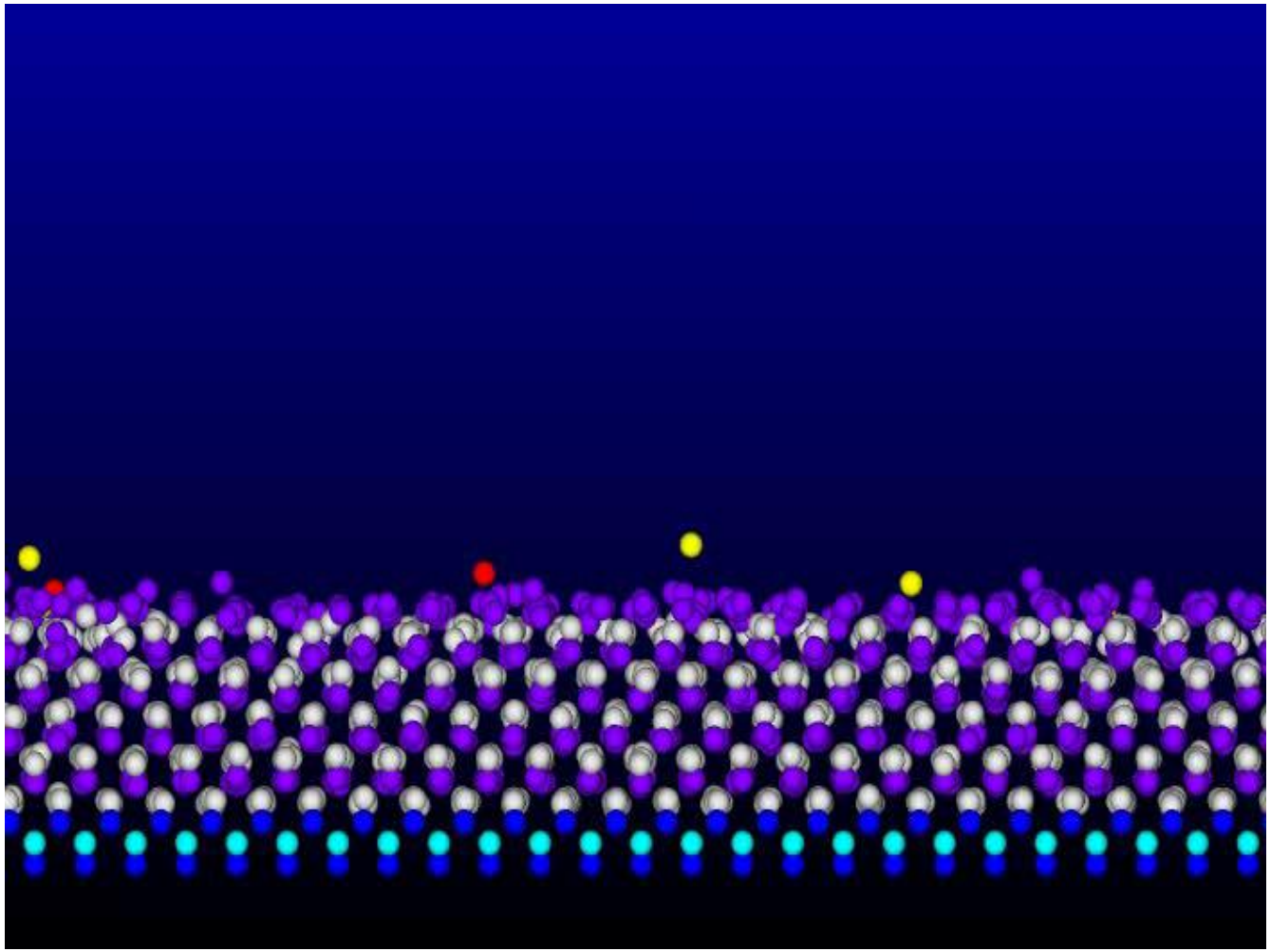


MD solves atom positions vs. time from Newton's equations for atomistic systems.

Example MD problems:

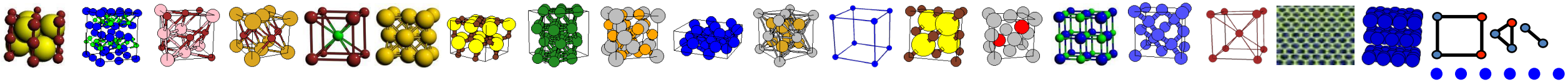
- Thermal transport / phonon calculations
- Mechanical testing simulations (strength)
- Defect studies (vacancy diffusion, dislocation energies, etc.)
- Structural evolution visualization during synthesis

Example simulation: CdTe on CdSe growth



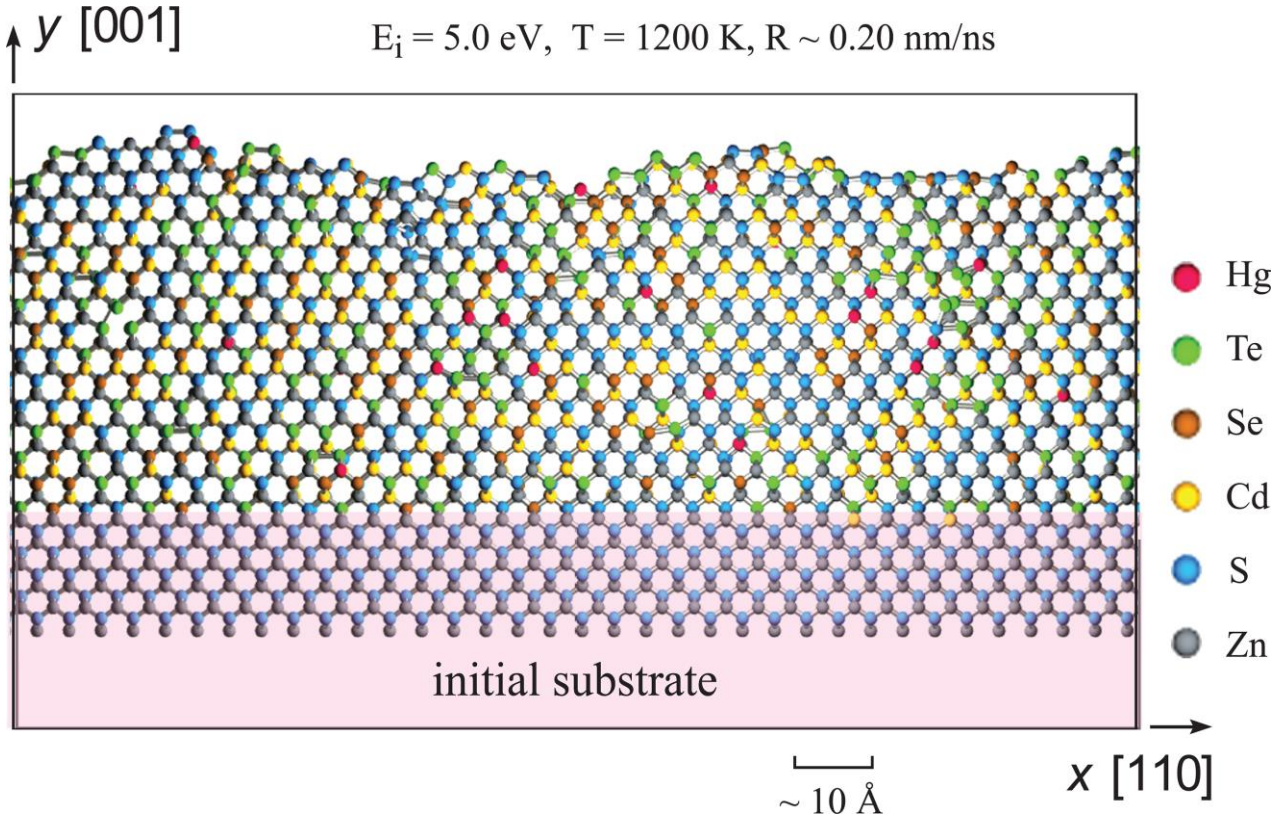
MD Challenge: Interatomic Potential

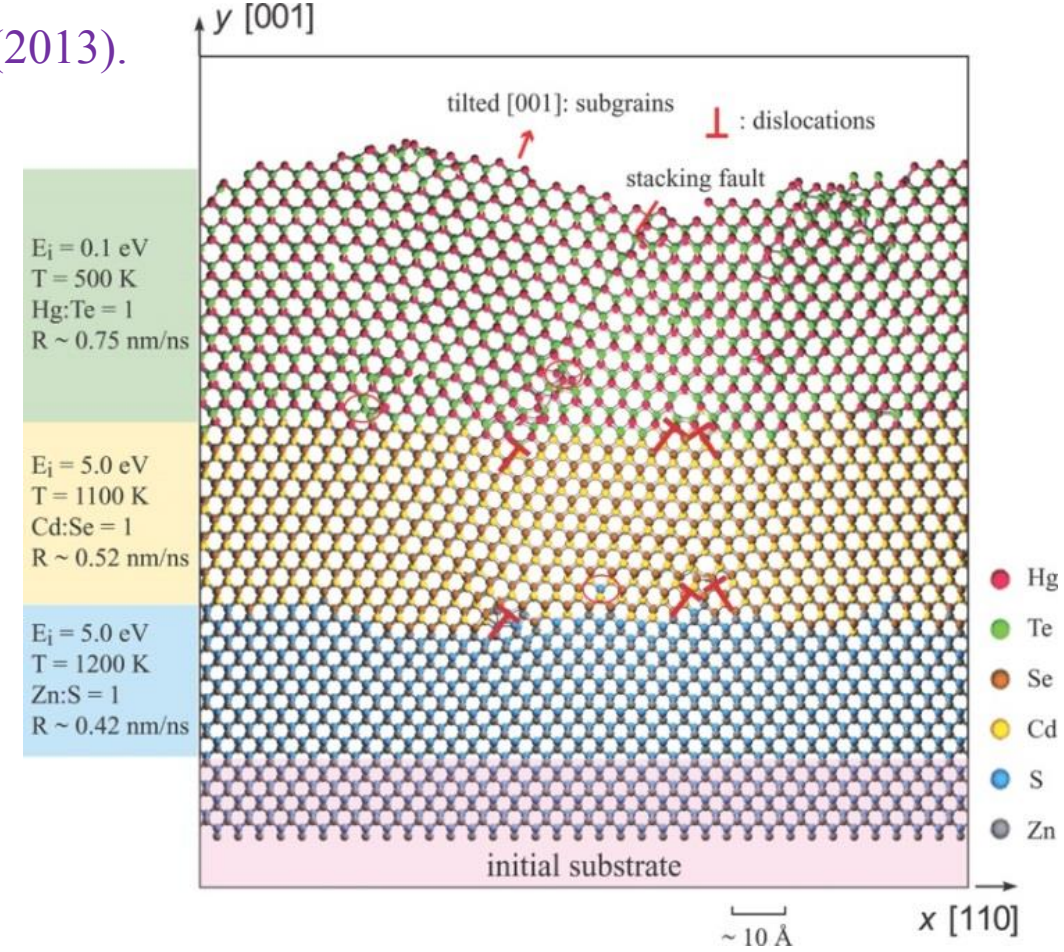
1. Potential of your material does not exist; 2. Literature potential is not good enough.



To simulate growth, a potential must ensure a lower energy for the growth phase as compared to **any other** configurations!

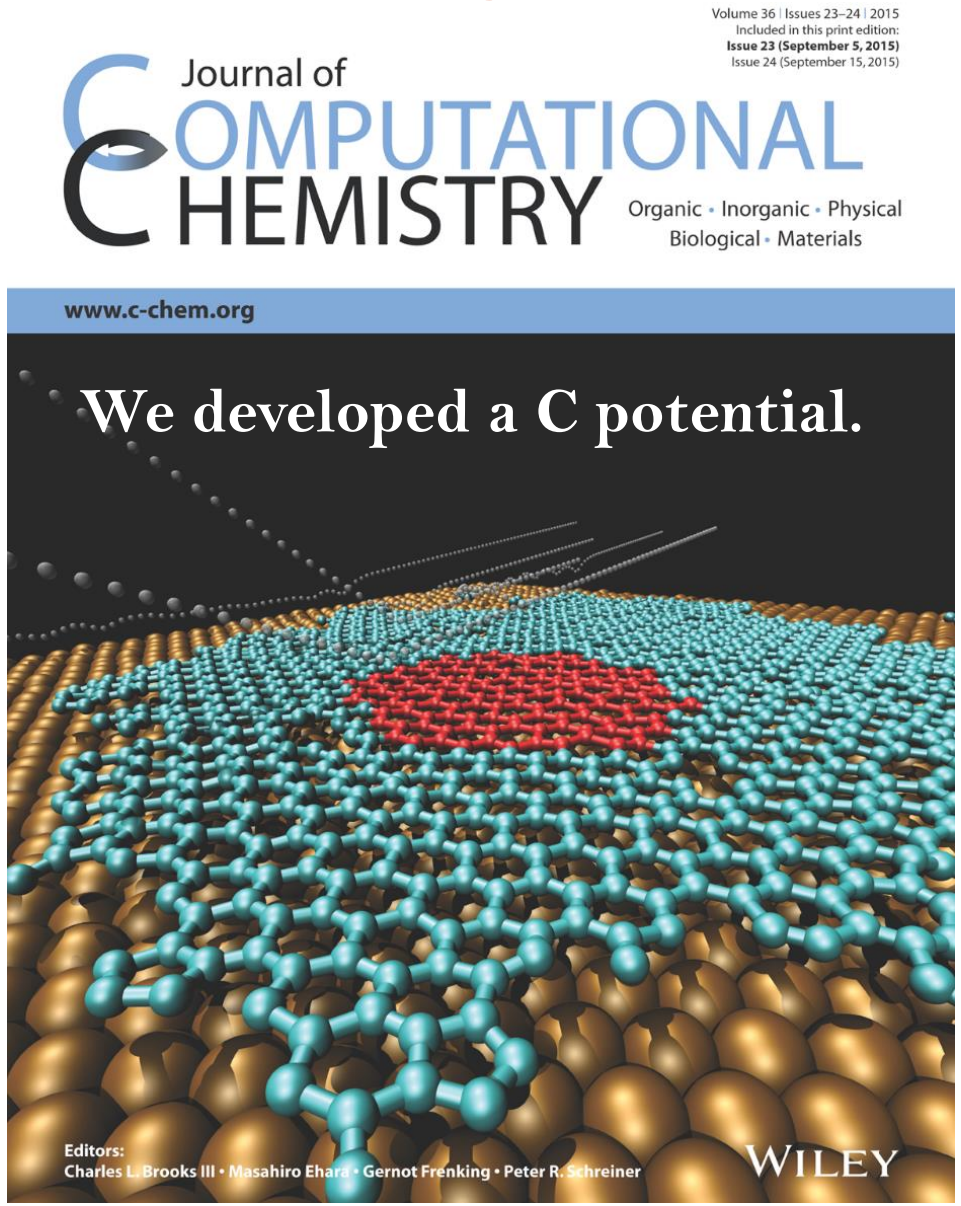
A Zn-Cd-Hg-S-Se-Te potential achieves this: Zhou et al, PRB, 88, 085309 (2013).



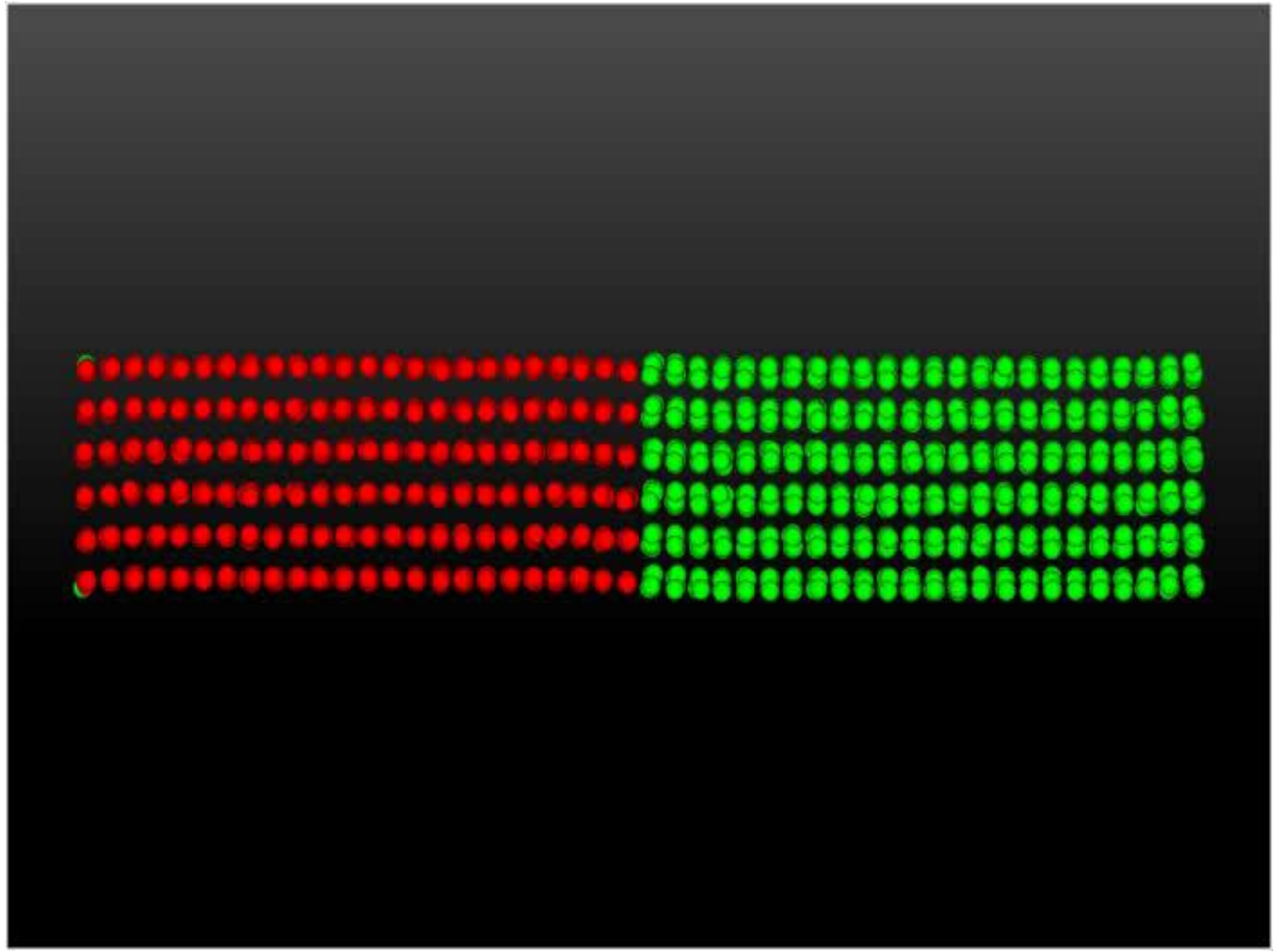


MD Study of Graphene Growth: Interatomic Potential

1. Defects impact graphene properties; 2. Can MD reveal defect formation mechanisms?



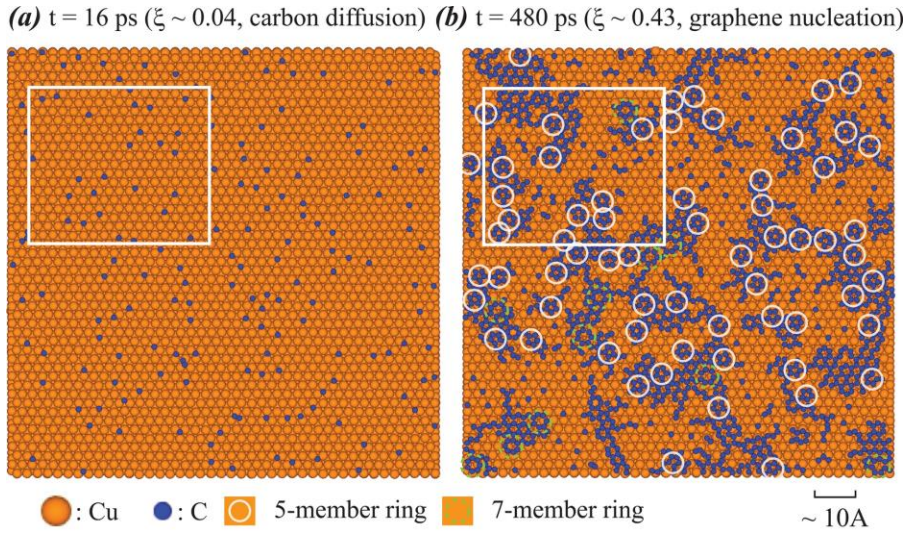
Validation of potential: Diamond formation



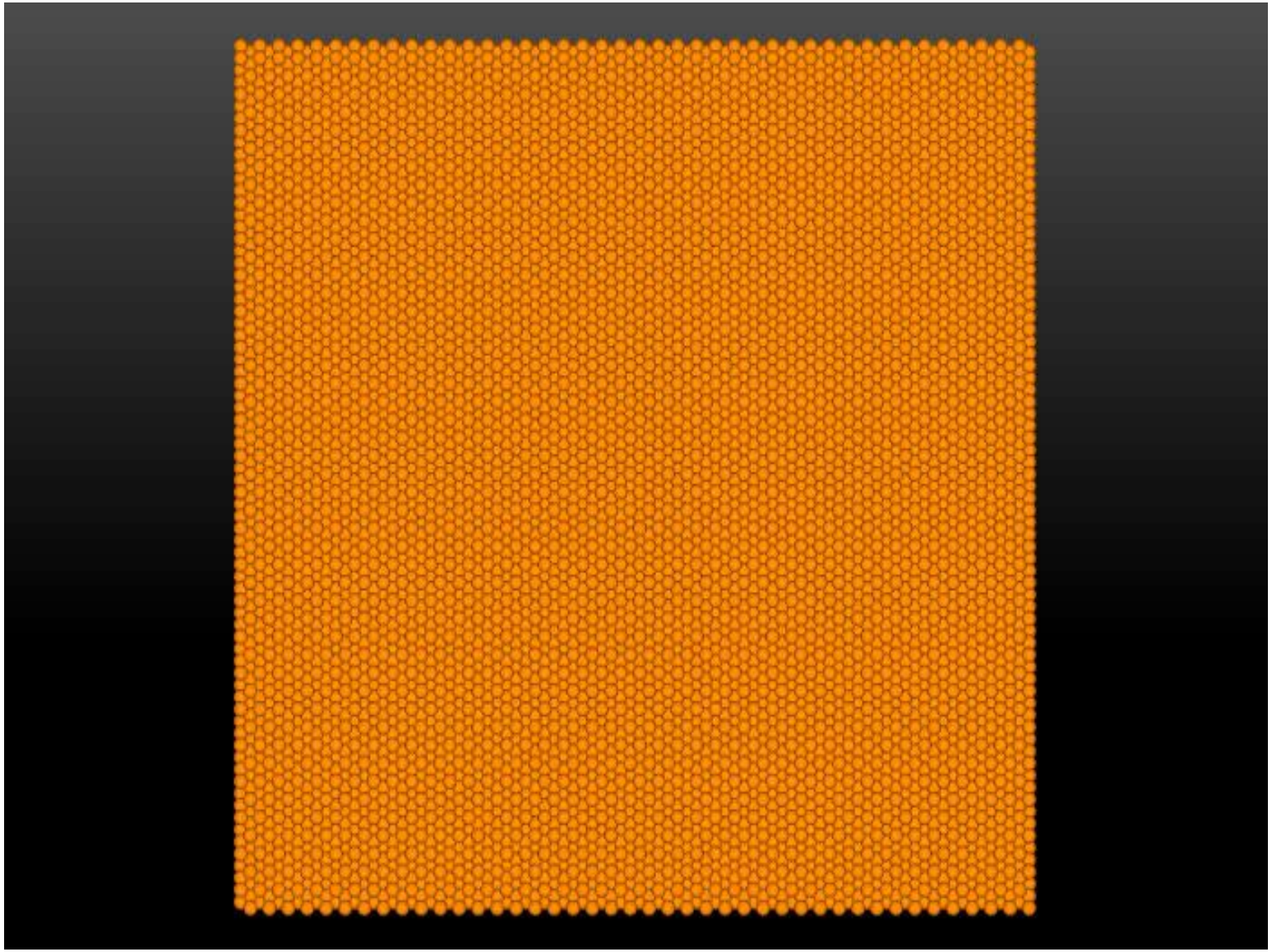
Red: Graphite Green: Diamond (T = 2000 K, P = 0.6 Mbars)

MD Simulations Graphene Growth on Copper

Defects at periphery of islands, not boundaries between islands



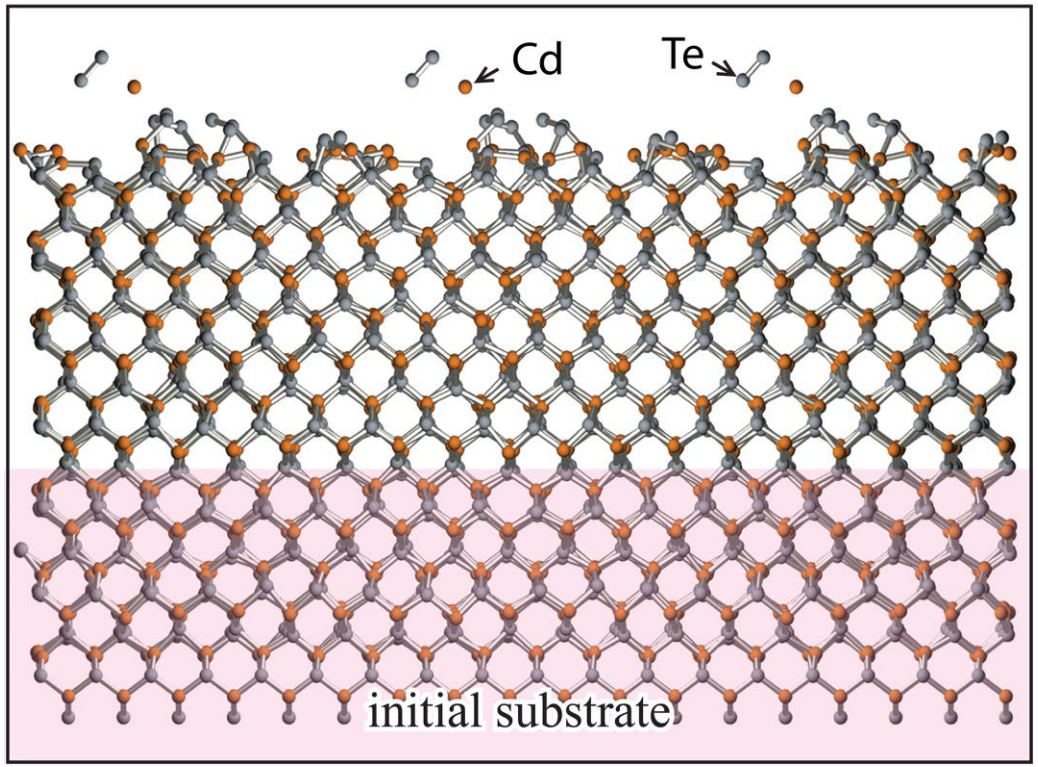
In-situ MD visualization

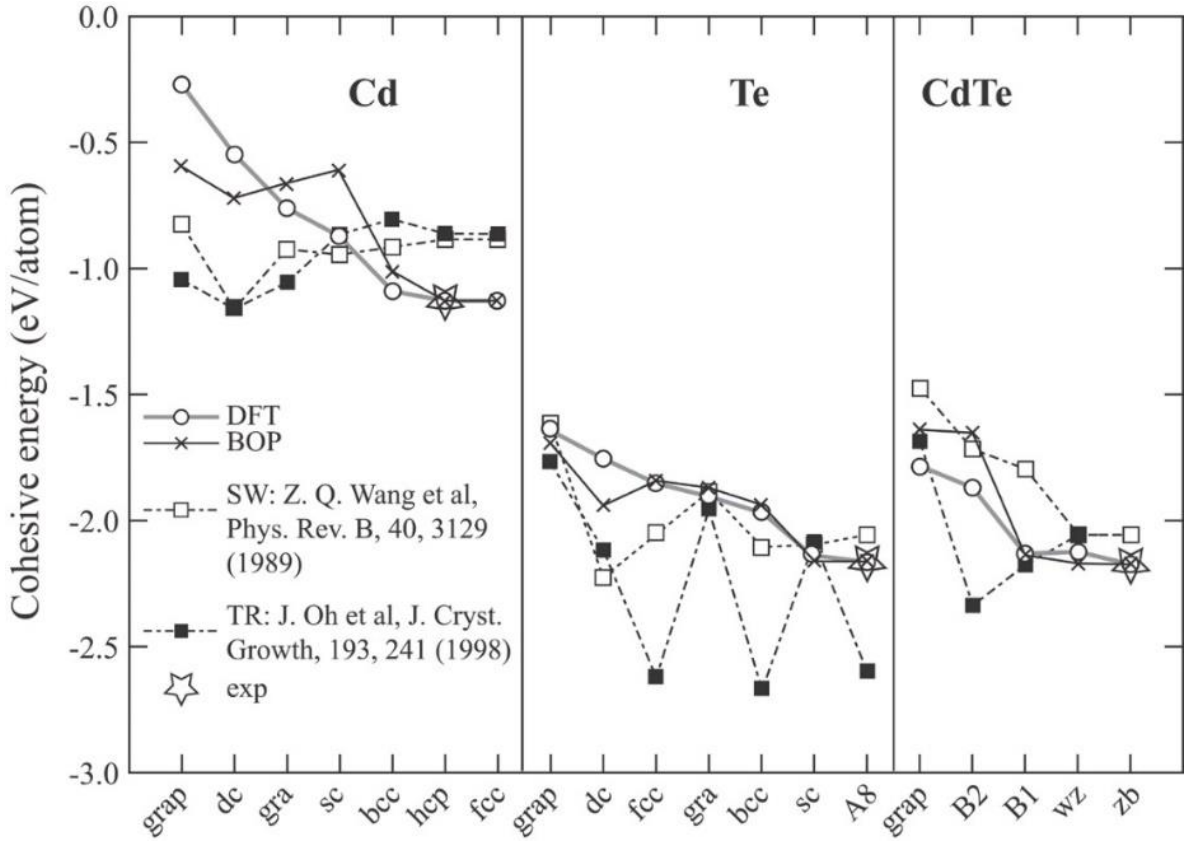


MD Study of CdTe/CdS Systems: Interatomic Potential

1. **Misfit dislocations limit photovoltaic properties of CdTe/CdS films.**
2. **Can MD be used to guide misfit dislocations reduction?**

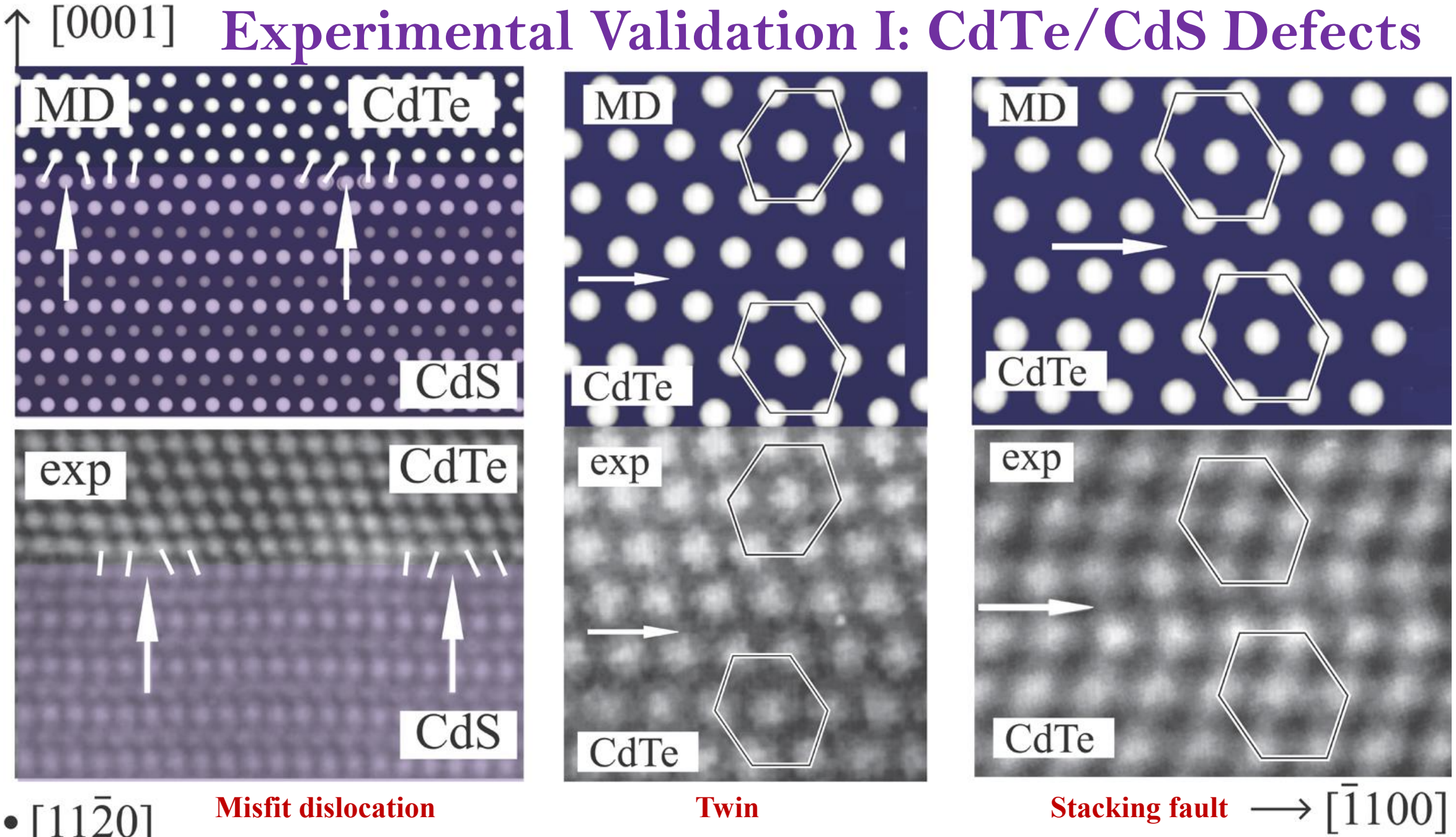
E_i = 1.0 eV, Cd:Te = 1, R = 2.2 nm/ns, T = 1000 K





- **We have developed a high-fidelity bond order potential (BOP) for Cd-Te-Zn** [Ward et al, PRB, 85, 115206 (2012); PRB, 86, 245203 (2012); J. Mol. Model., 19, 5469 (2013)].
- **This potential captures property trends of variety of phases in addition to enabling crystalline growth of zinc-blends CdTe**.

Experimental Validation I: CdTe/CdS Defects

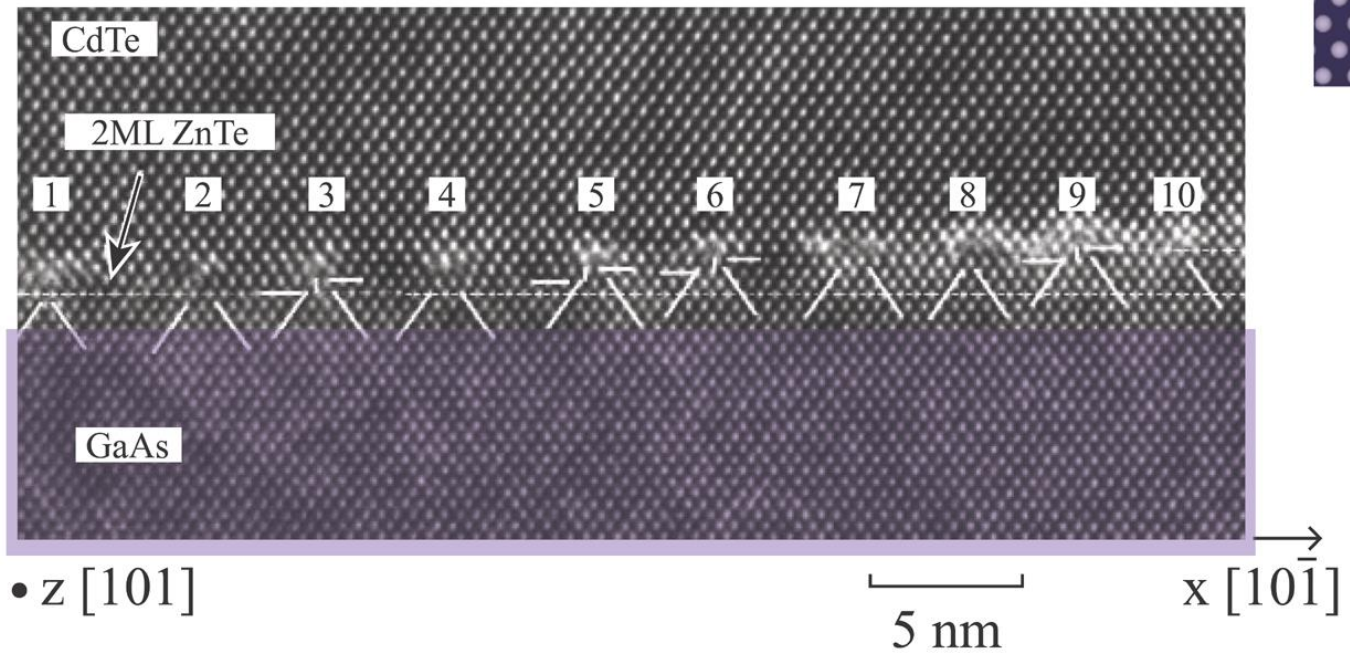


HRTEM from Yan et al, JAP, 89, 5844 (2001).

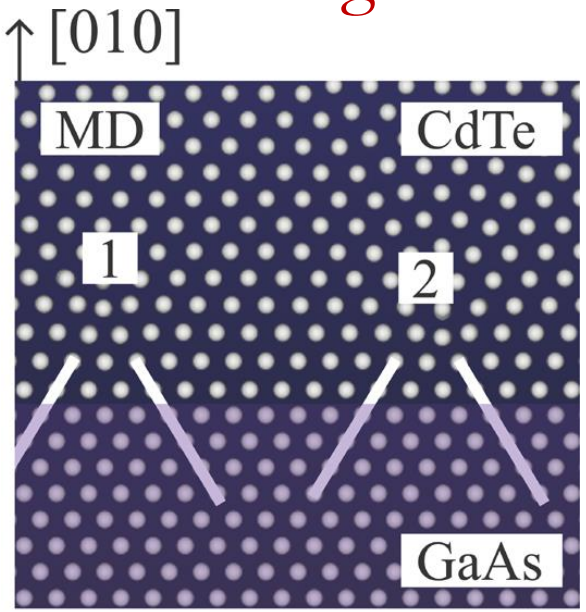
Experimental Validation II: CdTe/GaAs Misfit Dislocation

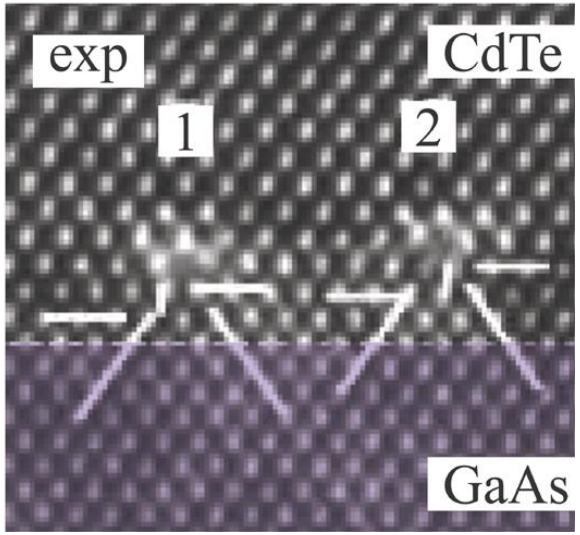
(a) BOP simulation (only Cd and the approximate "Ga" atoms are shown)

(b) HRTEM experimental image: S. Kret et al, Philo. Mag. 83, 231 (2003)



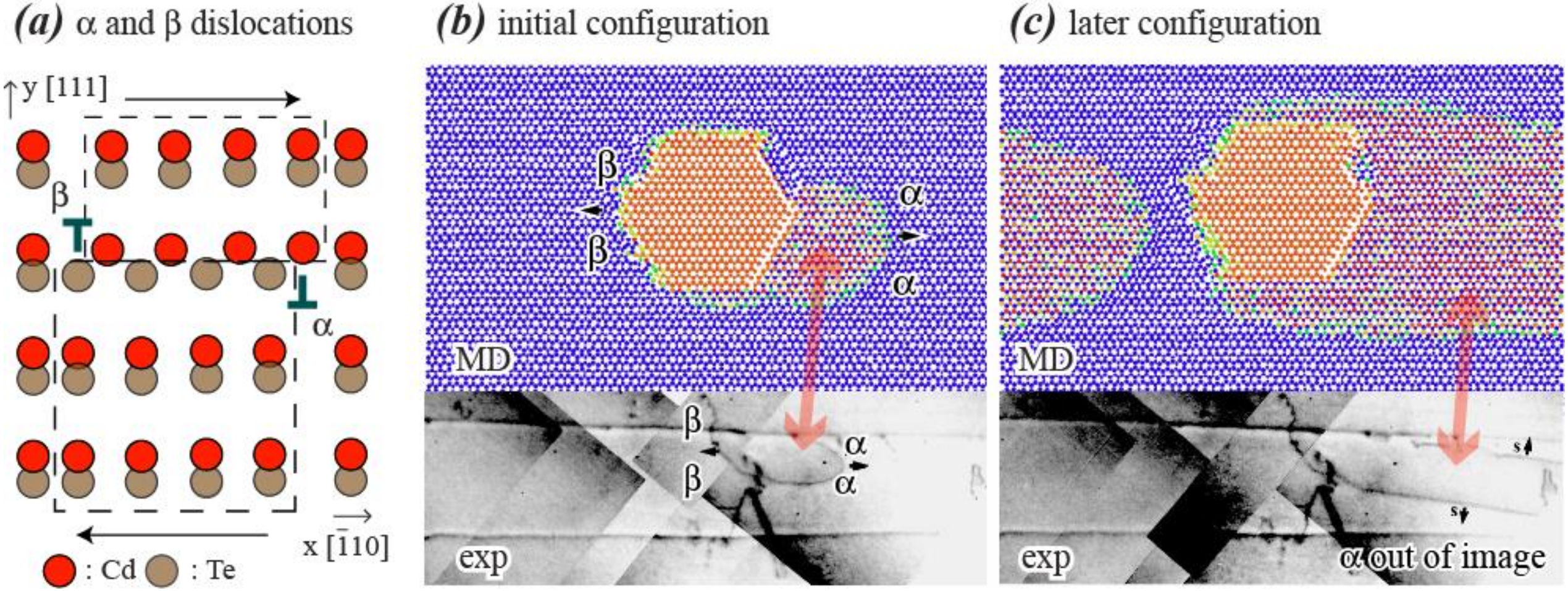
Magnified examination





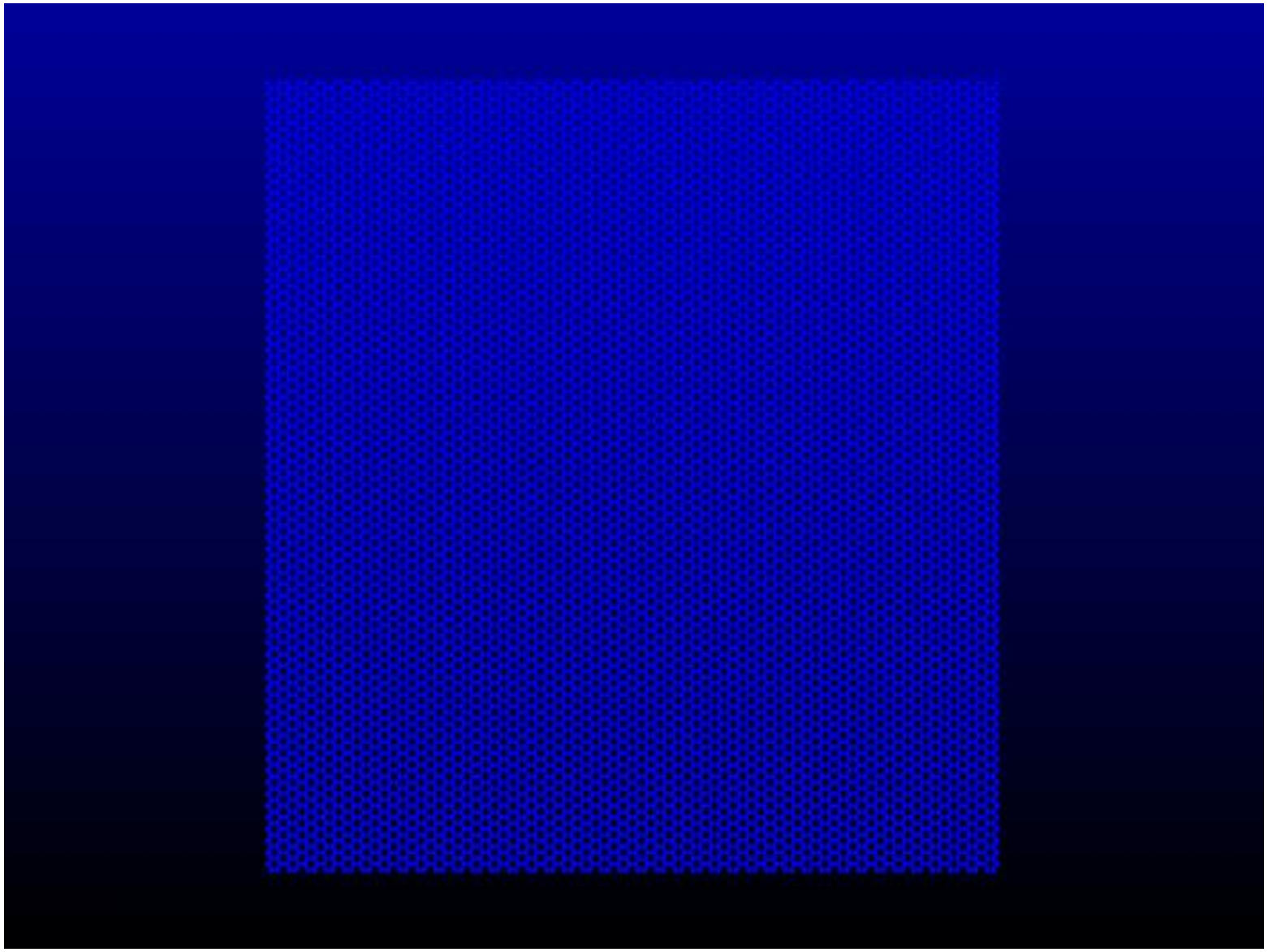
- **We only have Cd-Te-Zn potential, so GaAs is simulated as CdTe but lattice mismatch is accurately captured by fixing the "CdTe" at the GaAs lattice constant.**
- **Dislocation morphology and density obtained in MD simulations are similar to those seen in experiments.**

Dislocations in Radiation Detecting $Cd_xZn_{1-x}Te$



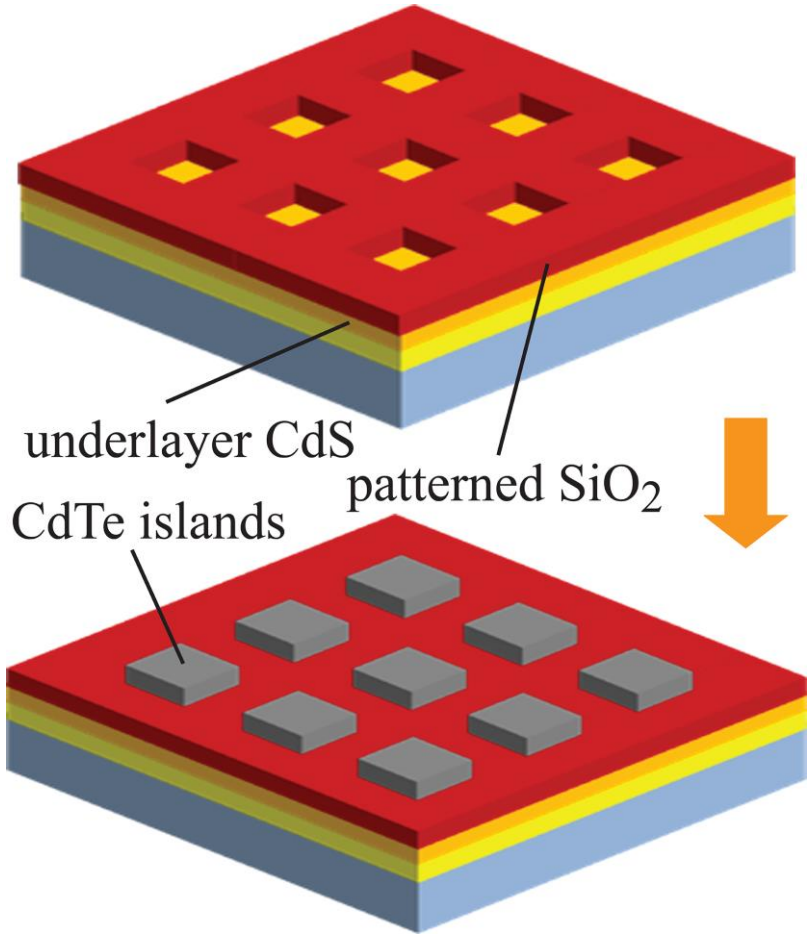
Experiments from Vanderschaeve et al, J. Phys.: Condens. Matter, 12, 10093 (2000).

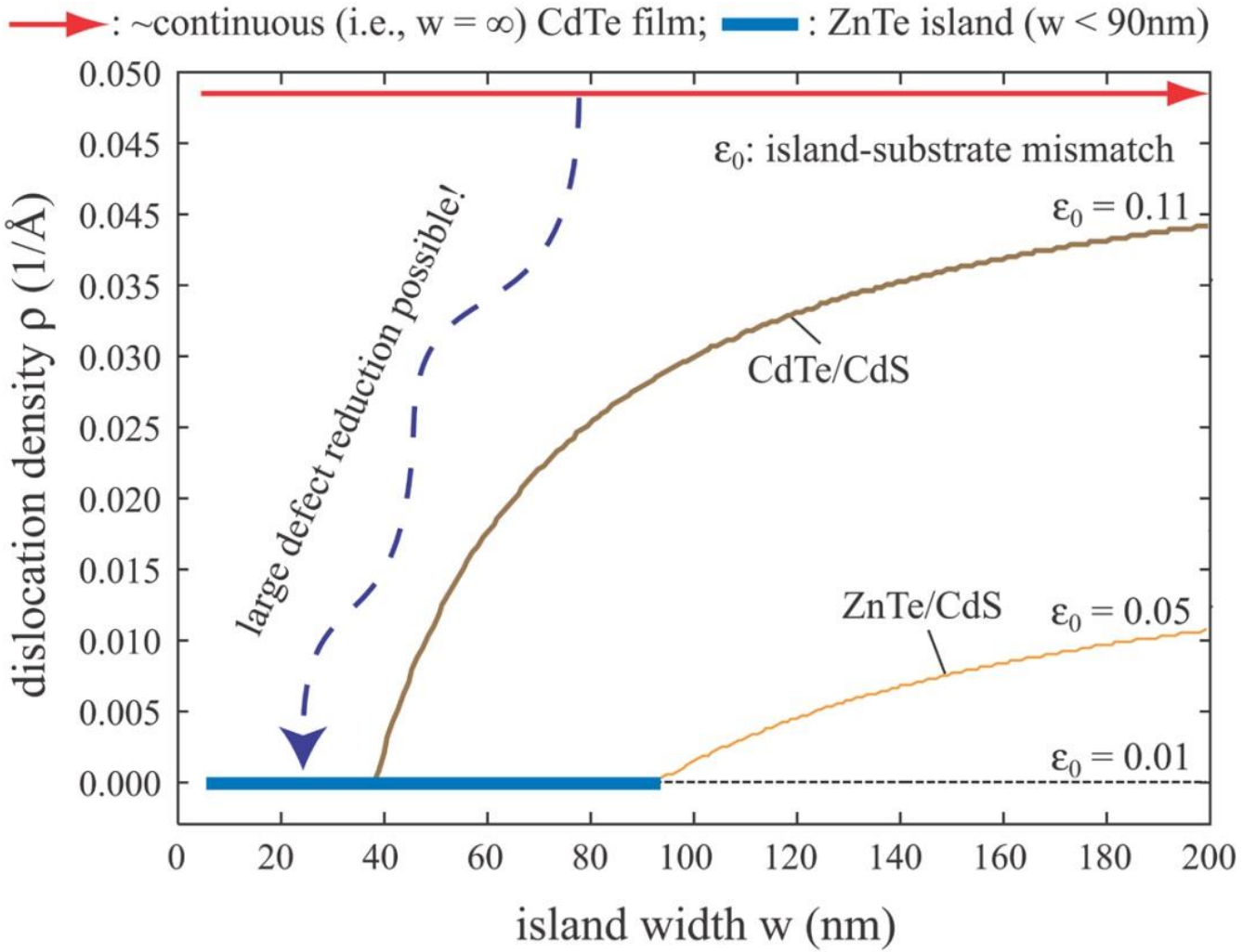
α and β Dislocation Mobility



MD Design of Dislocation-Free CdTe/CdS Solar Cells

Island growth technology:

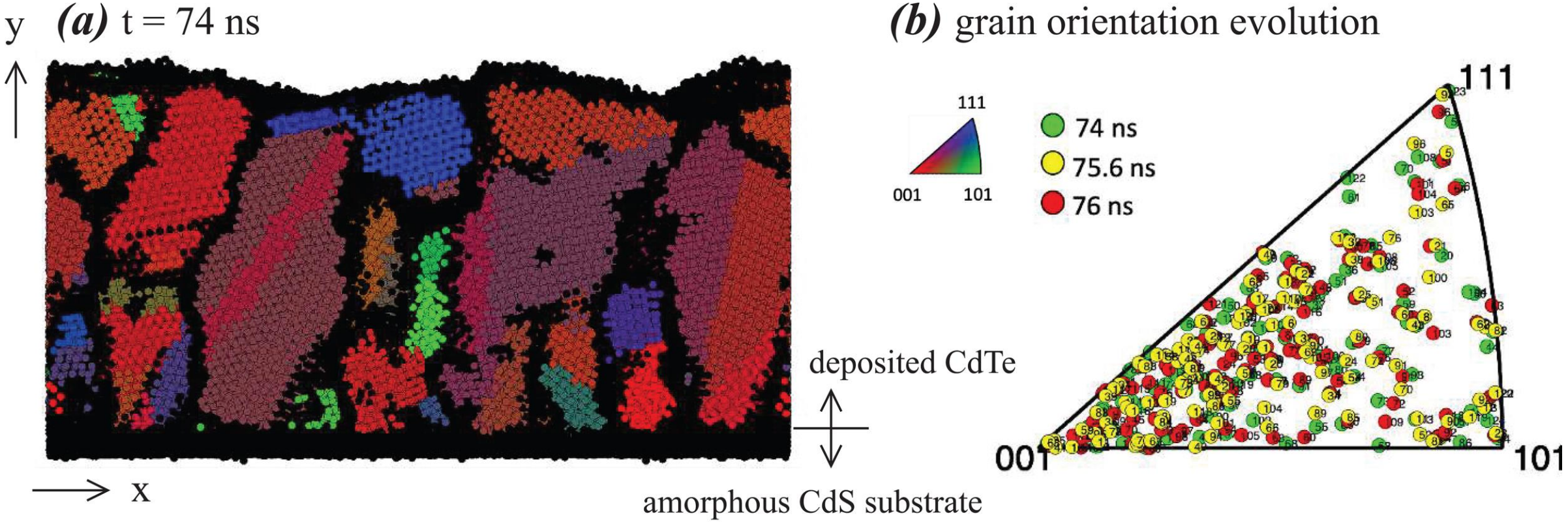




- Misfit dislocation always forms when misfit strain energy exceeds dislocation energy above critical film thickness.
- Islands relax misfit strain energy in 3D, can potentially prevent formation of misfit dislocations.
- MD enables calculations of misfit strain and dislocation energies in island configurations, which can be used to design dislocation-free nanostructures [Zhou et al, Prog. Photovoltaics., 23, 1837 (2015)].

MD Study of Grain Structure Evolution

1. Photovoltaic properties of CdTe/CdS films are limited by grain boundaries.
2. Can MD be used to analyze grain boundary structures and their evolution?



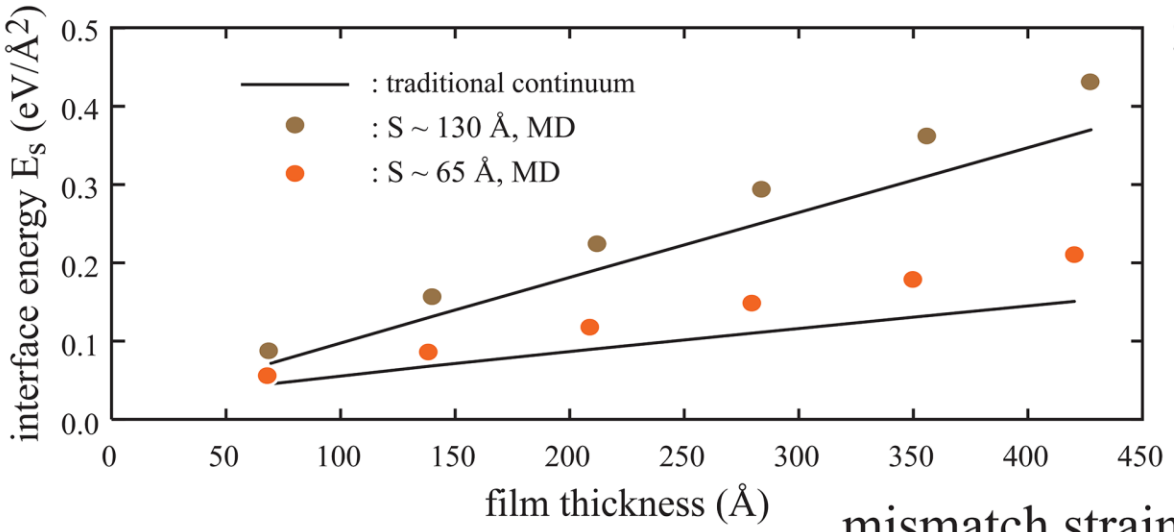
temperature = 1400 K, adatom energy 0.5 eV, growth rate 0.2 nm/ns

- ❑ MD can be used to simulate the growth of polycrystalline films on amorphous substrates.
- ❑ Grain Tracking Algorithm* can be used to analyze grain orientation evolution.

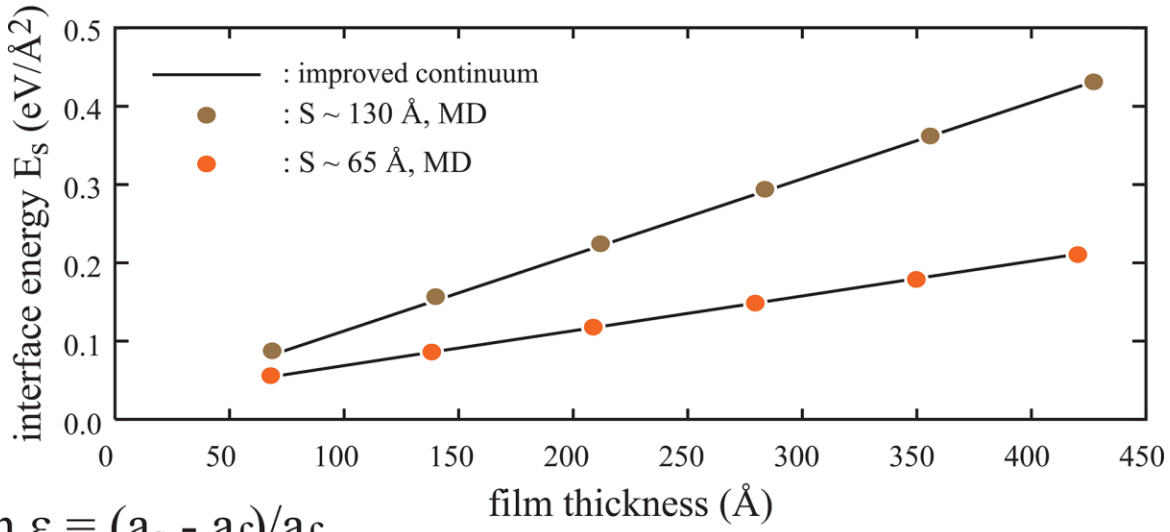
* Panzarino et al, JOM, 66, 417 (2014).

MD Guided Misfit Dislocation Theory Development

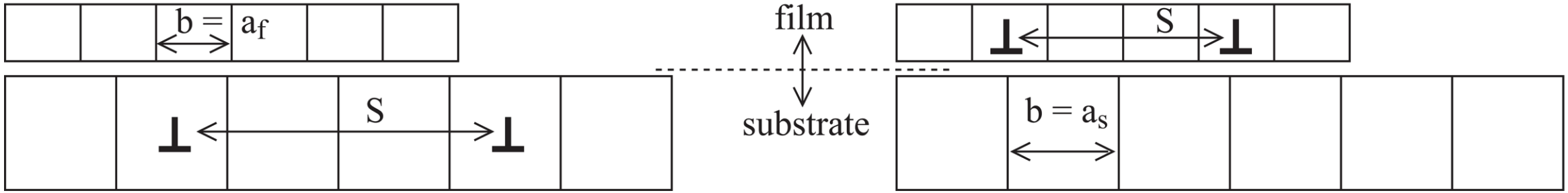
(a) MD. vs. traditional misfit dislocation theory



(b) MD vs. improved misfit dislocation theory



mismatch strain $\varepsilon = (a_s - a_f)/a_f$



1. In dislocation theory, system energy $E(b,S,\varepsilon) = E_\varepsilon(S,\varepsilon) + E_d(b,S)$ (misfit + dislocation energies).
2. Dislocation density is calculated by minimizing energy. Issues: Should b and S be measured from film or substrate? Is $E_d(b,S)$ expression accurate? Existing theories are only applicable for continuous films …
3. MD simulations guided more accurate $E_d(b,S)$ derivation, showed that b and S should be from substrate and film respectively.

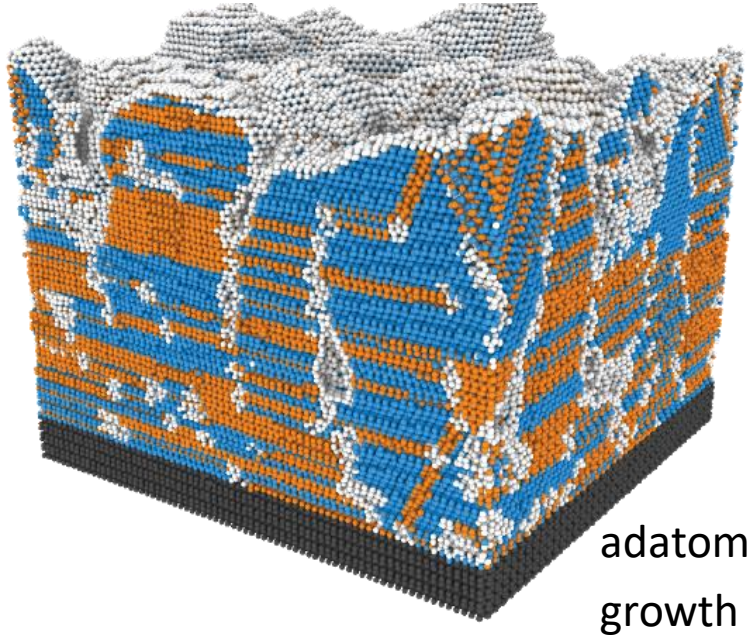
Zhou et al, J. Mech. Phys. Sol., 91, 265 (2016).

MD Study of Solid State Lighting InGaN Systems

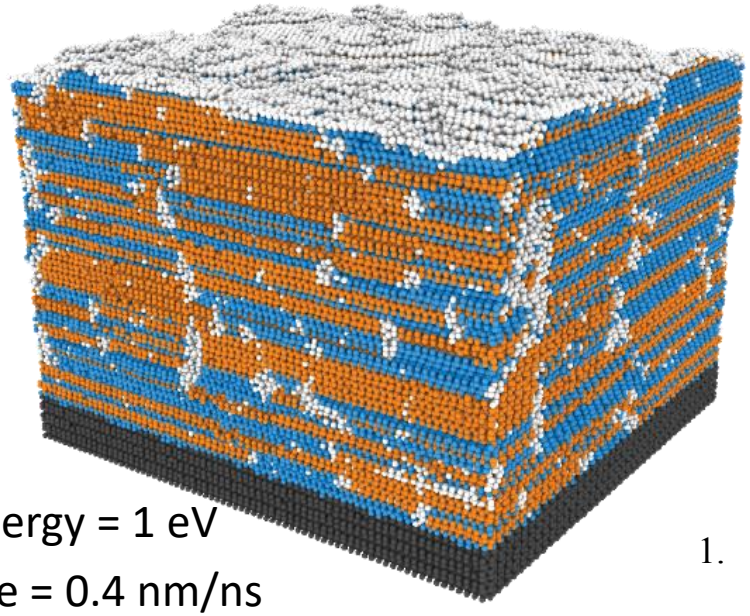
1. Misfit Defects limit InGaN properties; 2. Can MD guide defect reduction?

MD Simulation

(a) homologous temp (T/T_m = 0.56)



(b) Homologous temp (T/T_m = 0.78)

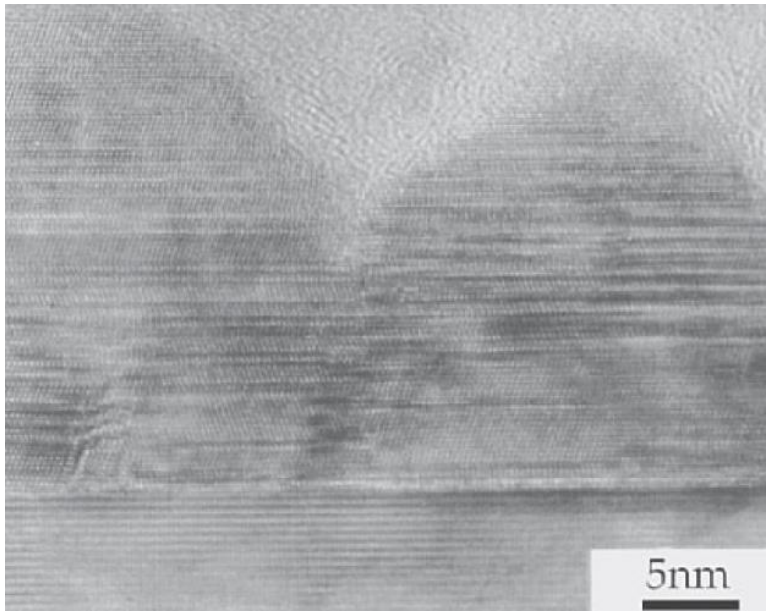


adatom energy = 1 eV

growth rate = 0.4 nm/ns

Wurtzite Zinc-Blende Substrate Other

Experiments



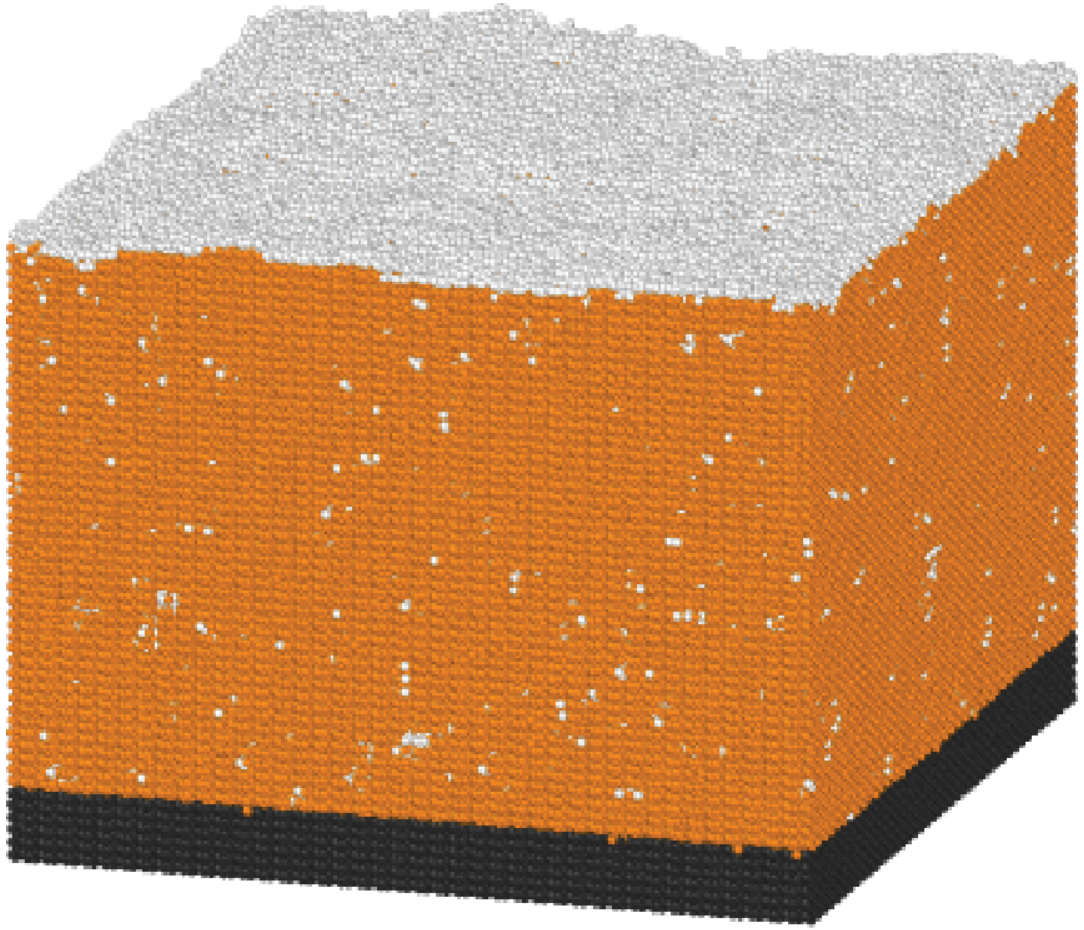
1. Zhou et al, J. Appl. Phys., 122, 235703 (2017); J. Mater. Sci. Res., 6, 88 (2017).
2. Gruber et al, JAP, 121, 195301 (2017).
3. Wu et al, APL, 68, 1372 (1996).

- Based on the InGaN potentials[1], MD is used to explore InGaN growth on (0001) GaN[2].
- Surface morphology is similar to experimental observation[3]. Significant polytypism is observed with the (0001) growth. Increasing temperature reduces surface roughness and associated defects

GaN on $(11\bar{2}0)$ GaN

GaN on a $(11\bar{2}0)$ GaN at $T/T_m = 0.78$

adatom energy = 1 eV, growth rate = 0.4 nm/ns

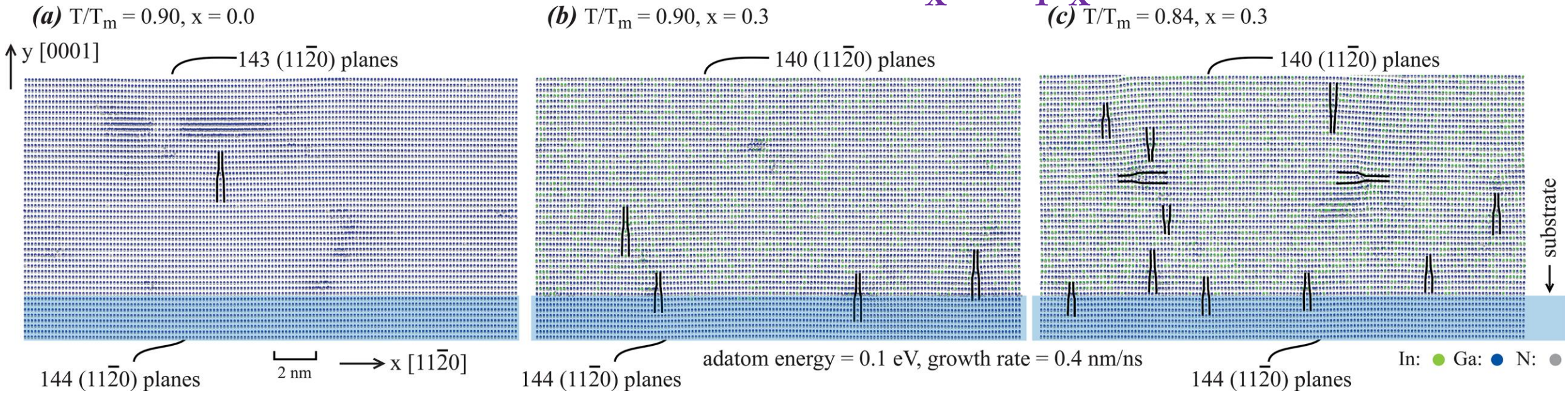


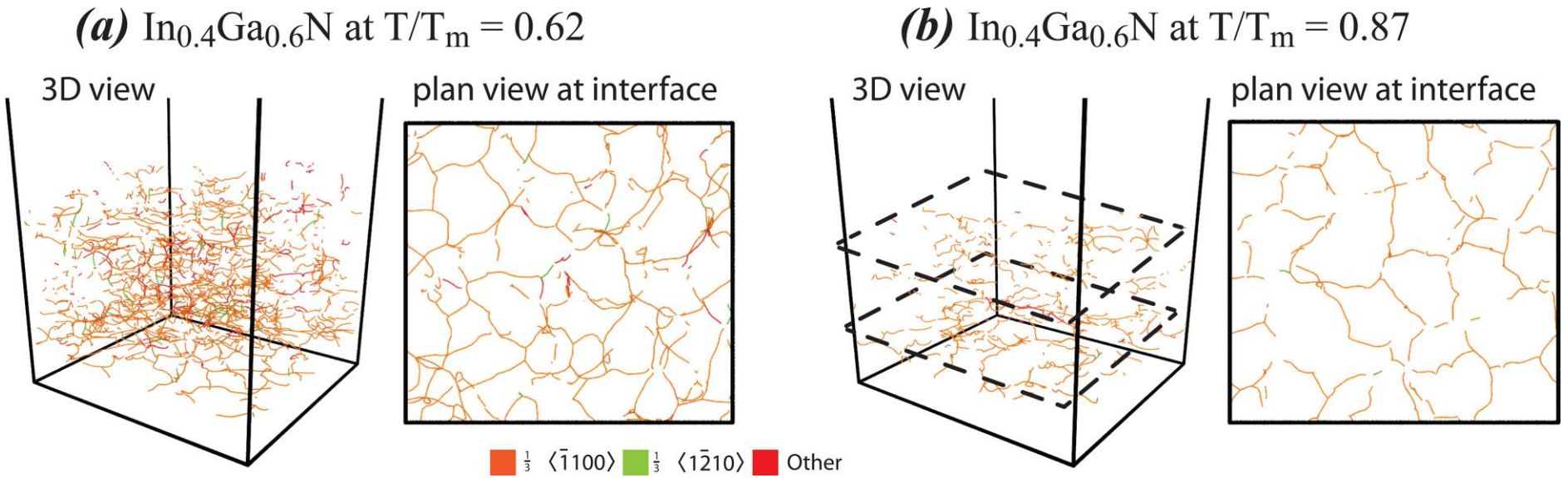
Wurtzite Zinc-Blende Substrate Other

- MD indicates that polytypism occurs on (0001) because there are three (0001) planes A, B, C so both B and C can form on A.
- We hypothesize that $(11\bar{2}0)$ growth can eliminate polytypism as there are only A and B $(11\bar{2}0)$ planes.
- MD simulations verifies this hypothesis.
- Reduced polytypism also helps reduce other defects such as dislocations.

Chu et al, Phys. Rev. Mater., 2, 013402 (2018).

Misfit Dislocation in $In_xGa_{1-x}N/GaN$

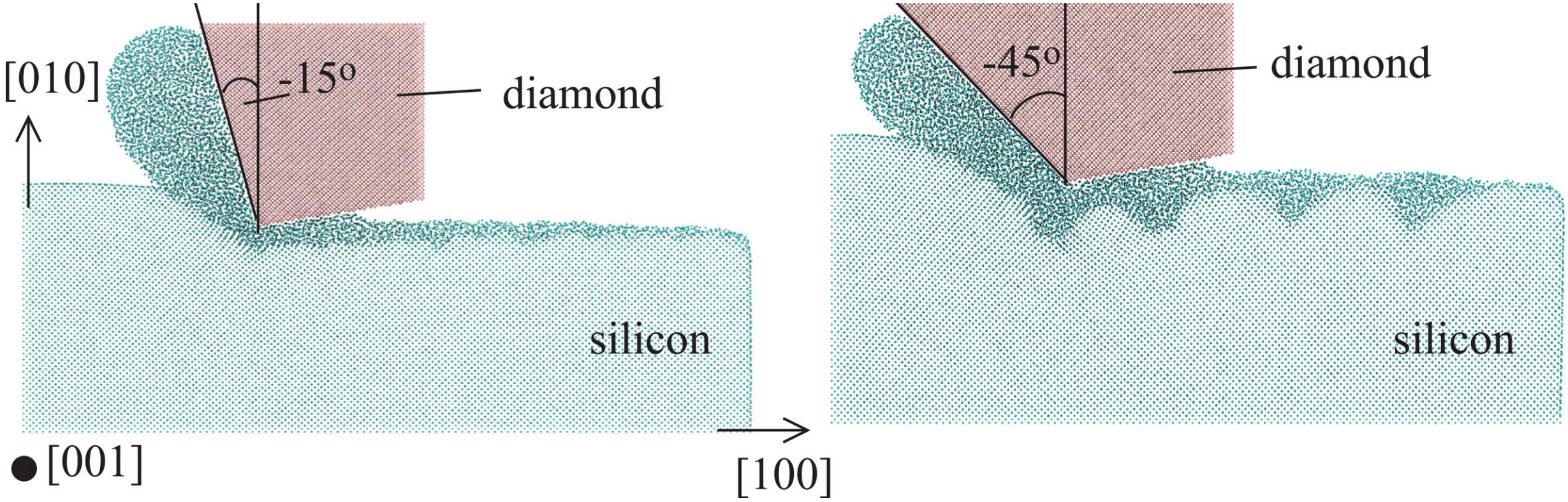




Misfit dislocation density increases when indium content is increased and temperature is decreased.

Gruber et al, J. Appl. Phys., 121, 195301 (2017).

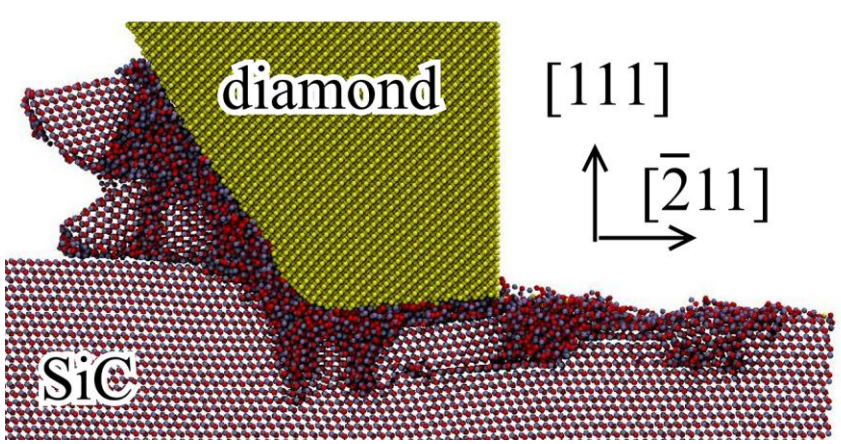
MD Study of Rake Angle Effects of Cutting Tool

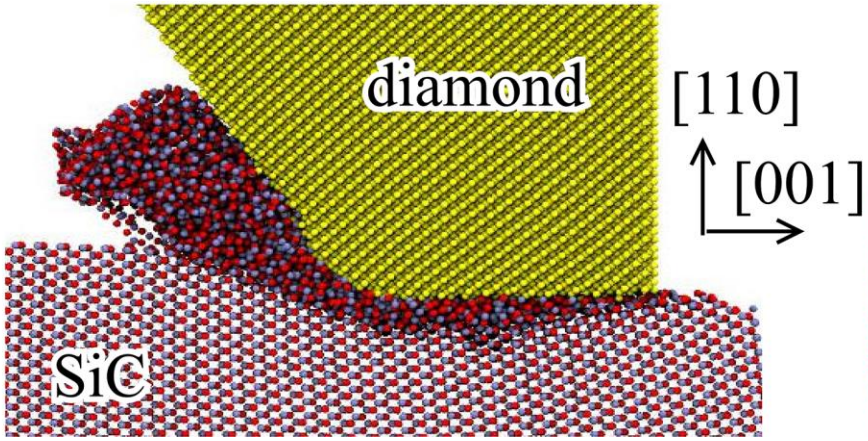


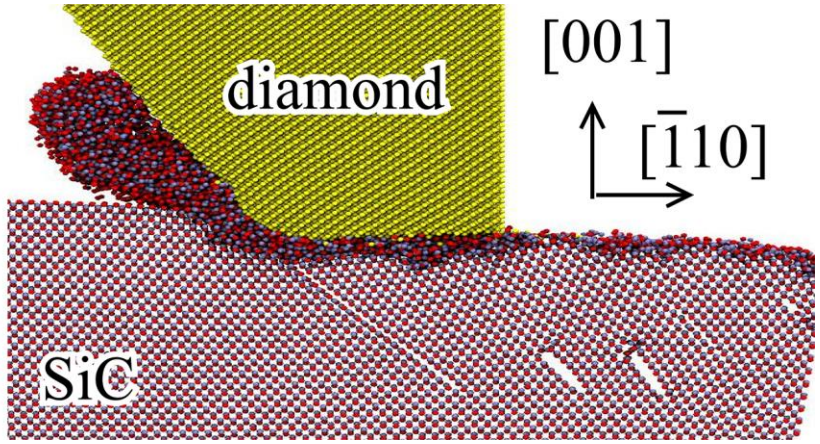
MD simulations indicated that the cutting tool rake angle sensitively impacts the damage. Large negative angles may increase the damage zone, but is needed to prevent fracture of brittle workpiece.

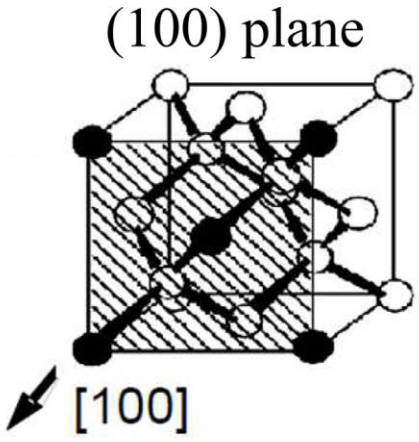
Goel et al, Inter. J. Machine Tools Manufac., 88, 131 (2015).

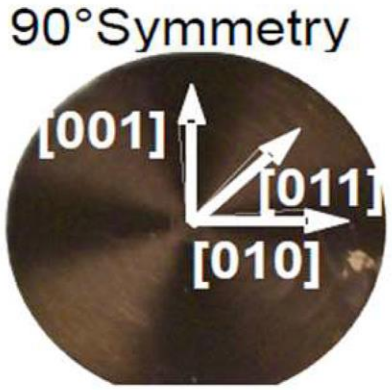
MD Study of Anisotropic Effects of SiC

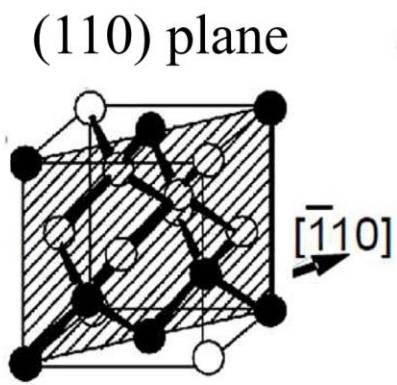


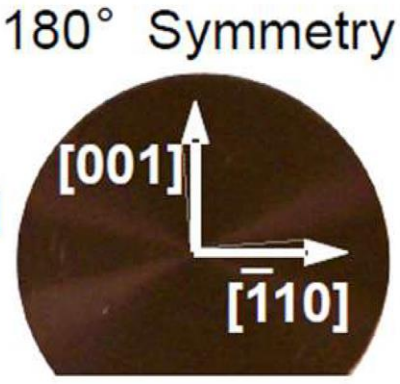


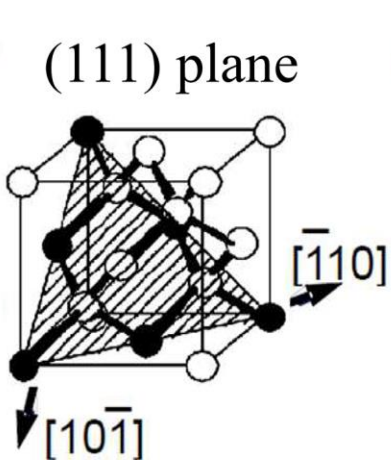


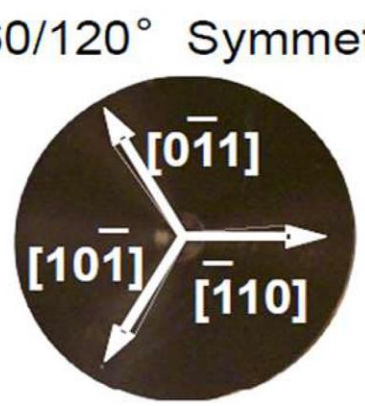








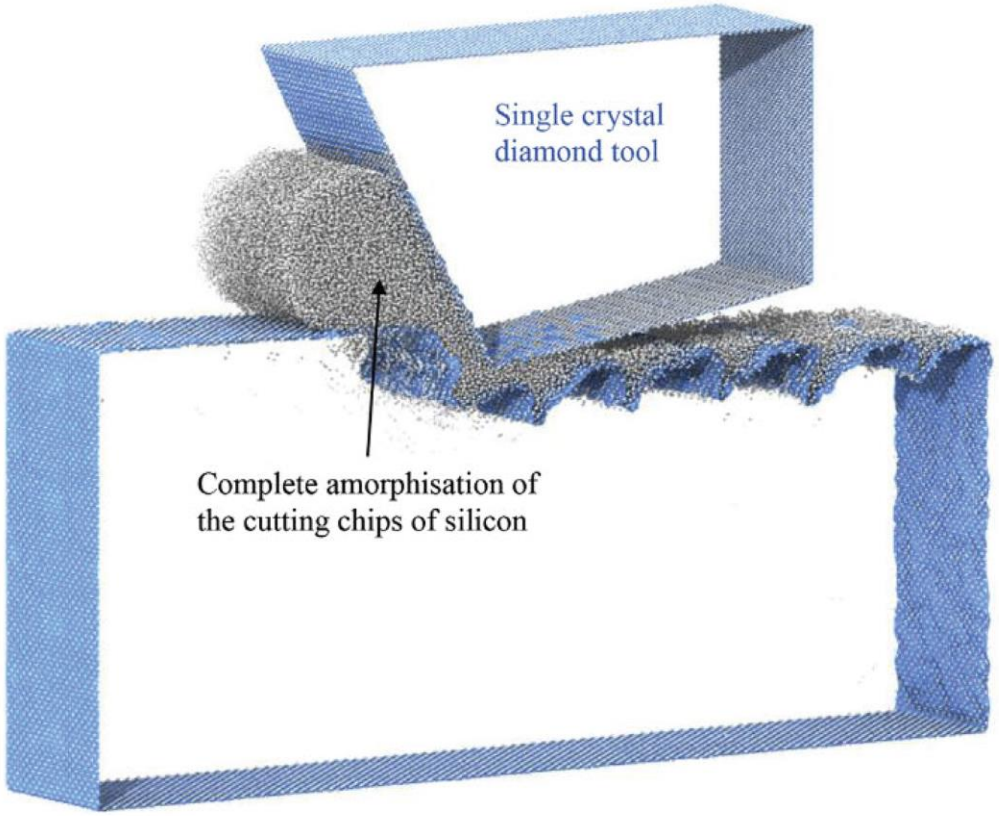




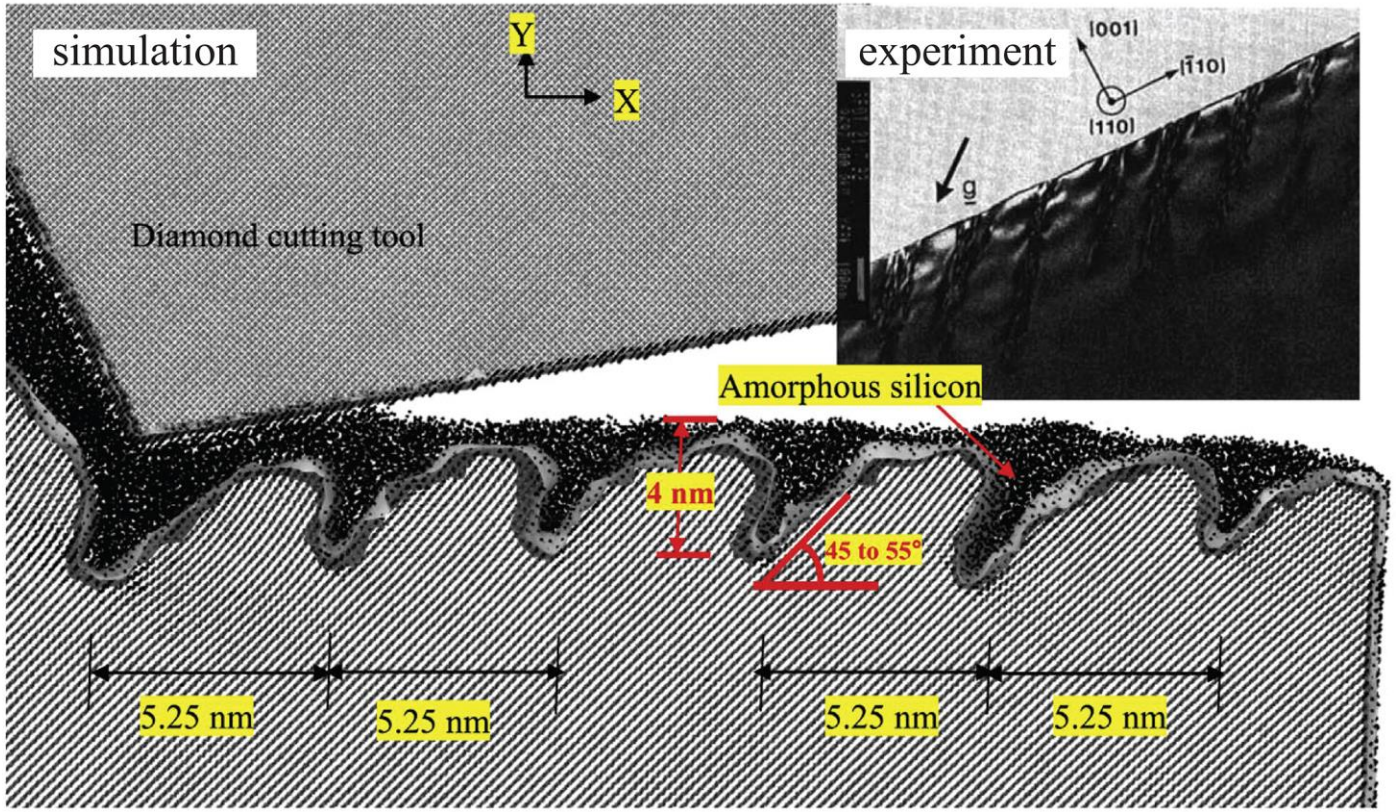
SiC was found to be highly anisotropic.

MD Study of Defect Zones on Surfaces

(a) 3D visualization of cutting



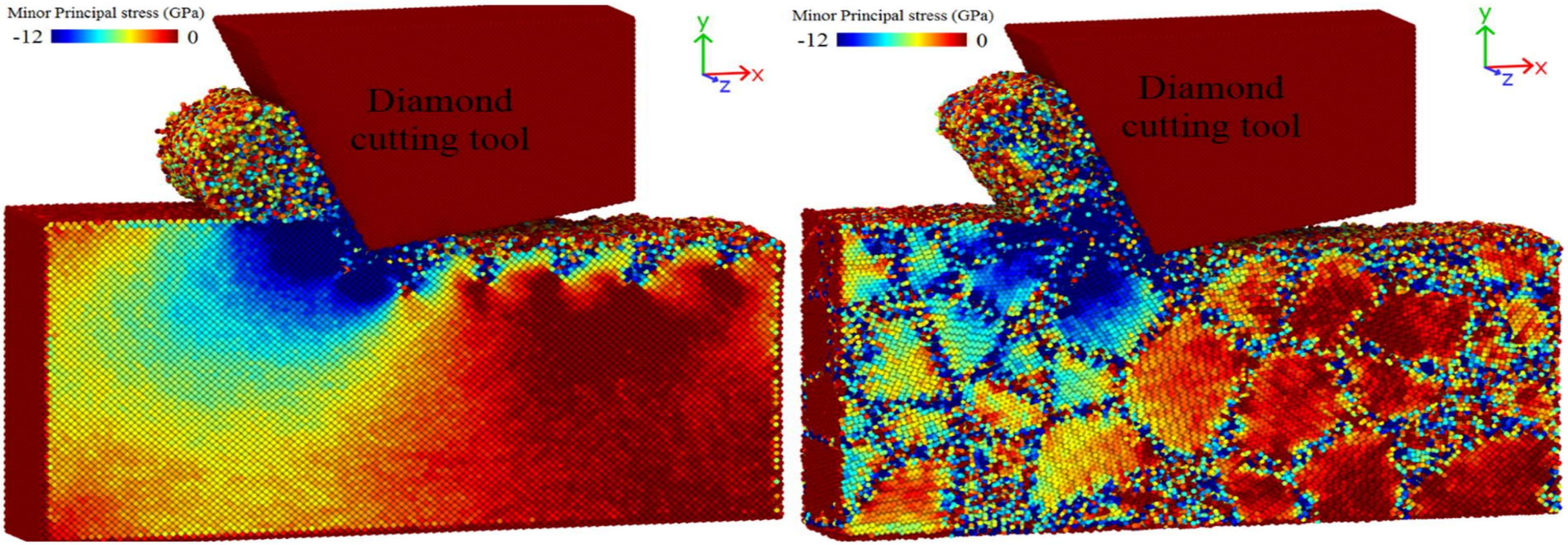
(b) 2D comparison with experimental image



- Unlike the conventional high pressure phase transformation mechanism, direct amorphization was identified as the root cause of plasticity in silicon cutting.
- The predicted formation of periodic nanogrooves at 45° to 55° agrees with experiments.

Goel et al, Acta Mater., 105, 464 (2016).

Single vs. Polycrystalline Samples



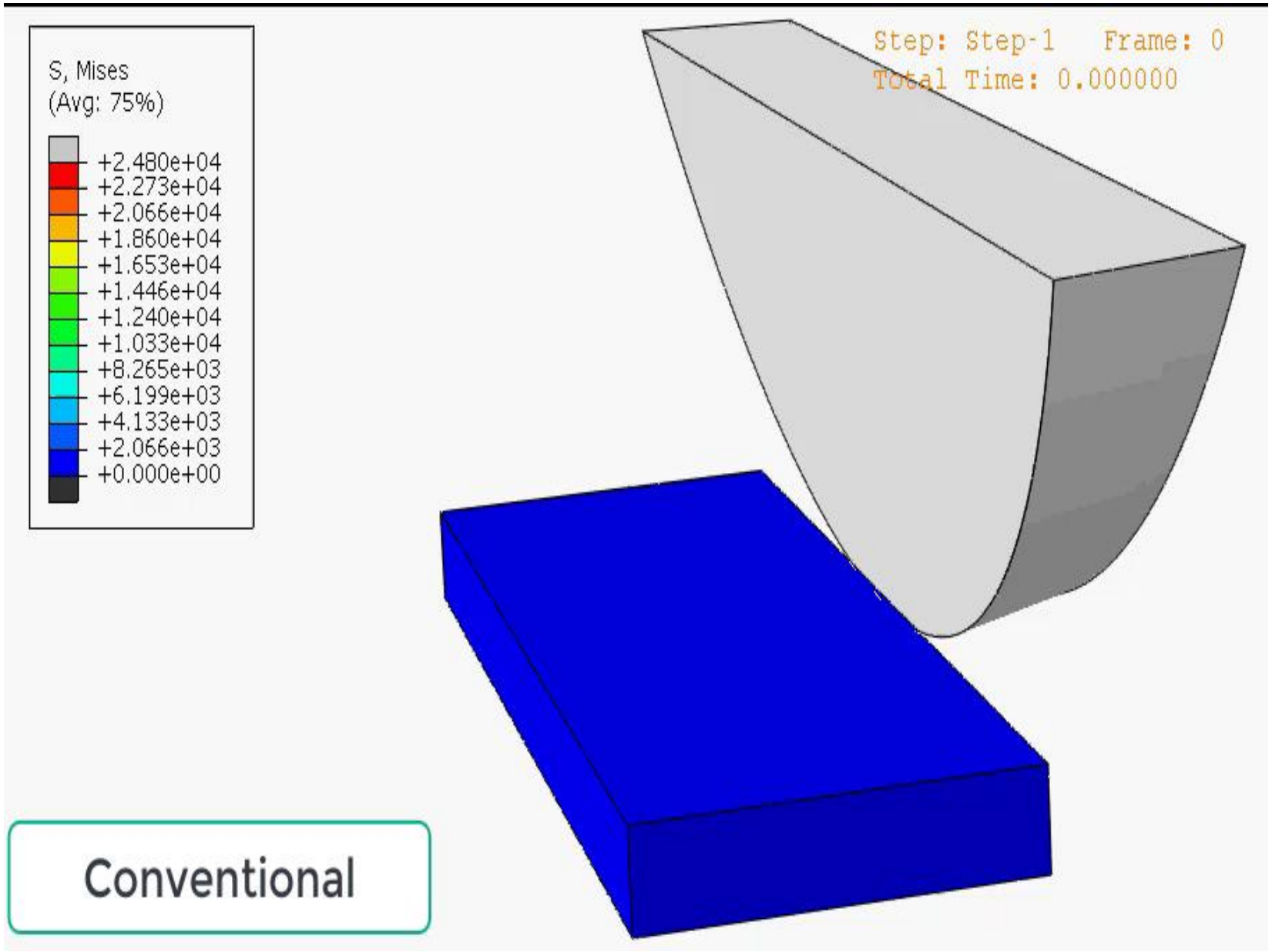
- Chips from single crystalline Si samples are far more curl.
- The stress non-uniformity in the polycrystalline samples reduces the cutting force.
- MD results in the “surface defect machining method” for reducing cutting strength, which has been experimentally demonstrated.

Goel et al, Acta Mater., 105, 464 (2016).

Summary

- MD indicated that defects in graphene are created at island periphery at early stage rather than after islands impinge.
- MD, validated by experimental defect characteristics, indicated that nanostructure can produce dislocation-free CdTe/CdS structures.
- MD can be used to study grain evolution.
- MD can guide the development of misfit dislocation theories.
- MD revealed dislocation formation mechanism in InGaN films, and indicated that polytypism in can be removed by changing the growth direction.
- MD provided insights to improve microfabrication.

Finite Element Method Exploration of Si Cutting



Graphene Growth Simulation