SAND2014-18012PE

Molecular Dynamics (MD) Simulations Based Design and Process Optimization of Solar Cells

Autumn School on Microstructural Characterization and Modelling of Thin-Film Solar Cells

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Outline

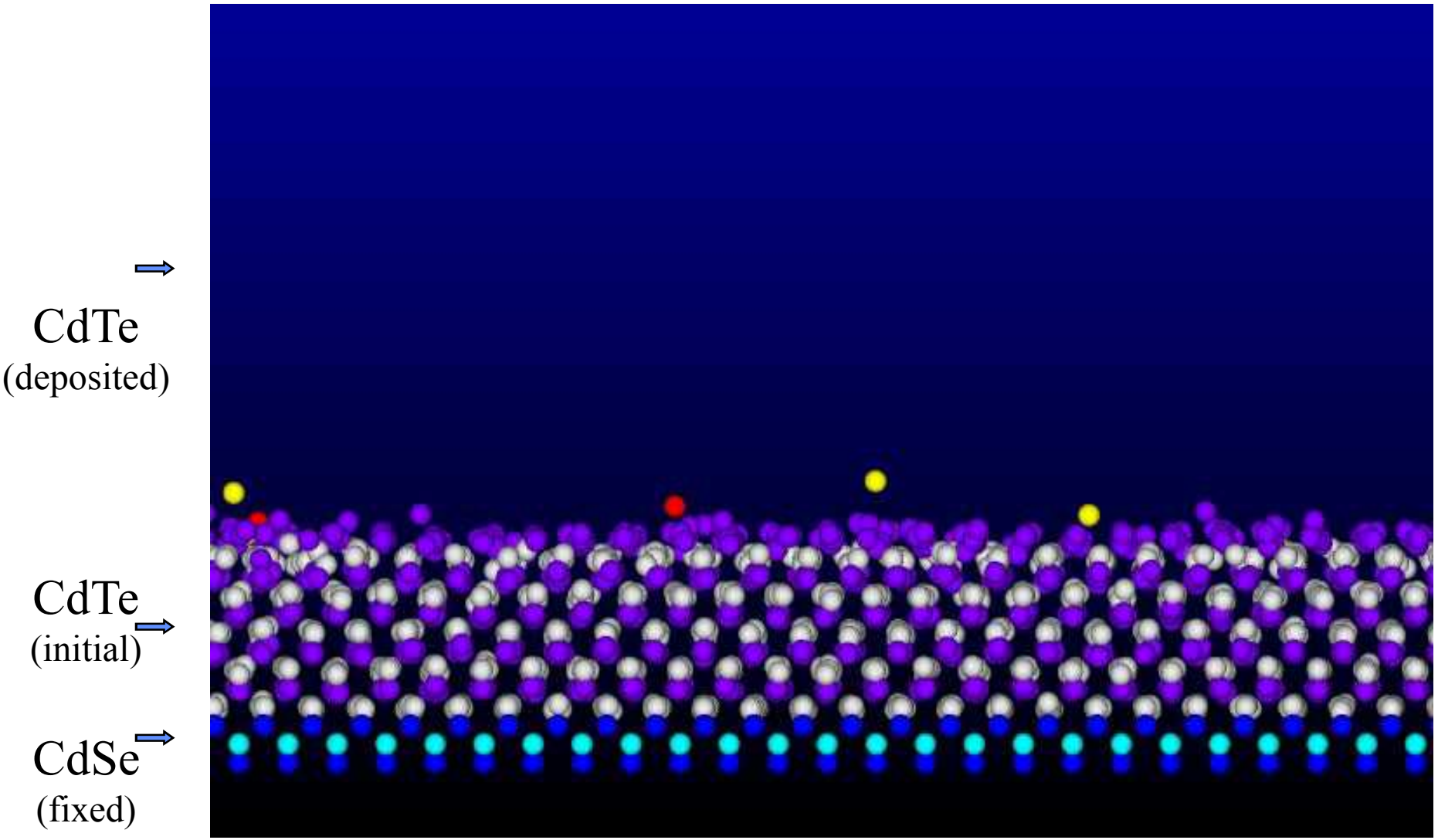
1. What MD can do
2. Quantum Mechanical Calculations
3. Interatomic Potentials
4. Molecular Dynamics / LAMMPS
5. Pre- and Post- Processing
6. MD Informed Continuum models
7. Exercises

Topic 1:
What MD can do

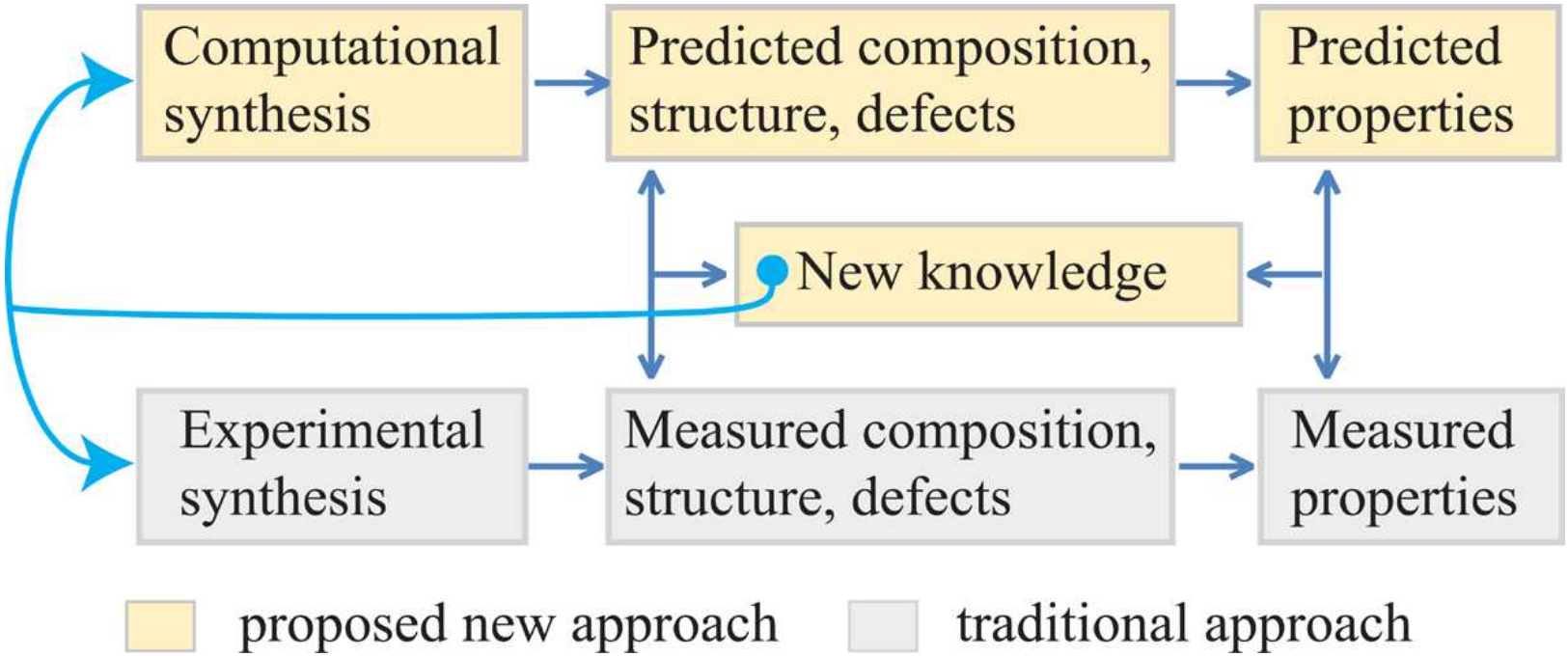
Molecular Dynamics (MD)

solves atom positions as a function of time from Newton's equation

reveal atomic scale structures and is applicable for synthesis processes



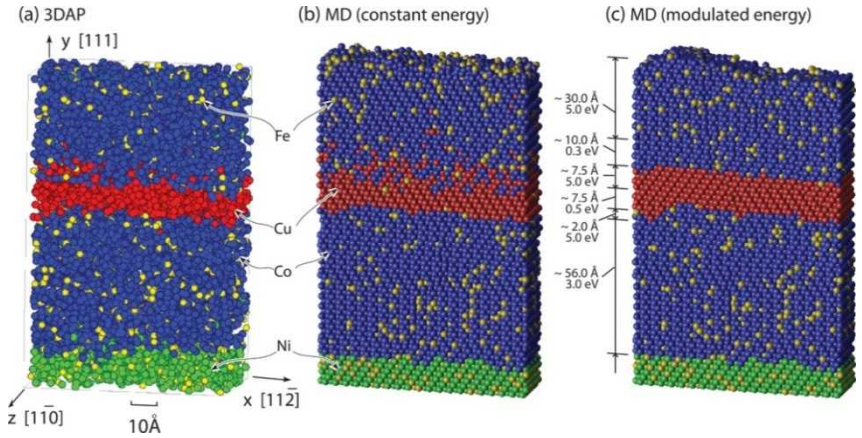
Defect Reduction through Computational Synthesis



1. No sample preparation;
2. Numerical details of defect configurations;
3. In situ observations;
4. Mechanism studies;
5. Test prior to experimental investment.

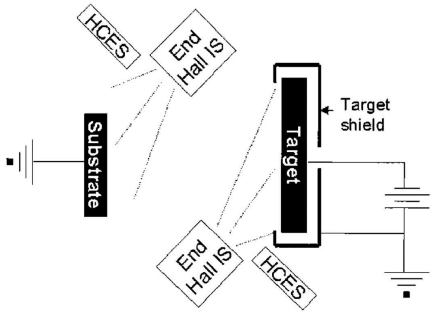
The proposed approaches do work!

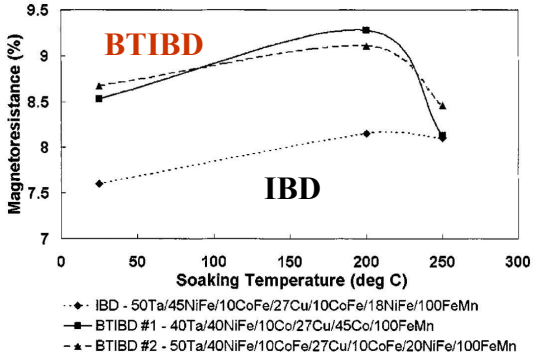
MD prediction of improved synthesis
(giant magnetoresistive spin valve)



X. Zhou, et al, Acta Mater., 49, 4005 (2001).

MD leads to a new BTIBD growth method
(by CVC, Inc.)





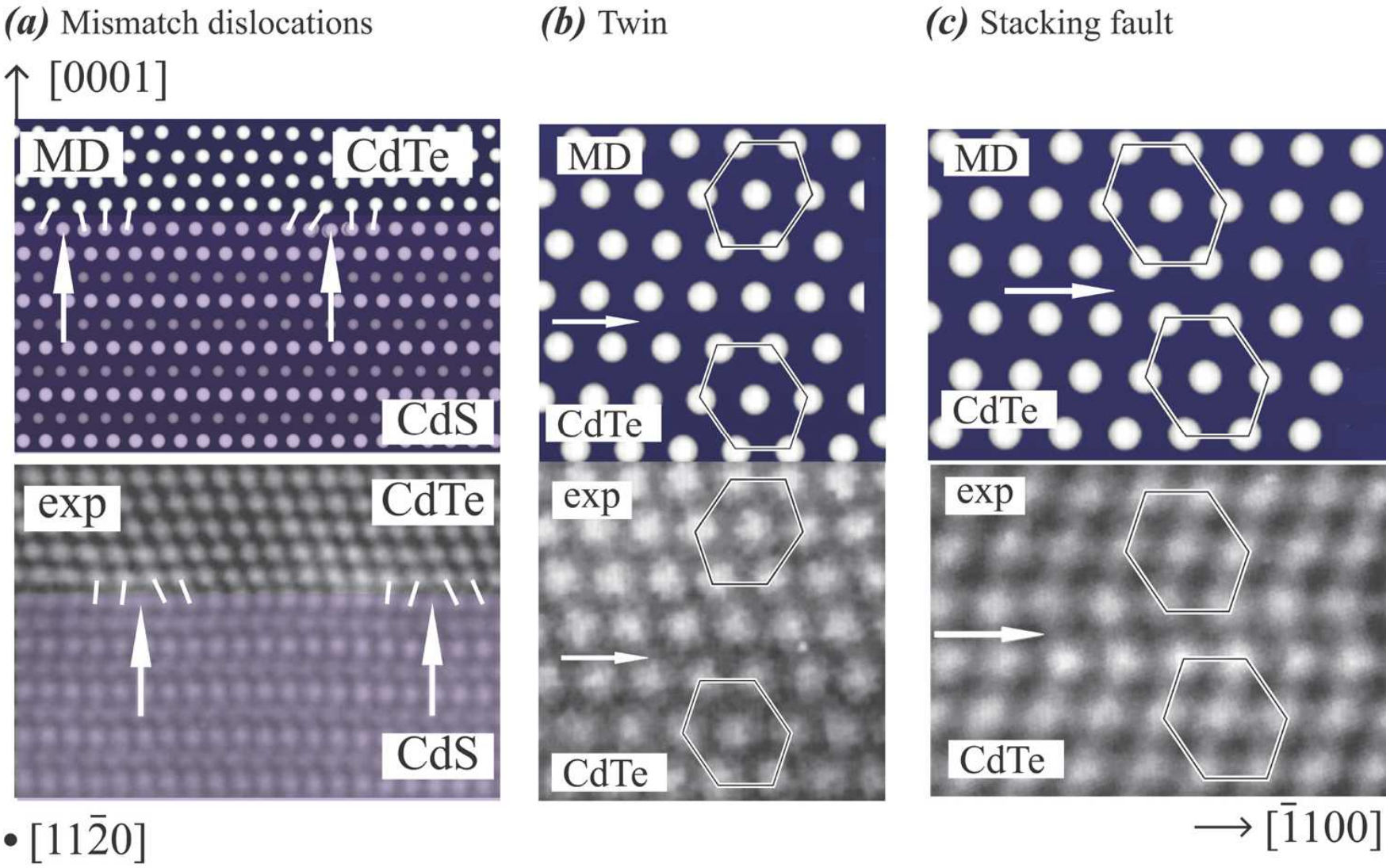
T. L. Hylton, et al, IEEE Trans. Mag., 36, 2966 (2000).

High-fidelity simulations enable us to:

- visualize strain relaxation defect formation in situ;
- thoroughly explore growth conditions;
- brainstorm novel synthesis (e.g., intra layer modulation of conditions).
- design of defect-free nanostructures;

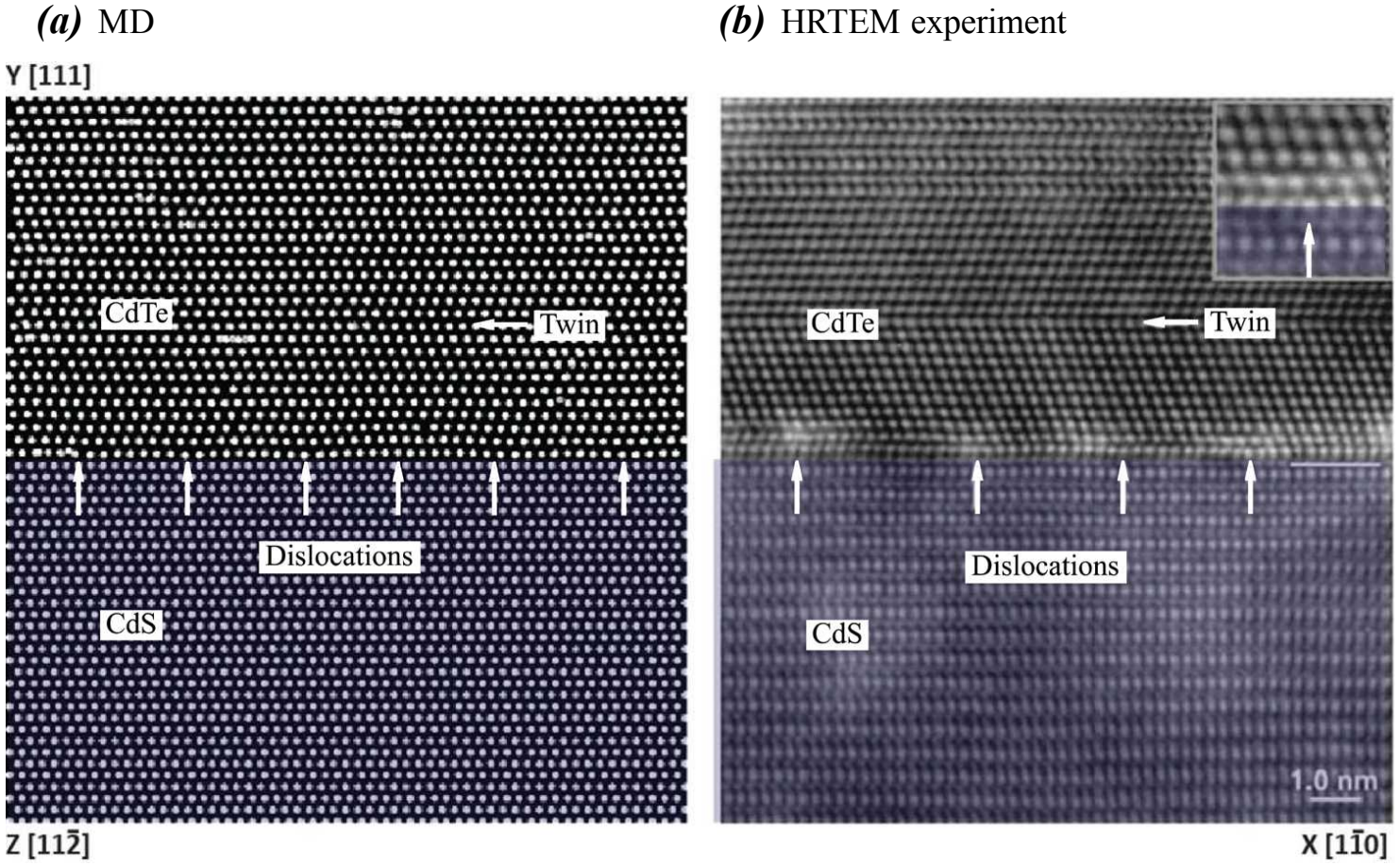
Similar successes with NA22 on three funded projects, CZT, $LaBr_3$, and elpasolites...

1st Example of MD Fidelity: CdTe/CdS Defects



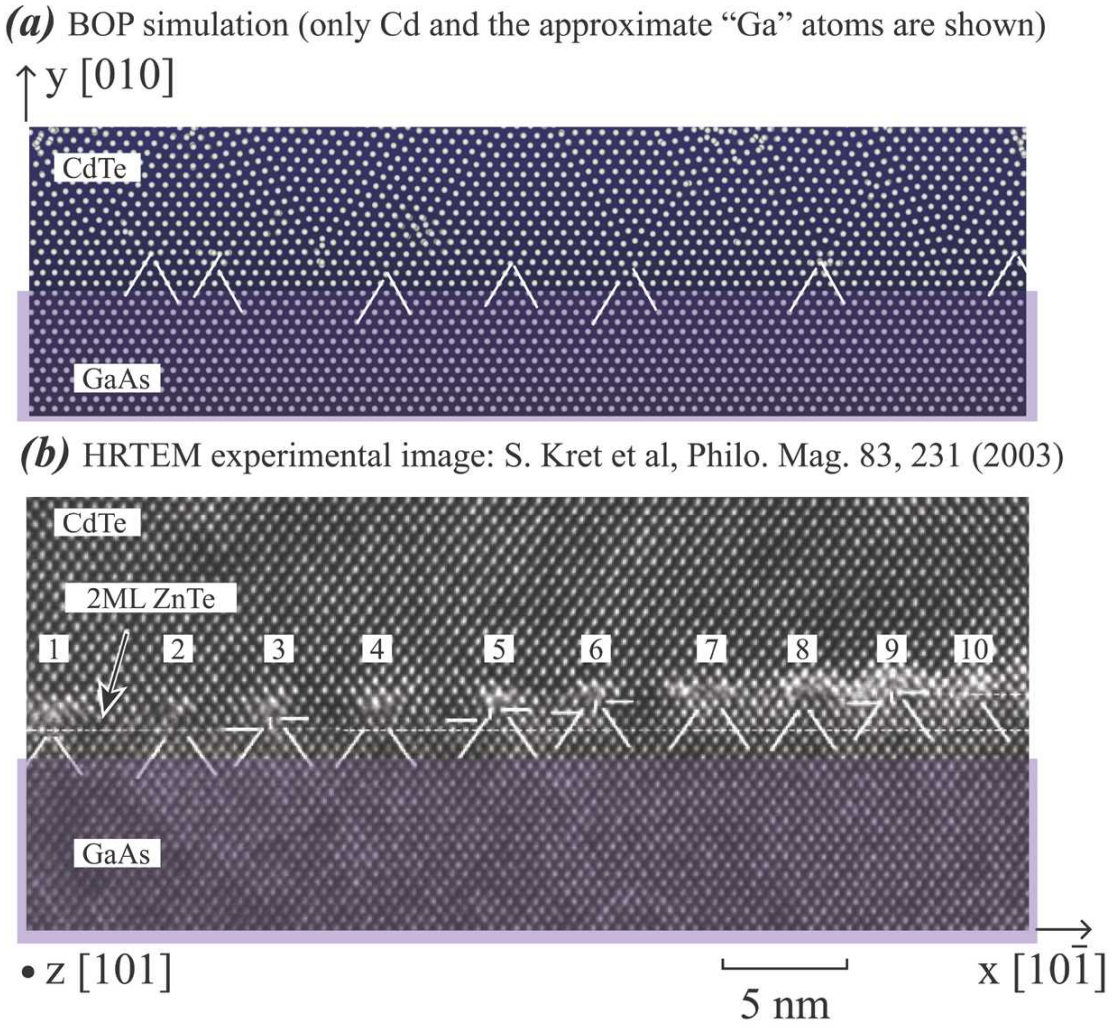
HRTEM from Y. Yan, R. G. Dhere, K. M. Jones, and M. M. Al-Jassim, J. Appl. Phys. 89, 5844 (2001).

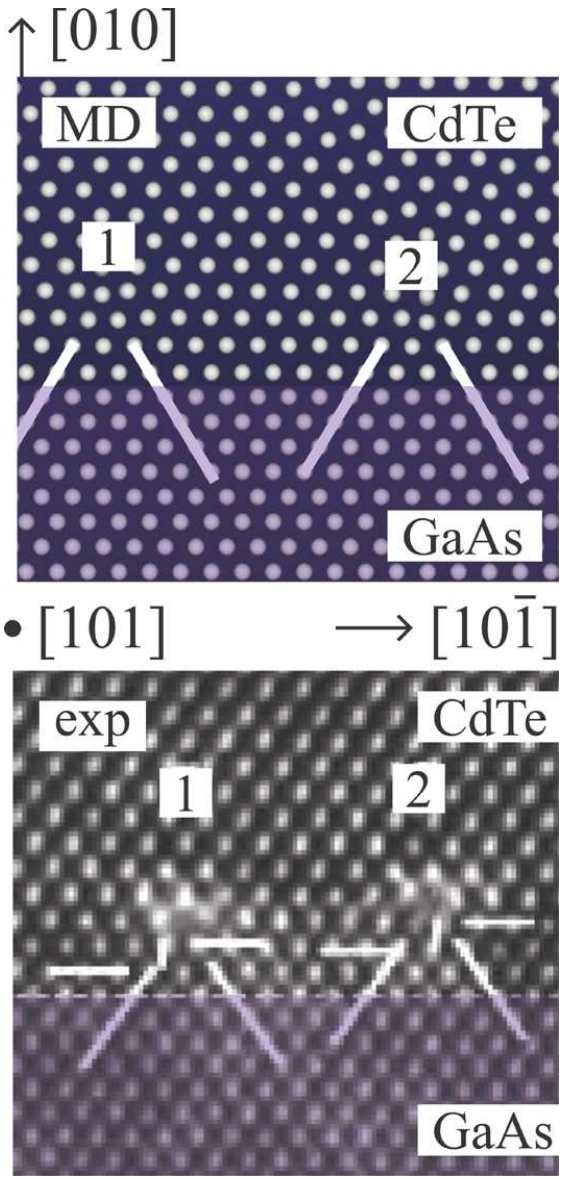
2nd Example of MD Fidelity: CdTe/CdS Defects



HRTEM from Y. Yan, R. G. Dhere, K. M. Jones, and M. M. Al-Jassim, J. Appl. Phys., 89, 5944 (2001).

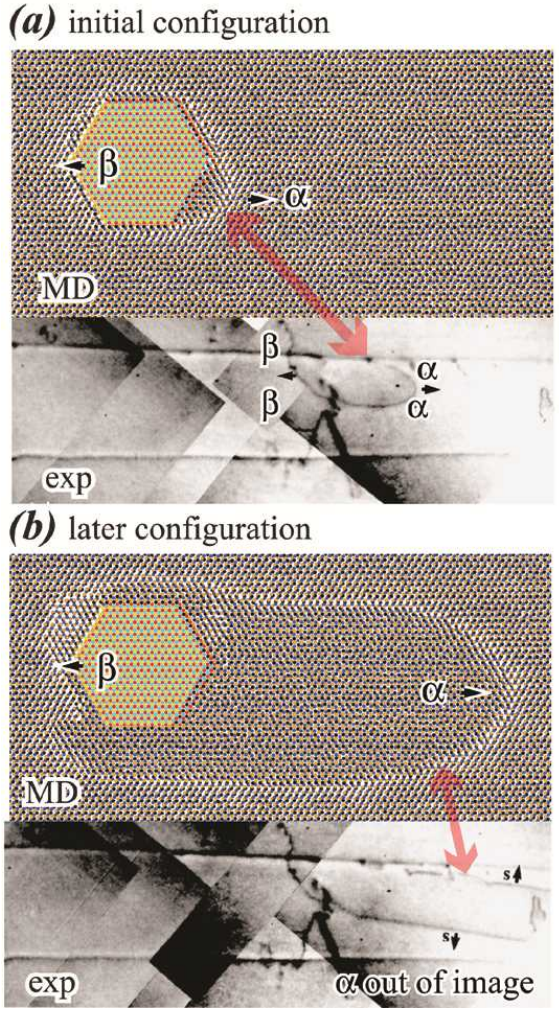
3rd Example of MD Fidelity: CdTe/GaAs Defects

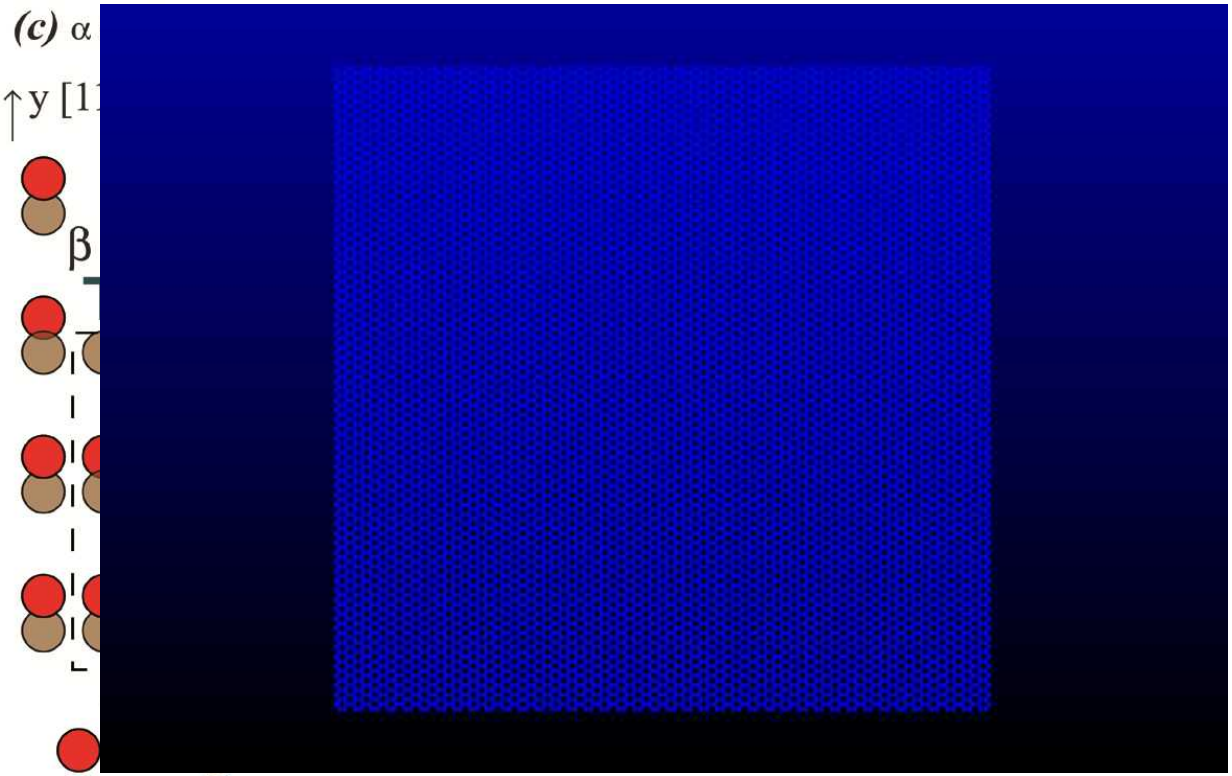




J. J. Chavez, D. K. Ward, B. M. Wong, F. P. Doty, J. L. Cruz-Campa, G. N. Nielson, V. P. Gupta, D. Zubia, J. McClure, and X. W. Zhou, Phys. Rev. B, 85, 245316 (2012).

4th Example of MD Fidelity: α-Dislocation Moves Faster than β-Dislocation

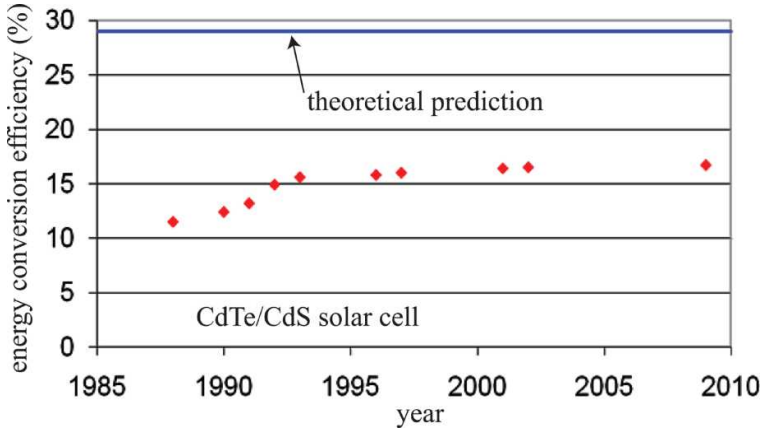


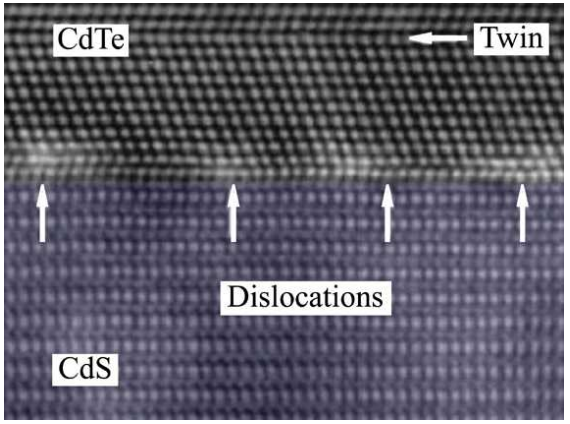


X. Zhou, D. K. Ward, B. M. Wong, F. P. Doty, and J. A. Zimmerman,
J. Phys. Chem., 116, 17563 (2012)

A Case Study: CdTe/CdS Solar Cells

1. CdTe/CdS solar cell electricity → \$0.15/kWh, lower than any other photovoltaic technology[1];
2. Current 19.6% record efficiency[1] significantly lower than the theoretical 29%[2,3];
3. Defects (misfit dislocations) have not been reduced from experiments in the past 15+ years;
4. Possible improvement: reduce defects.

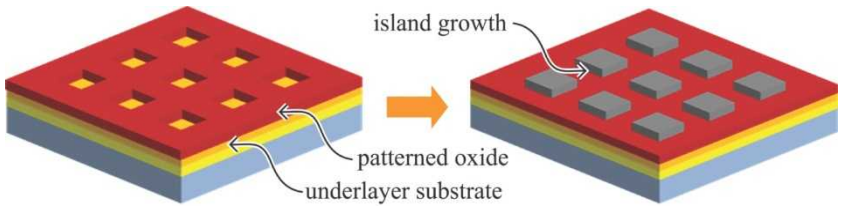




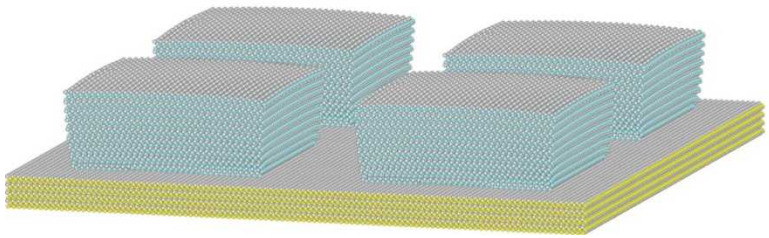
1. M. A. Green, K. Emery, Y. Hishikawa, W. Warta, and E. D. Dunlop, Prog. Photovol.: Res. Appl., 22, 1 (2014).
2. K. D. Dobson, I. Visoly-Fisher, G. Hodes, and D. Cahen, Solar Energy Mater. Solar Cells, 62, 295 (2000).
3. A. Shah, P. Torres, R. Tscharner, N. Wyrsch, and H. Keppner, Science, 285, 692 (1999).
4. K. Zweibel, Science, 328, 699 (2010).

Graded Island Growth

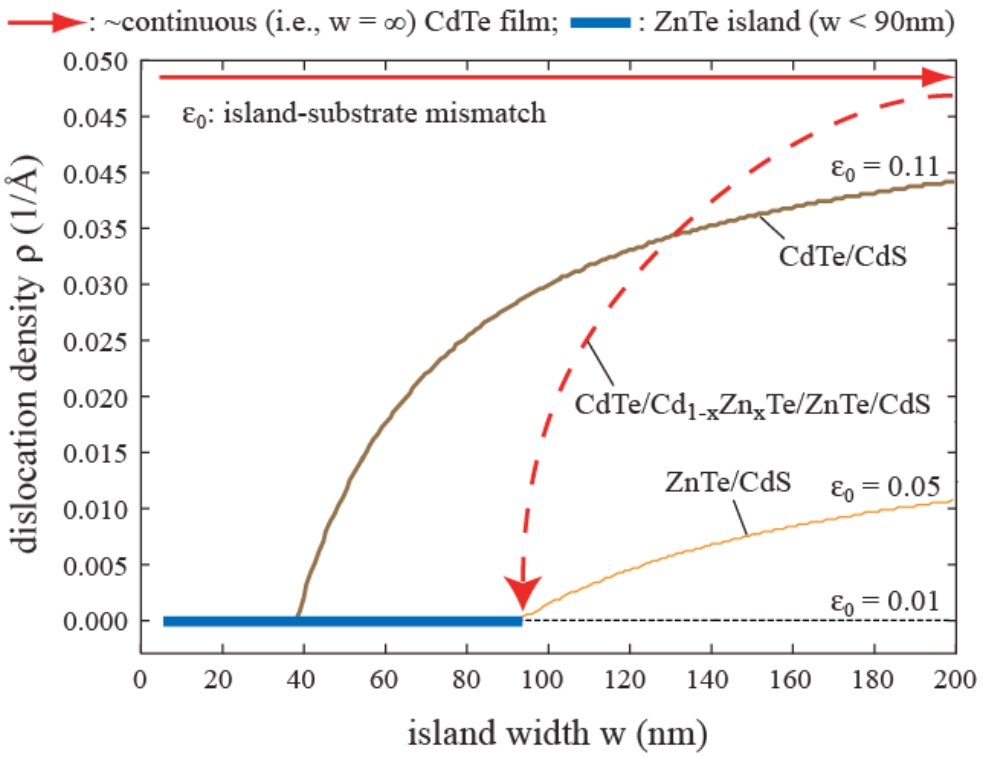
Modern nano technology:



Molecular dynamics simulation:



MD informed calculations:



Molecular dynamics energy calculations predict that using island growth and composition grading, dislocation free $CdTe/Cd_{1-x}Zn_xTe/Zn/Te/CdS$ solar cells can be synthesized at ~90 nm island dimension!

MD Virtual Processing (Patterned Growth + Composition Grading)

Fig. 1- Selective area bilayer deposition

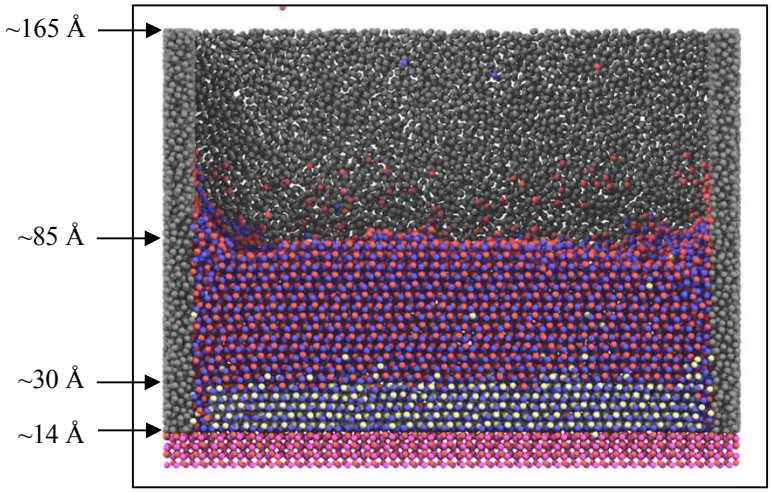


Fig. 2- Composition Profile Reveals $Cd_{1-x}Zn_xTe$ alloying

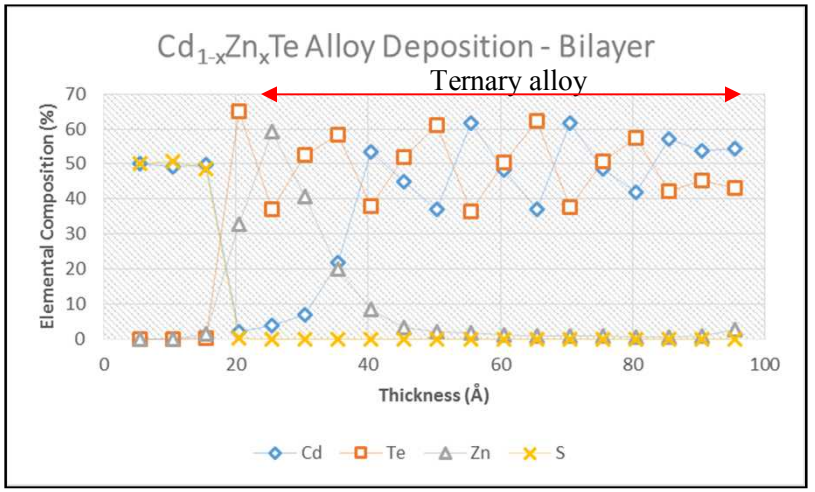


Fig. 3- Selected area linear grading deposition

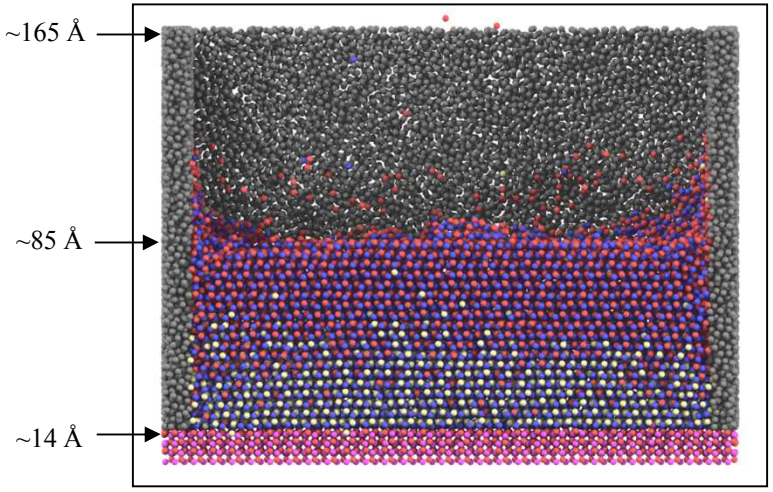
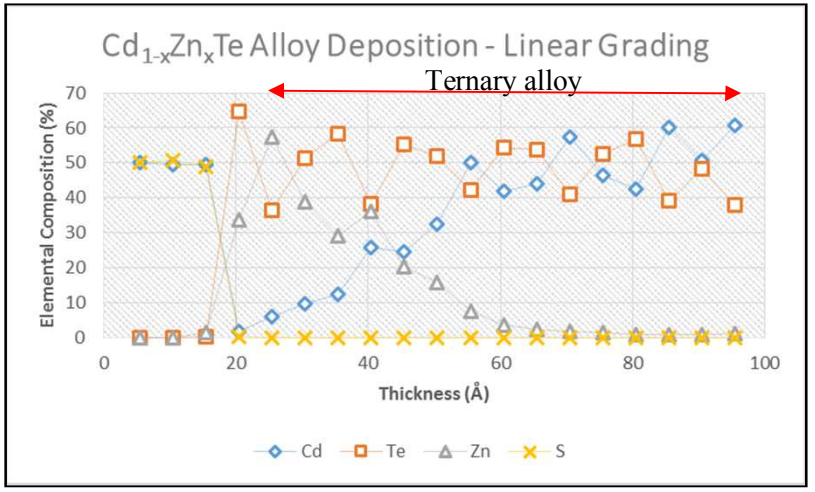


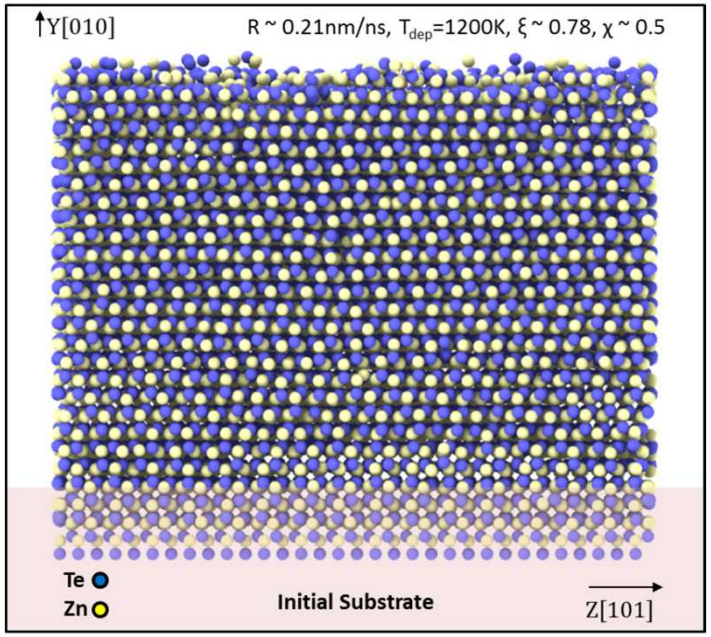
Fig. 4- Composition Profile Reveals $Cd_{1-x}Zn_xTe$ alloying

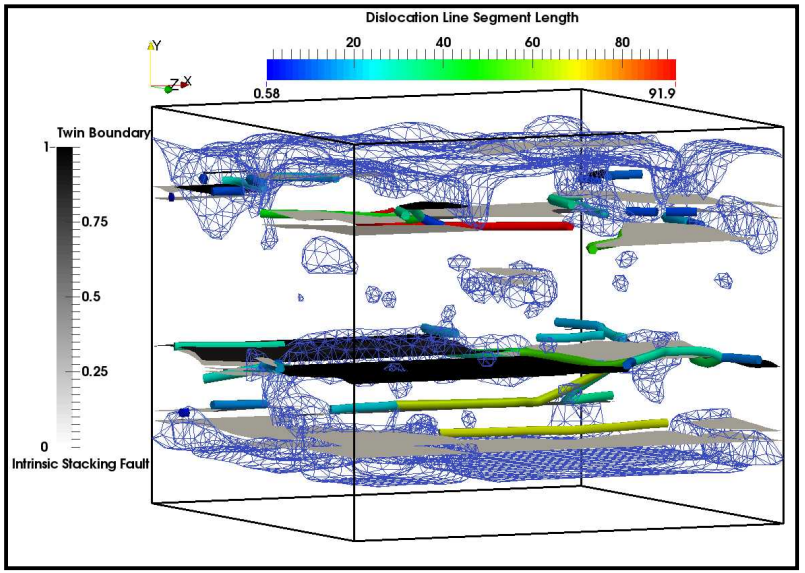


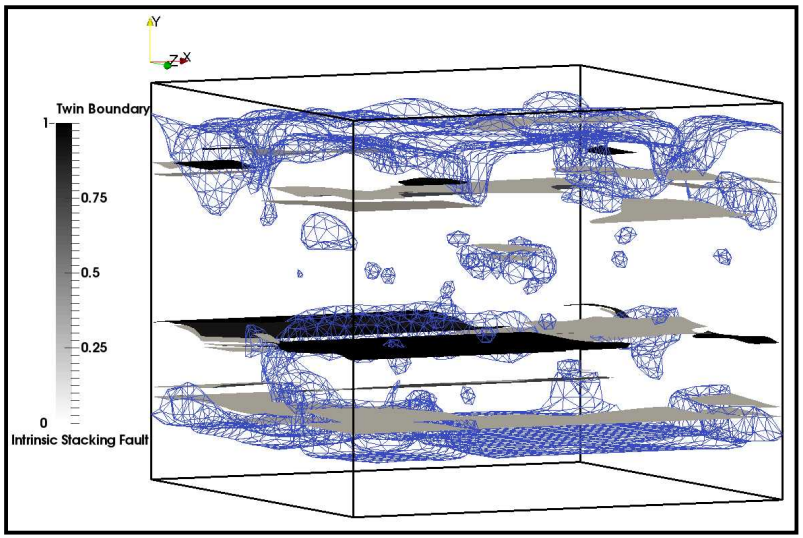
Planar ZnTe (111)

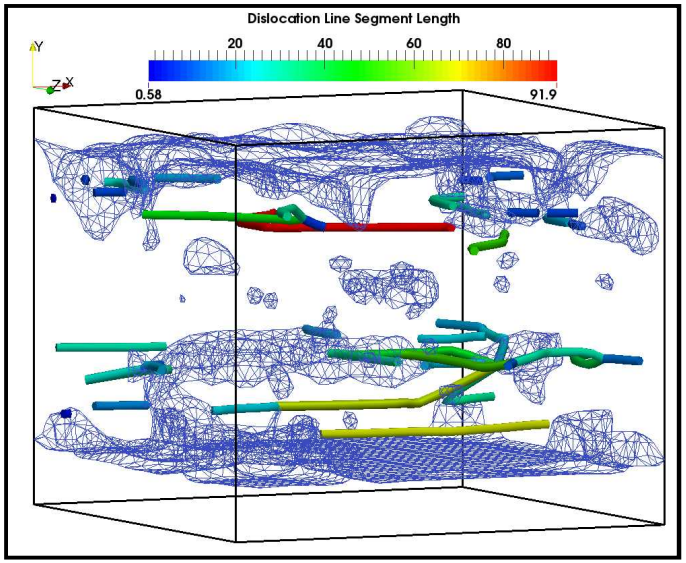
film dimension of measurement: ~130 by 90 by 130 Å^3

dislocations # = 33
avg. length = 23.5 Å
max. Length = 92.0 Å





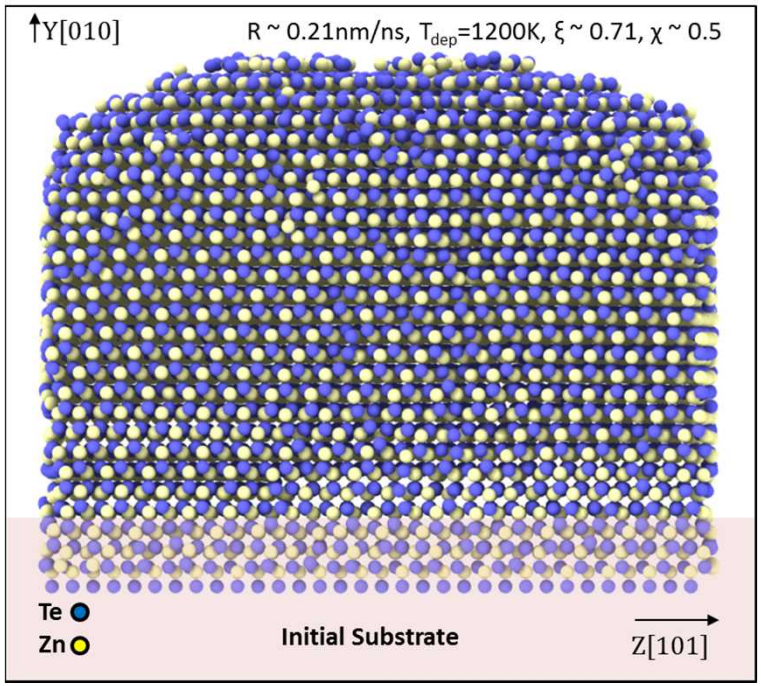


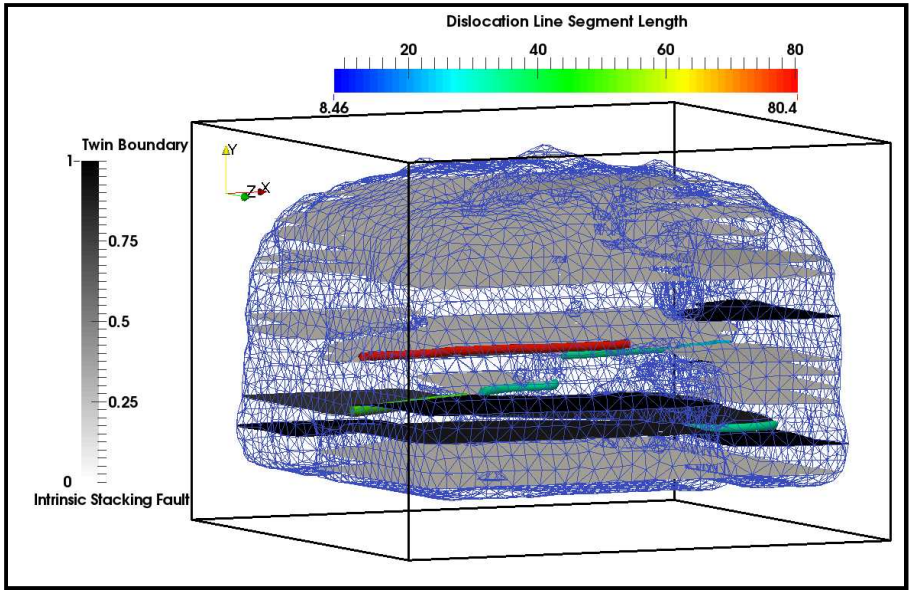


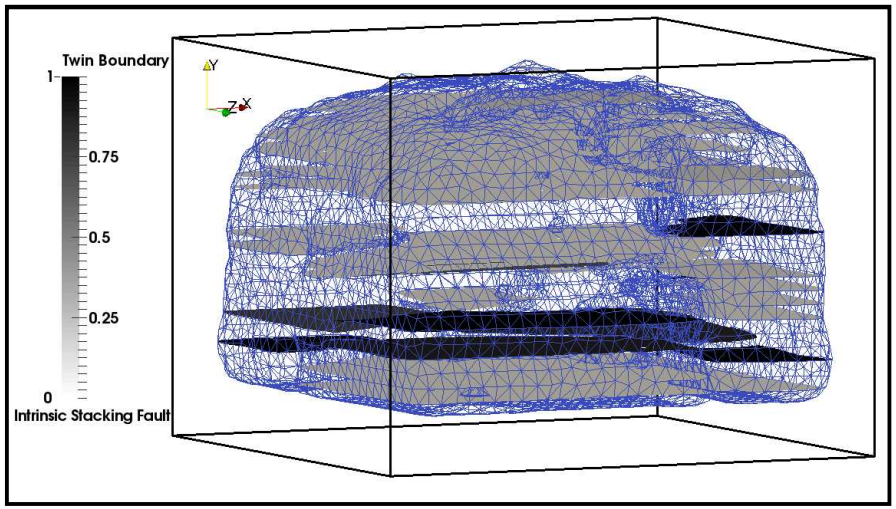
Patterned ZnTe (111)

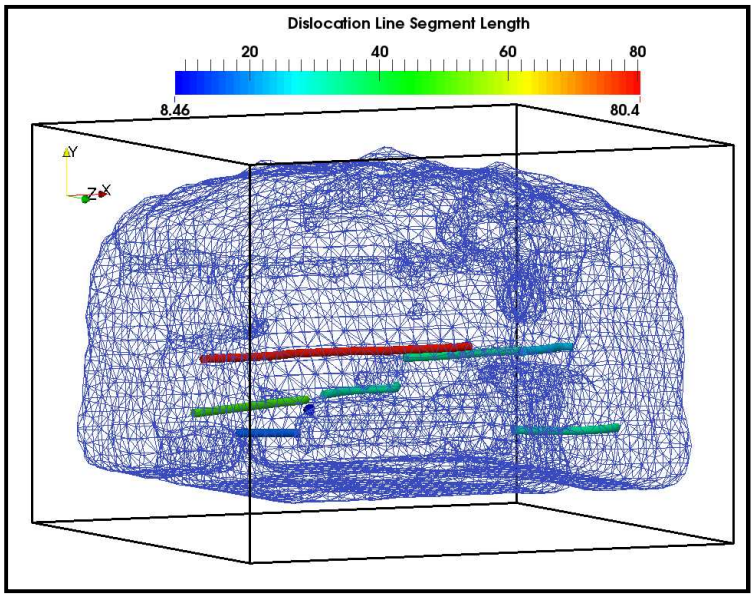
film dimension of measurement: ~130 by 90 by 130 Å^3

dislocations # = 7
avg. length = 34.4 Å
max. Length = 78.5 Å





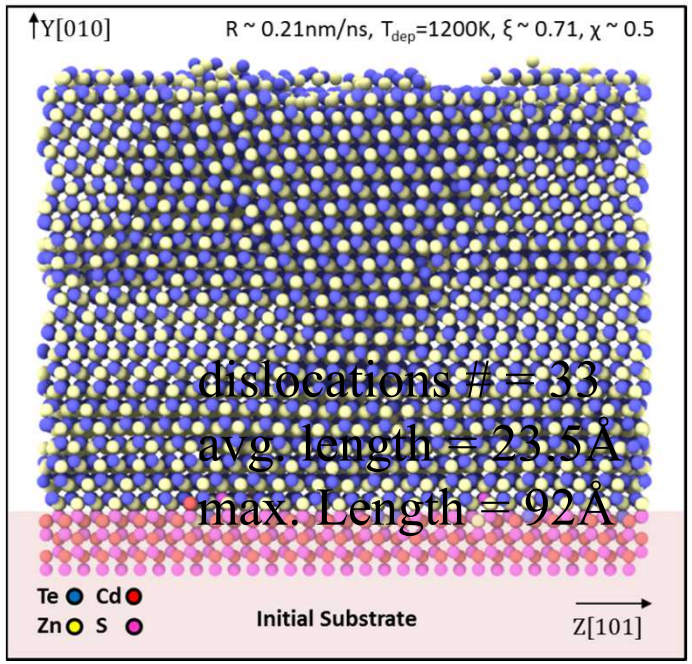


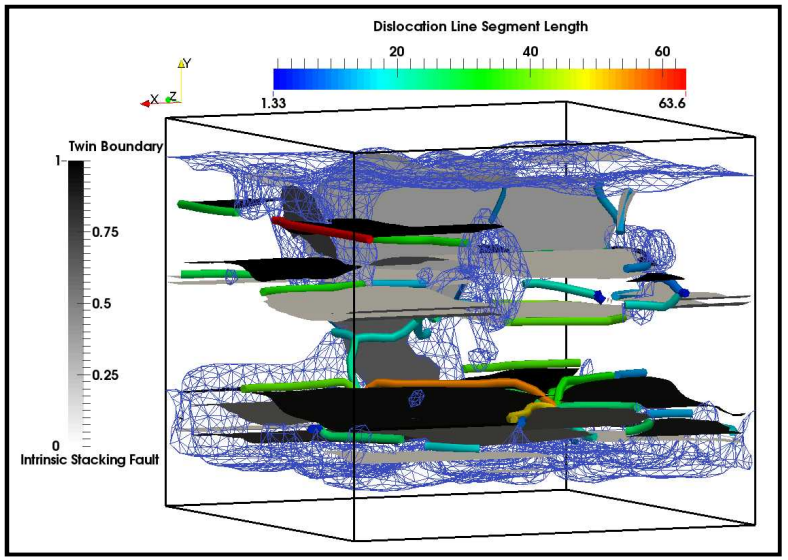


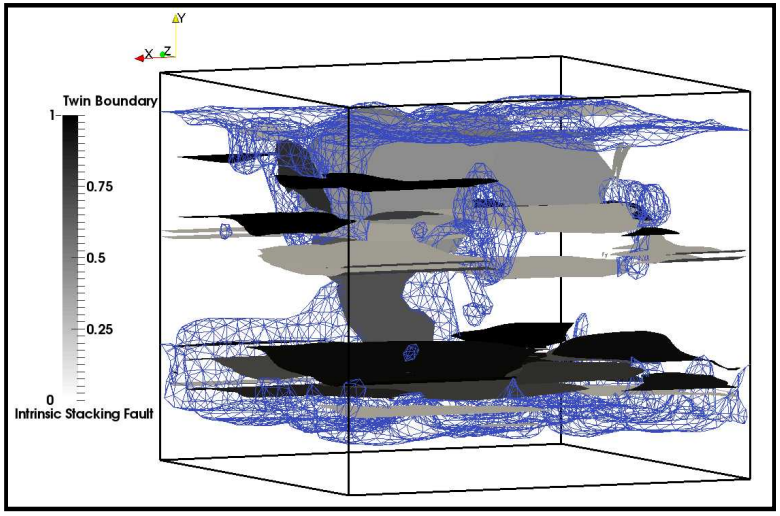
Planar ZnTe-on-CdS (111)

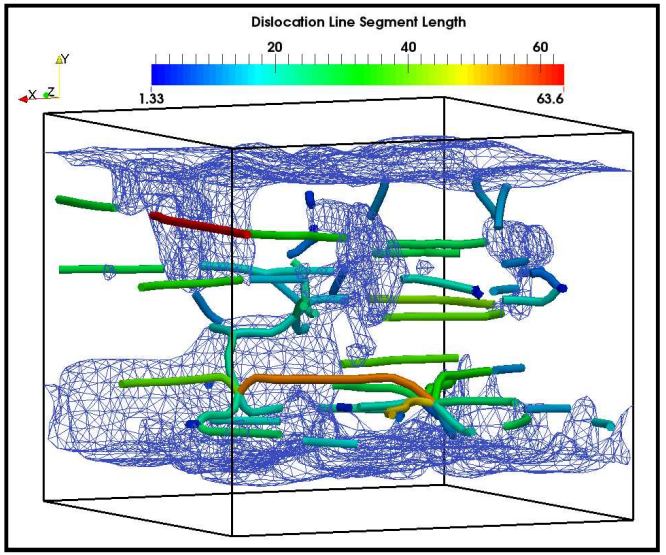
dislocations # = 56
avg. length = 19.7 Å
max. Length = 63.6 Å

film dimension of measurement: ~130 by 90 by 130 Å^3





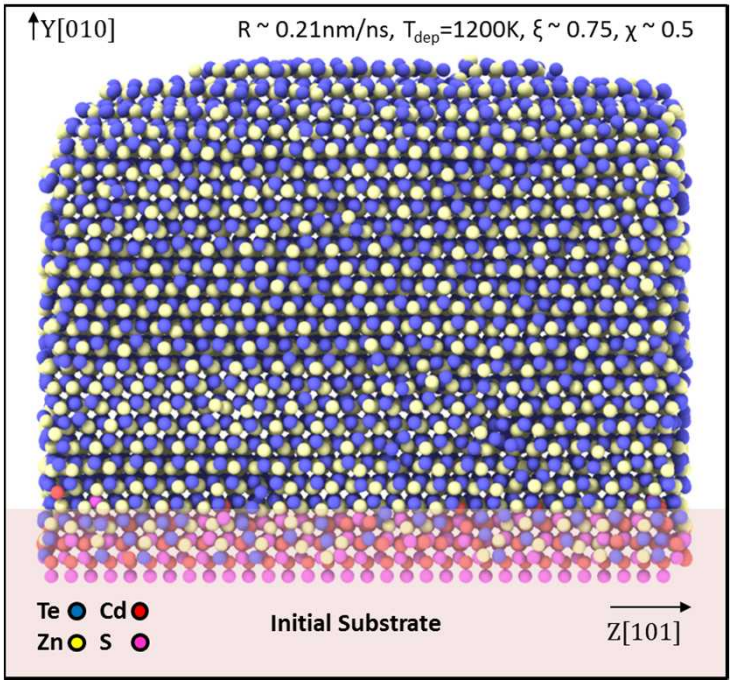


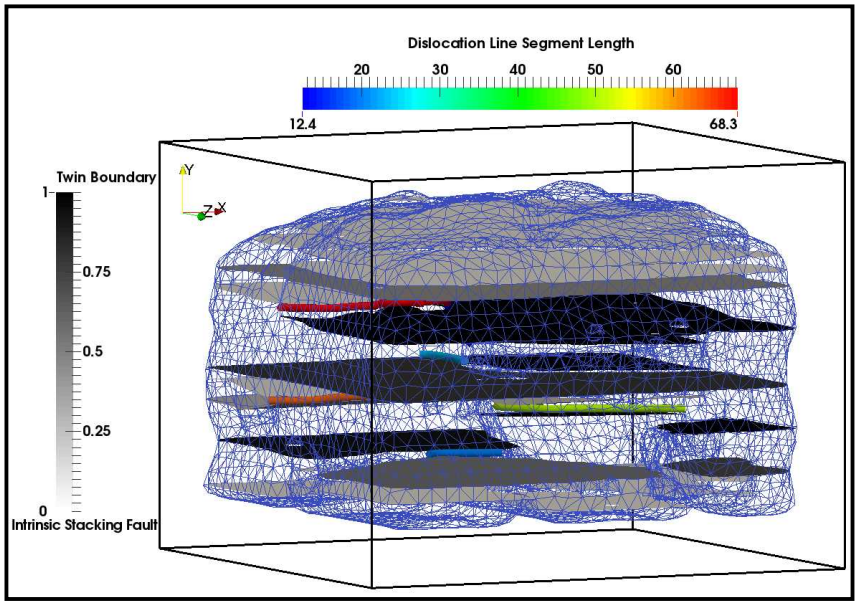


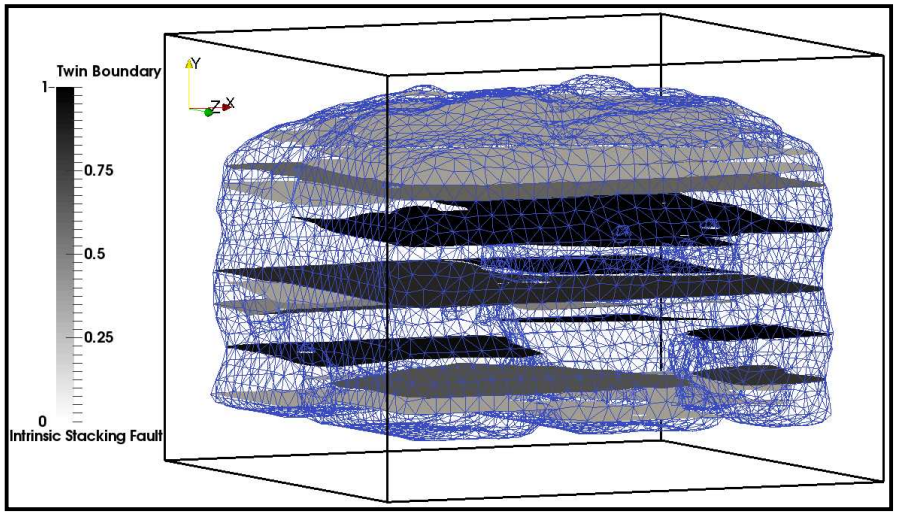
Patterned ZnTe-on-CdS (111)

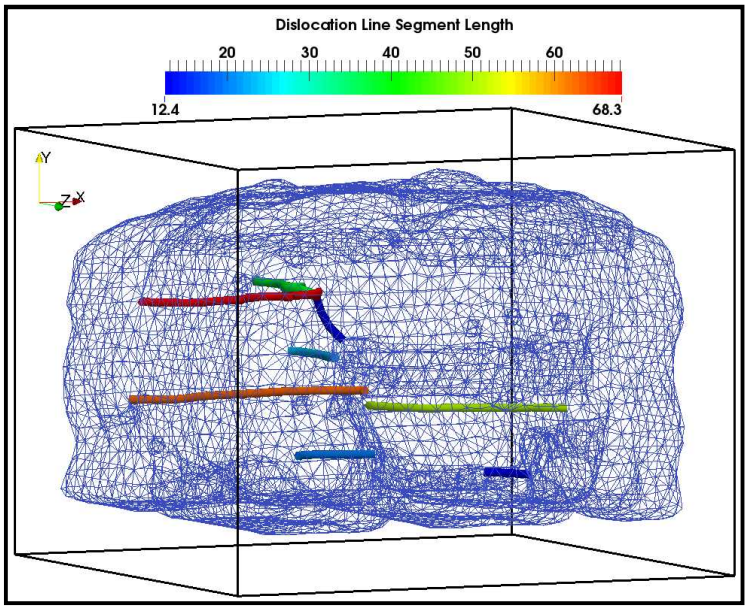
film dimension of measurement: ~130 by 90 by 130 Å^3

dislocations # = 10
avg. length = 35.8 Å
max. Length = 68.2 Å

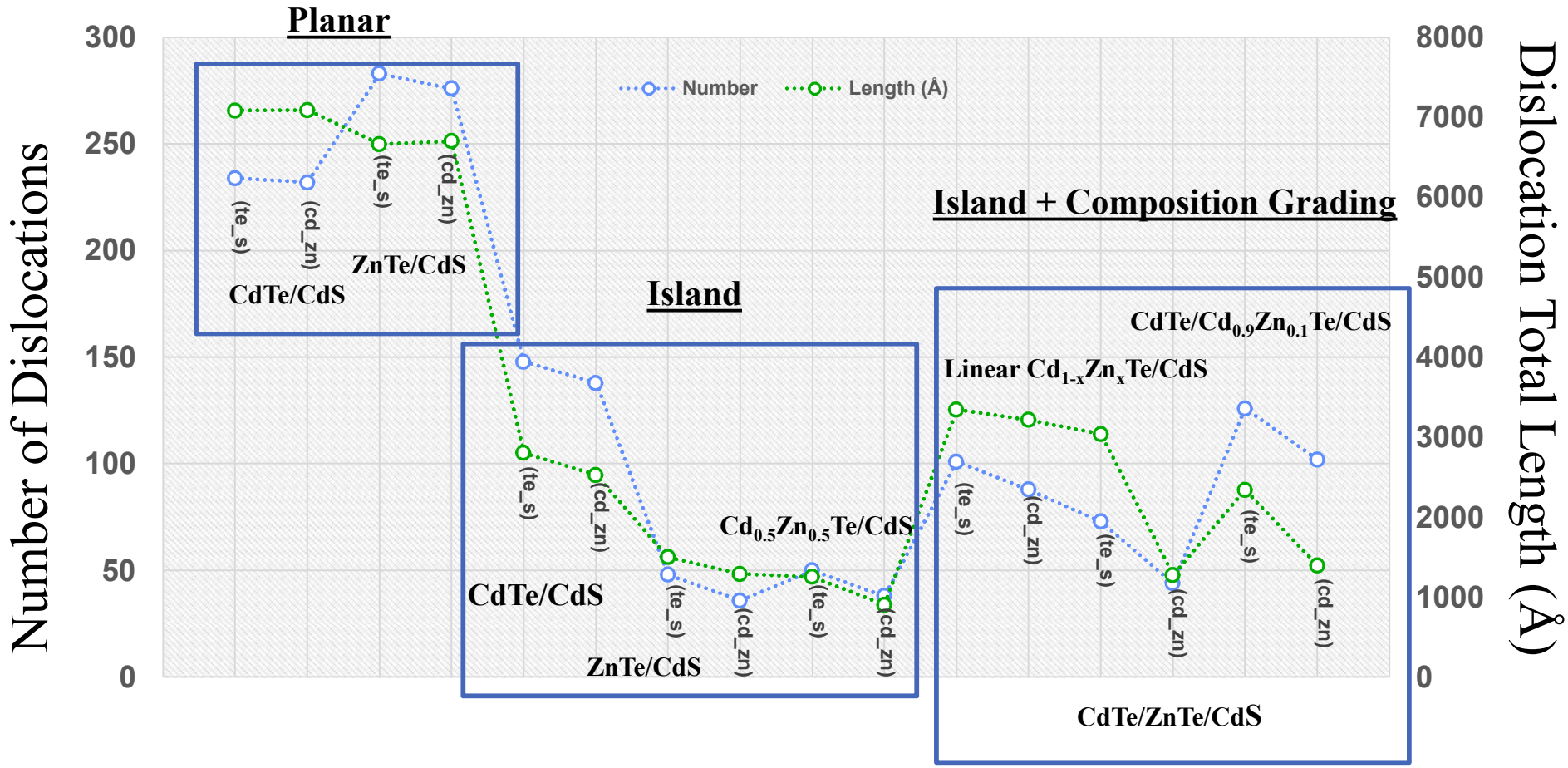








Dislocation Reduction in Nanostructures from MD Prediction



TEM Observations: Defect Reduces When CdTe Island Sizes Decrease

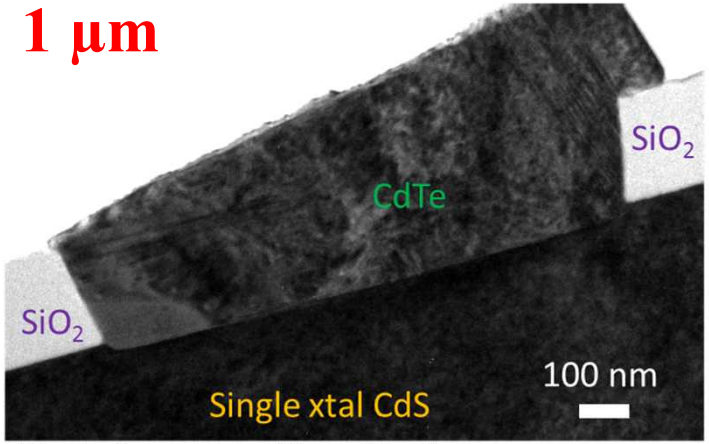


Fig. 1a Low mag. of 1 um island

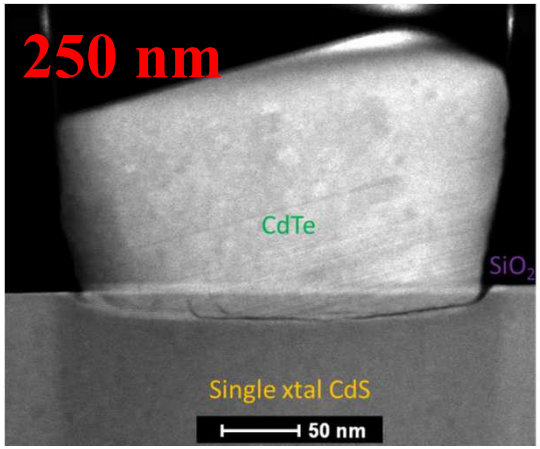


Fig. 2a Low mag. of 250 nm island

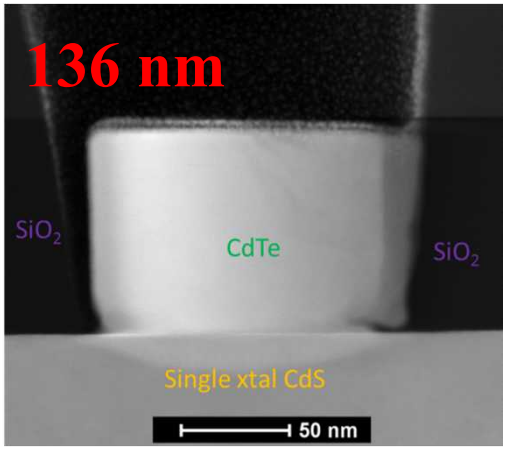


Fig. 3a Low mag. of 136 nm island

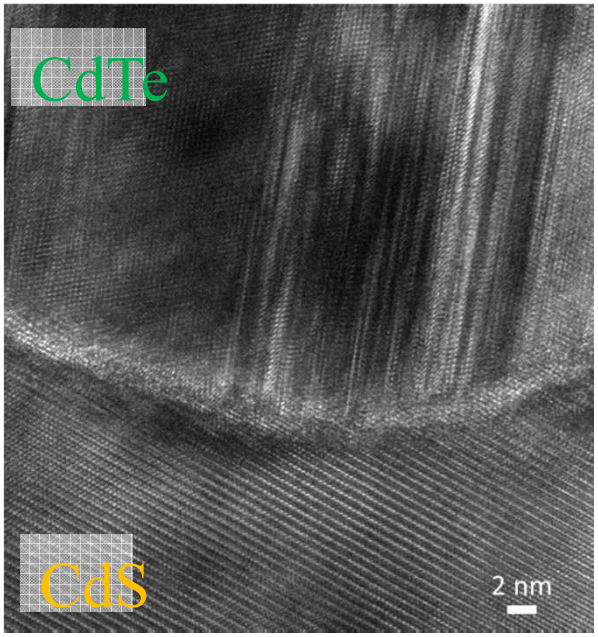


Fig. 1b High mag. of 1 um island

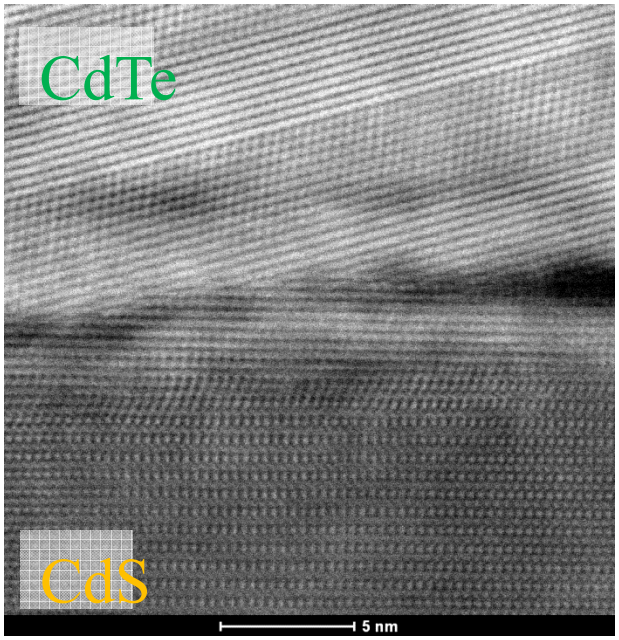


Fig. 2b High mag. of 250 nm island

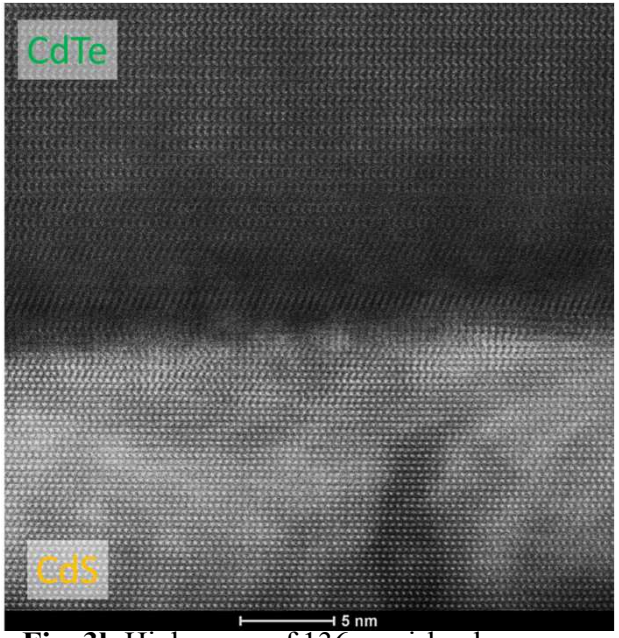


Fig. 3b High mag. of 136 nm island

Topic 2:
Quantum Mechanical Calculations

Density Functional Theory (DFT)

Schrödinger equation for electrons i = 1, …, N:

$$\hat{H}\Psi = \left[\hat{T} + \hat{V} + \hat{U}\right]\Psi = \left[\sum_{i=1}^{N}\left(-\frac{\hbar^2}{2m_i}\nabla_i^2\right) + \sum_{i=1}^{N} V(\vec{r}_i) + \sum_{i=1}^{N}\sum_{j>i}^{N} U(\vec{r}_i, \vec{r}_j)\right]\Psi = E\Psi$$

$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$, $\hbar = \frac{h}{2\pi}$, h: Planck constant, $\hat{T}$: kinetic energy, $\hat{V}$ potential energy from the external field due to positively charged nucli, $\hat{U}$: electron-electron interaction energy

Directly solving Schrödinger equation not possible for many bodies.

DFT: electron density $\rho(\vec{r})$ uniquely determines all properties of the system.

This leads to Kohn-Sham equation:

$$\left[\frac{\hbar^2}{2m_i}\nabla^2 + V_s(\vec{r})\right]\phi_i(\vec{r}) = \varepsilon_i\phi_i(\vec{r})$$

The effective single particle potential $V_s(\vec{r}) = V(\vec{r}) + \int \frac{e^2\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r' + V_{XC}[\rho(\vec{r})]$, $\rho(\vec{r}) = \sum_{i=1}^{N}|\phi_i(\vec{r})|^2$,

$\int \frac{e^2\rho(\vec{r}')}{|\vec{r}-\vec{r}'|}d^3r'$: electron-electron Coulomb repulsion, $V_{XC}[\rho(\vec{r})]$: exchange-correlation potential.

Beginner's Calculations

Many quantum mechanical codes are available. Here we use a free package Quantum Espresso as an example:

1. Download the codes at http://www.quantum-espresso.org;
2. Compile/install the codes following the instructions;
3. Download appropriate pseudopotentials of your elements at http://www.quantum-espresso.org;
4. Create an input file, where atom types/positions, system geometry, pseudopotential files, energy cutoff, k-point mesh, etc., can all be specified;
5. Run the calculation with the input file, wait till the calculation completes, and analyze the results in the result files.
6. Detailed information on how to create the input file can be found at http://www.quantum-espresso.org;
7. An example input file is included in the supplemental materials of this lecture.

Topic 3:
Interatomic Potentials

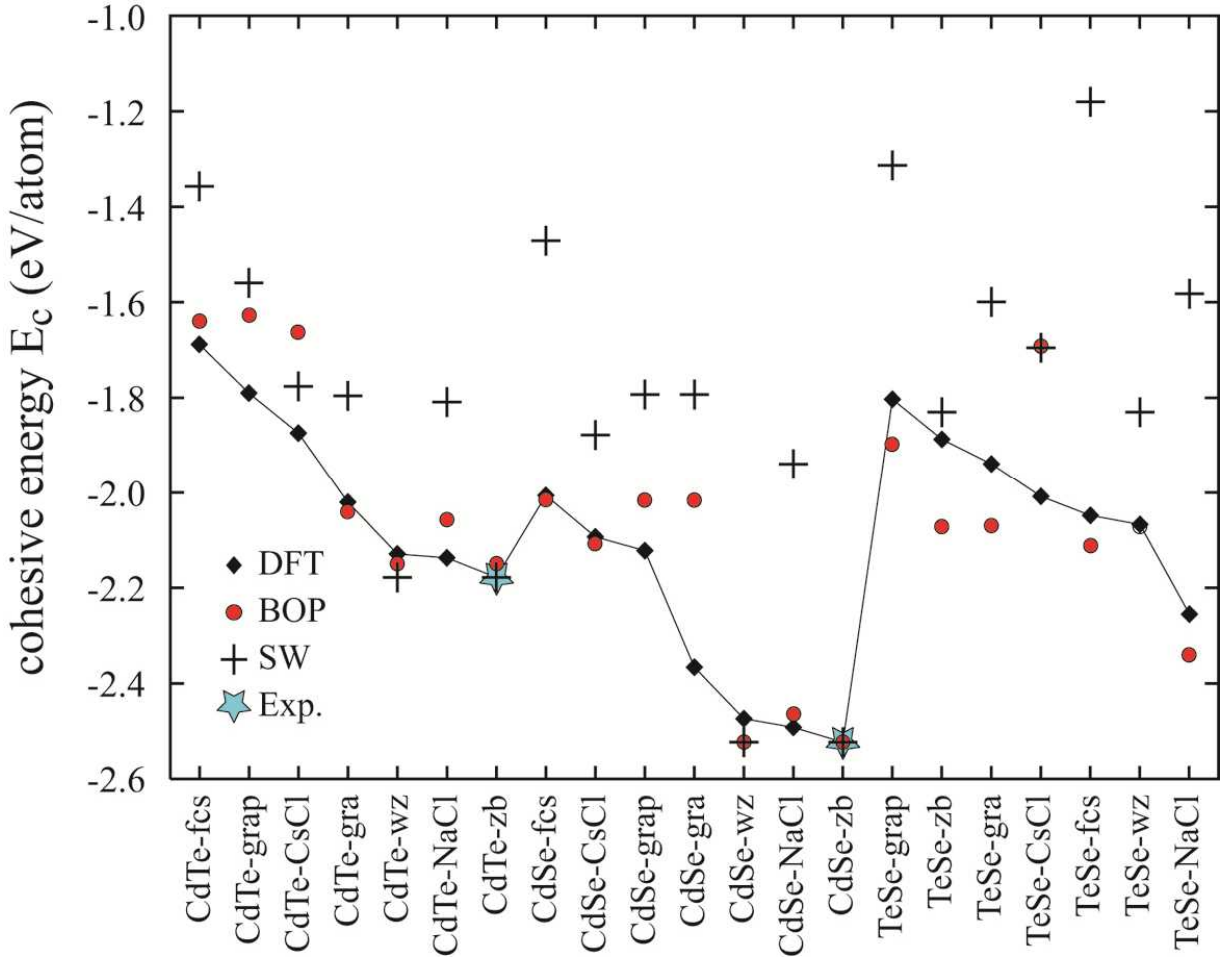
Recommended Semiconductor Potentials

1. Stillinger-Weber potentials[1]
2. Tersoff potentials[2]
3. Analytical bond order potentials[3-9]

1. F.H. Stillinger and T.A. Weber, Phys. Rev. B 31, 5262 (1985).
2. J. Tersoff, Phys. Rev. B 39, 5566 (1989).
3. D. G. Pettifor, M. W. Finnis, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, and H. N. G. Wadley, Mater. Sci. Eng. A, 365, 2 (2004).
4. R. Drautz, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, TMS Lett., 1, 31 (2004).
5. R. Drautz, D. A. Murdick, D. Nguyen-Manh, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, Phys. Rev. B, 72, 144105 (2005).
6. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, and D. G. Pettifor, Phys. Rev. B, 73, 45206 (2006).
7. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 59, 8487 (1999).
8. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).
9. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 65, 172103 (2002).

Strength / Weakness of Various Potentials

Stillinger-Weber potentials only work well for the equilibrium structures.
More advanced potentials are much more difficult to develop!

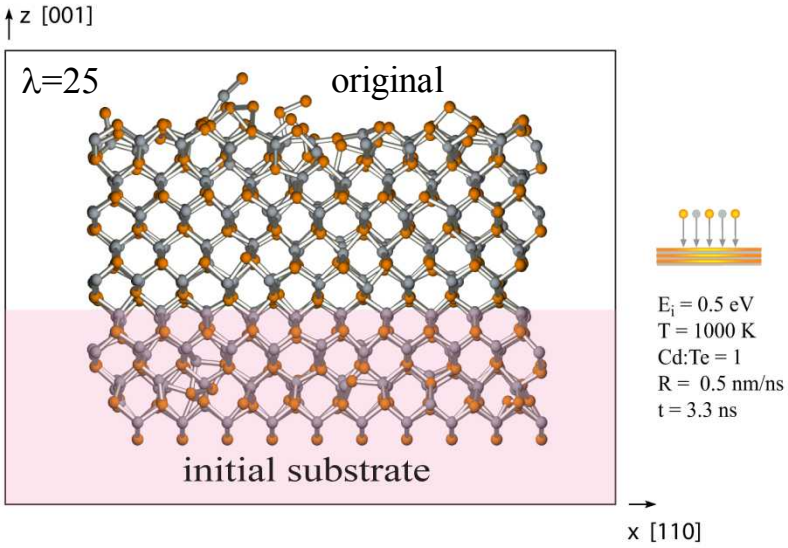


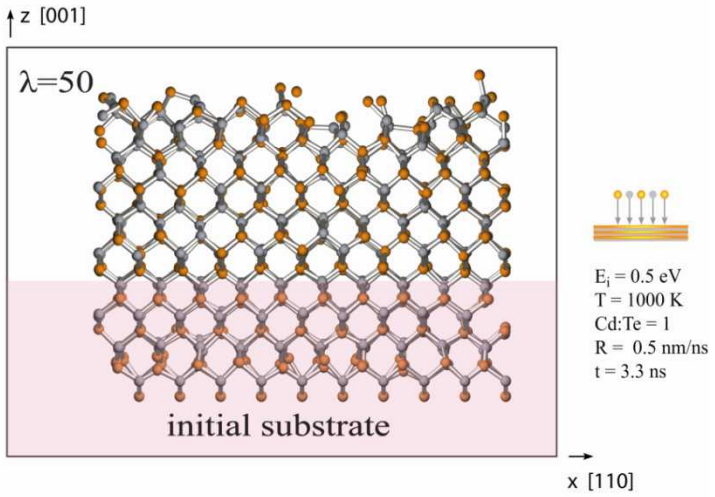
X. W. Zhou, M. E. Foster, F. B. van Swol, J. E. Martin, and B. M. Wong, J. Phys. Chem. C, in press (2014).

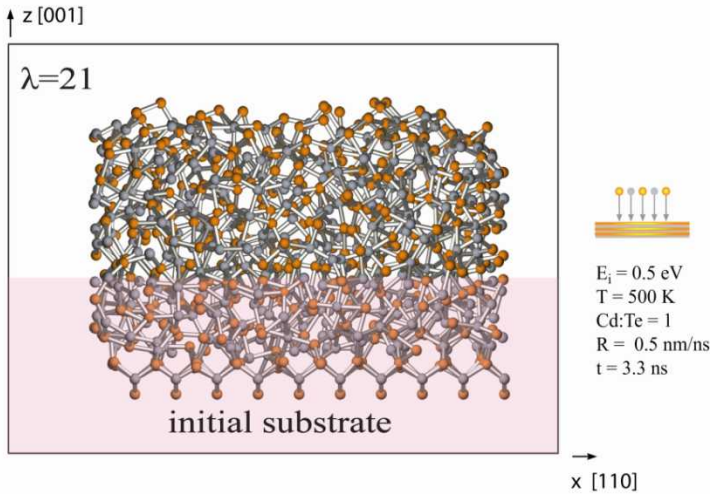
SW Potentials Are Easy to Develop

SW potentials use an energy penalty approach to capture the equilibrium phase

$$E \sim \lambda \cdot \left(\cos\theta + \frac{1}{3} \right)^2$$



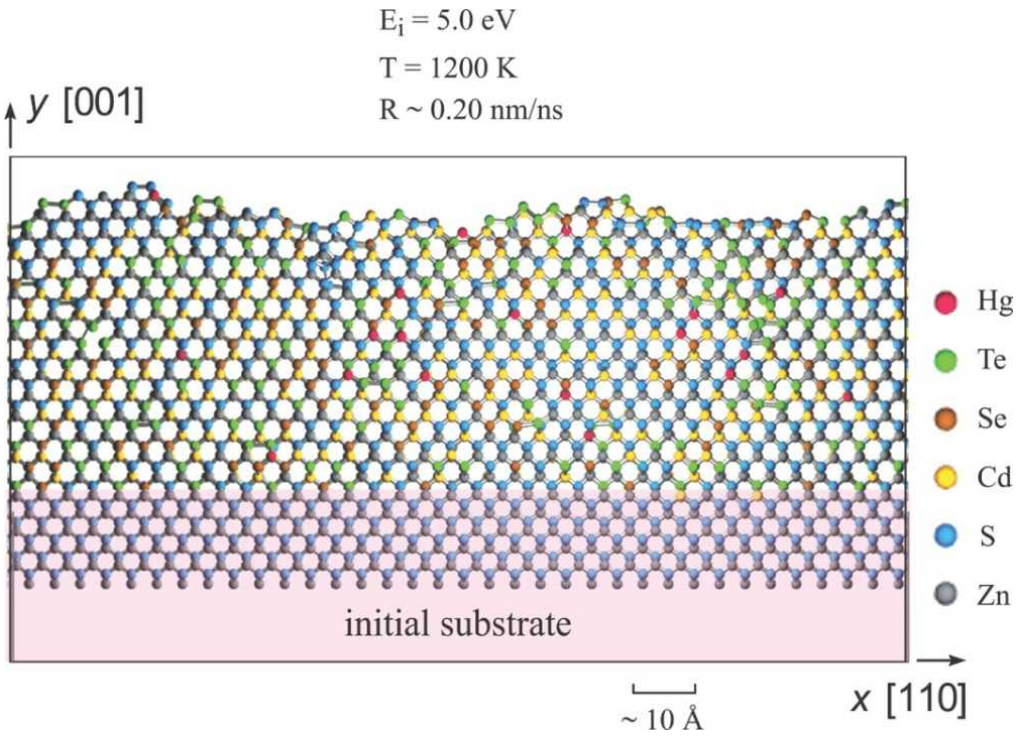




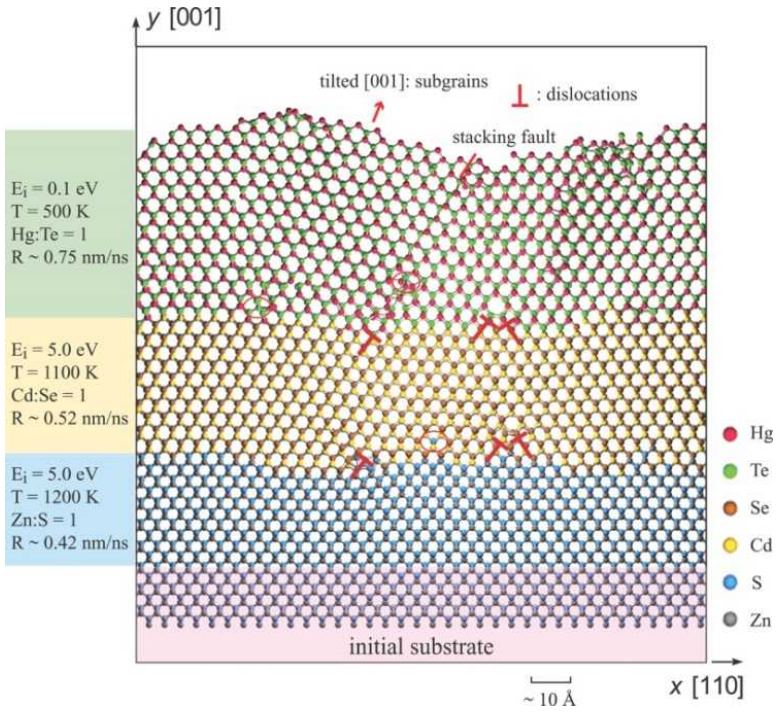
CdTe potential from Z. Q. Wang et al, Phys. Rev. B, 40, 3129 (1989).

Cd-Zn-Te-Se-Te-S SW Potential

$(Cd_{0.28}Zn_{0.68}Hg_{0.04})(Se_{0.20}Te_{0.68}S_{0.12}/ZnS)$ Growth



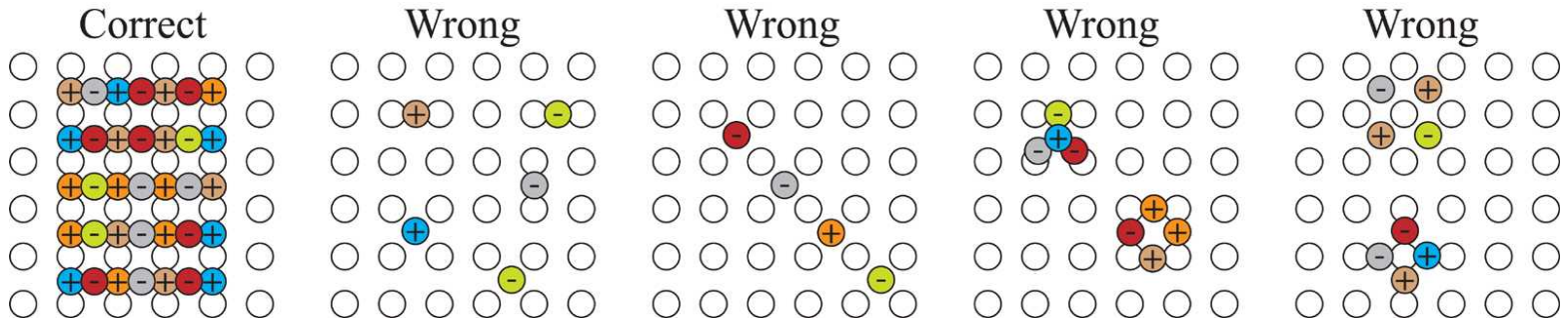
HgTe/CdSe/ZnS Growth



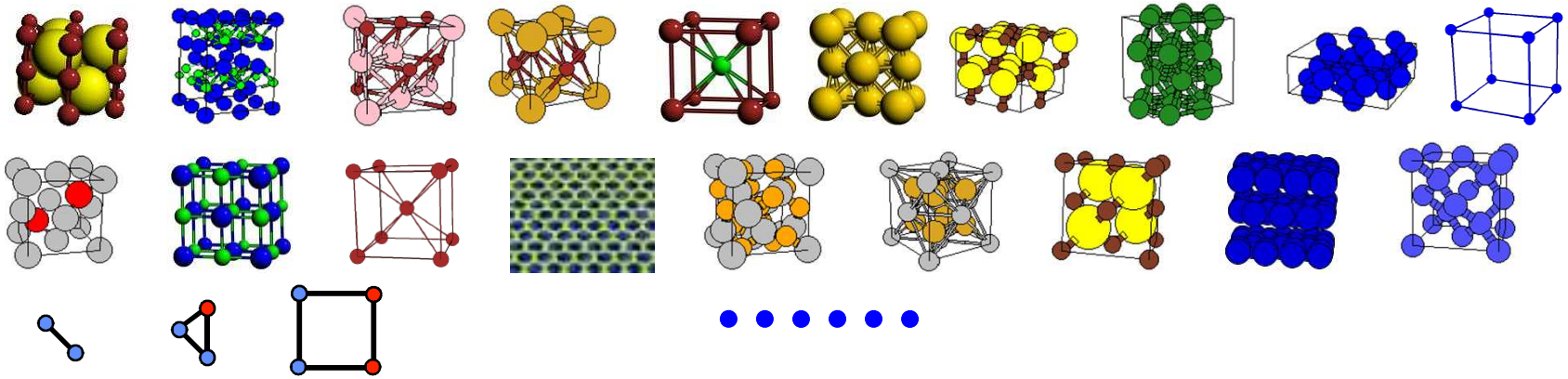
X. W. Zhou, D. K. Ward, J. E. Martin, F. B. van Swol, J. L. Cruz-Campa, and D. Zubia, Phys. Rev. B, 88, 085309 (2013).

Computational synthesis Extremely Challenging

- **Wrong configurations should and will nucleate due to random condensation of adatoms, but they must all evolve to the correct crystal structure;**

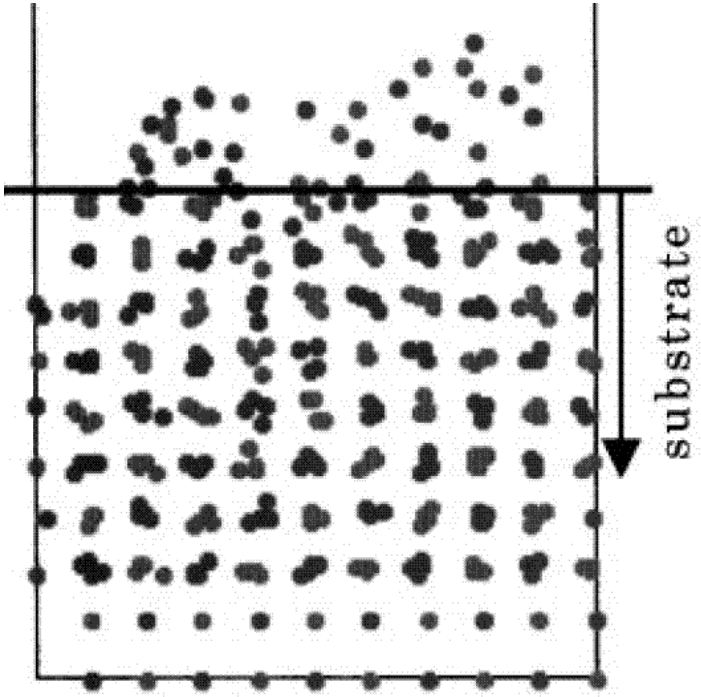


- **Only when property trends of a large number of clusters, lattices, and defects (enormous computation intensity) are captured will a growth simulation be successful.**

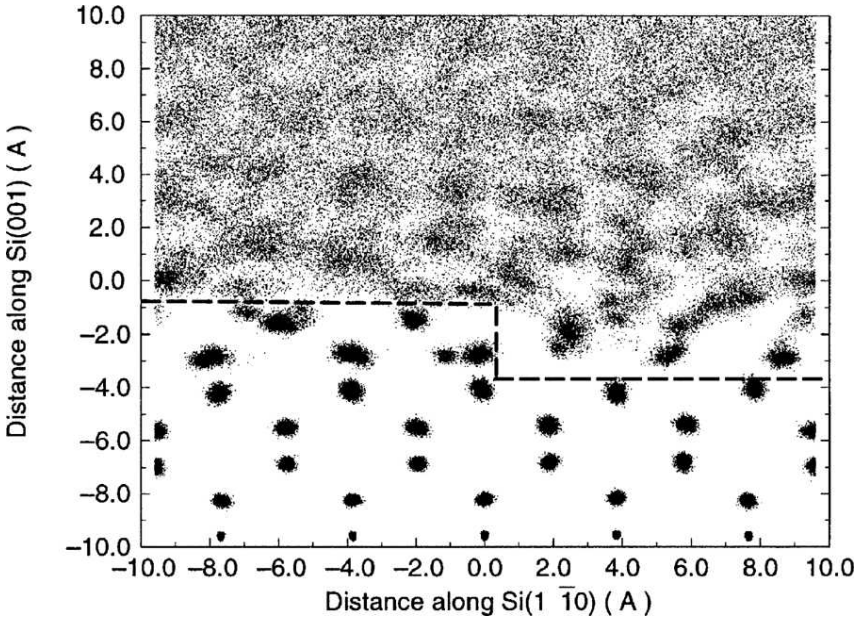


Literature Examples of Tersoff Potentials

InAs on (110) GaAs[1].



CdTe on (100) Si[5].



None of the potentials listed below predicts the crystalline growth.

1. M. Nakamura, H. Fujioka, K. Ono, M. Takeuchi, T. Mitsui, and M. Oshima, J. Cryst. Growth, 209, 232(2000).
2. J. Tersoff, Phys. Rev. B, 39, 5566(1989). – for Si (amorphous growth, but can re-crystallize at 2200 K through bulk transformation).
3. P. A. Ashu, J. H. Jefferson, A. G. Cullis, W. E. Hagston, and C. R. Whitehouse, J. Cryst. Growth, 150, 176(1995). – for GaAs.
4. R. Smith, Nucl. Instru. Meth. B, 67, 335(1992). – for GaAs.
5. J. Oh, C.H. Grein, J. Crys. Growth, 193, 241 (1998).

Examples of Growth Enabling Non-SW Potentials

1. K. Albe, K. Nordlund, J. Nord, and A. Kuronen, “Modeling of compound semiconductors: Analytical bond-order potential for Ga, As, and GaAs”, Phys. Rev. B, 66, 035205 (2002).
2. J. Nord, K. Albe, P. Erhart, and K. Nordlund, “Modelling of compound semiconductors: analytical bond-order potential for gallium, nitrogen and gallium nitride”, J. Phys.: Condensed Matter, 15, 5649 (2003).
3. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, D. G. Pettifor, “Analytic bond-order potential for the gallium arsenide system”, Phys. Rev. B, 73, 045206 (2006).
4. D. K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, “Analytical bond-order potential for the Cd-Zn-Te ternary system”, Phys. Rev. B, 86, 245203 (2012).
5. D. K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, “Analytical bond-order potential for the cadmium telluride binary system”, Phys. Rev. B, 85, 115206 (2012).
6. D. K. Ward, X. W. Zhou, B. M. Wong, and F. P. Doty, “A refined parameterization of the analytical Cd-Zn-Te bond-order potential”, J. Mol. Model., 19, 5469 (2013).

Topic 4:
Molecular Dynamics / LAMMPS

Fundamental Principles of MD: Newton Equations

$$\vec{f}_i = \frac{\partial E(\vec{r}_1, \vec{r}_N, ..., \vec{r}_N)}{\partial \vec{r}_i} = m_i \vec{a}_i = m_i \frac{\partial^2 \vec{r}_i}{\partial t^2}$$

$$\vec{r}_i(t+\delta t) = \vec{r}_i(t) + \vec{v}_i(t)\cdot\delta t + \frac{1}{2}\vec{a}_i(t)\cdot\delta t^2 + \frac{1}{6}\vec{b}_i(t)\cdot\delta t^3 + \frac{1}{24}\vec{c}_i(t)\cdot\delta t^4 + ...$$

$$\vec{v}_i(t+\delta t) = \vec{v}_i(t) + \vec{a}_i(t)\cdot\delta t + \frac{1}{2}\vec{b}_i(t)\cdot\delta t^2 + \frac{1}{6}\vec{c}_i(t)\cdot\delta t^3 + ...$$

$$\vec{a}_i(t+\delta t) = \vec{a}_i(t) + \vec{b}_i(t)\cdot\delta t + \frac{1}{2}\vec{c}_i(t)\cdot\delta t^2 + ...$$

$$\vec{b}_i(t+\delta t) = \vec{b}_i(t) + \vec{c}_i(t)\cdot\delta t + ...$$

where $\vec{r}_i$, $\vec{v}_i$, and $\vec{a}_i$ are position, velocity, and acceleration of atom i, and $\vec{b}_i$ and $\vec{c}_i$ are higher derivatives with respect to time. Solving position of atoms (strucure) and velocity (temperature) as a function of time. Stresses can also be calculated.

Force can be modified to allow isothermal control, and Newton's equation can be reformulated to Lagrangian equations to allow system size (L_x, L_y, L_z) to change under external stresses.

LAMMPS (A Widely Used MD package)

Large-scale Atomic/Molecular Massively Parallel Simulator

LAMMPS and manual can be downloaded at http://lammps.sandia.gov. You can compile the codes following the instructions.

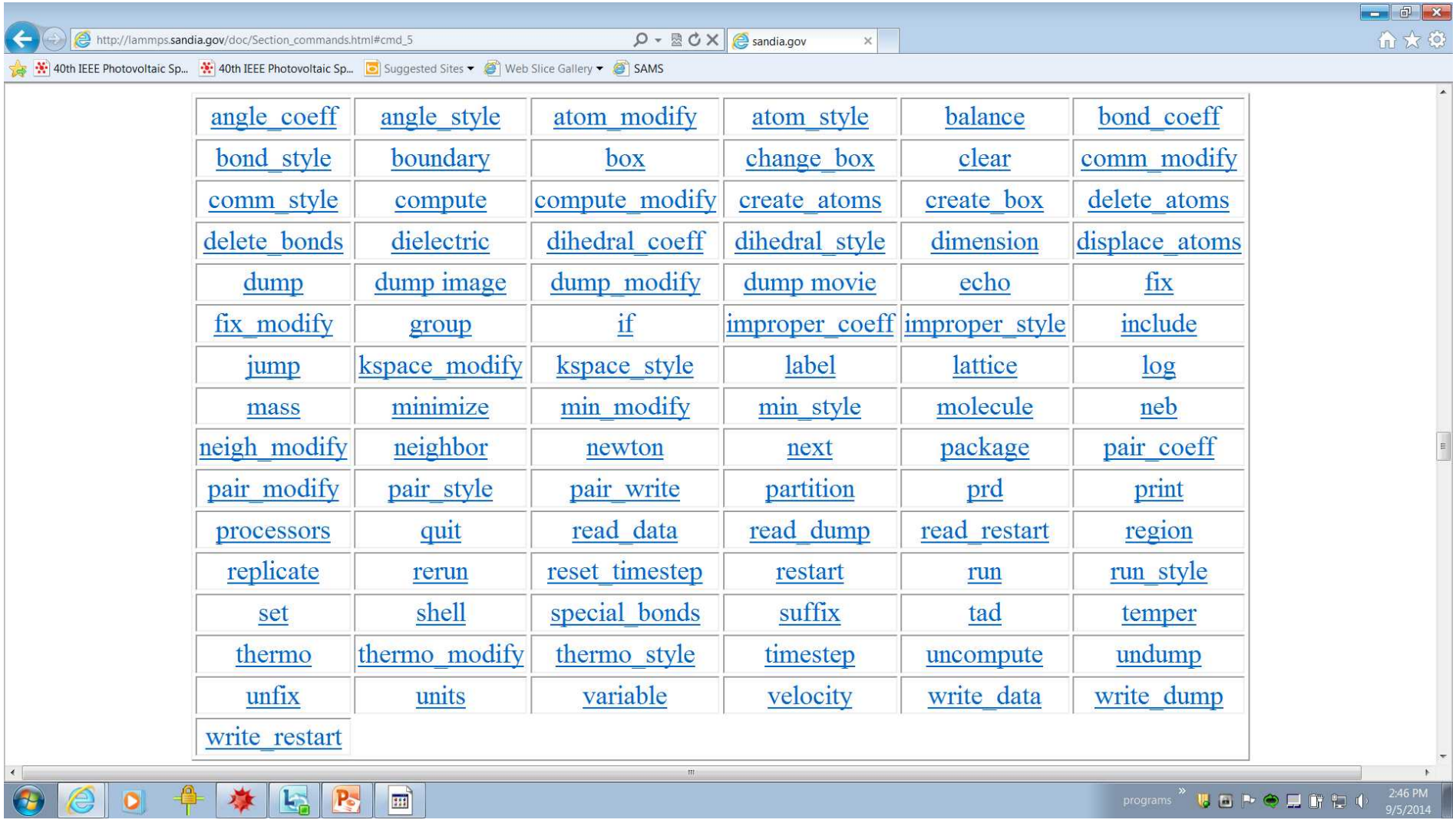
In most cases, you will need three files to run LAMMPS: a LAMMPS input file (say file name a.i), an interatomic potential file (say file name CdTeZnSeHgS0.sw), and an initial configuration file (say file name r0).

If the executable of the compiled LAMMPS is called lmp, then you can execute the run by executing the command "lmp < a.i" at the prompt of your command window.

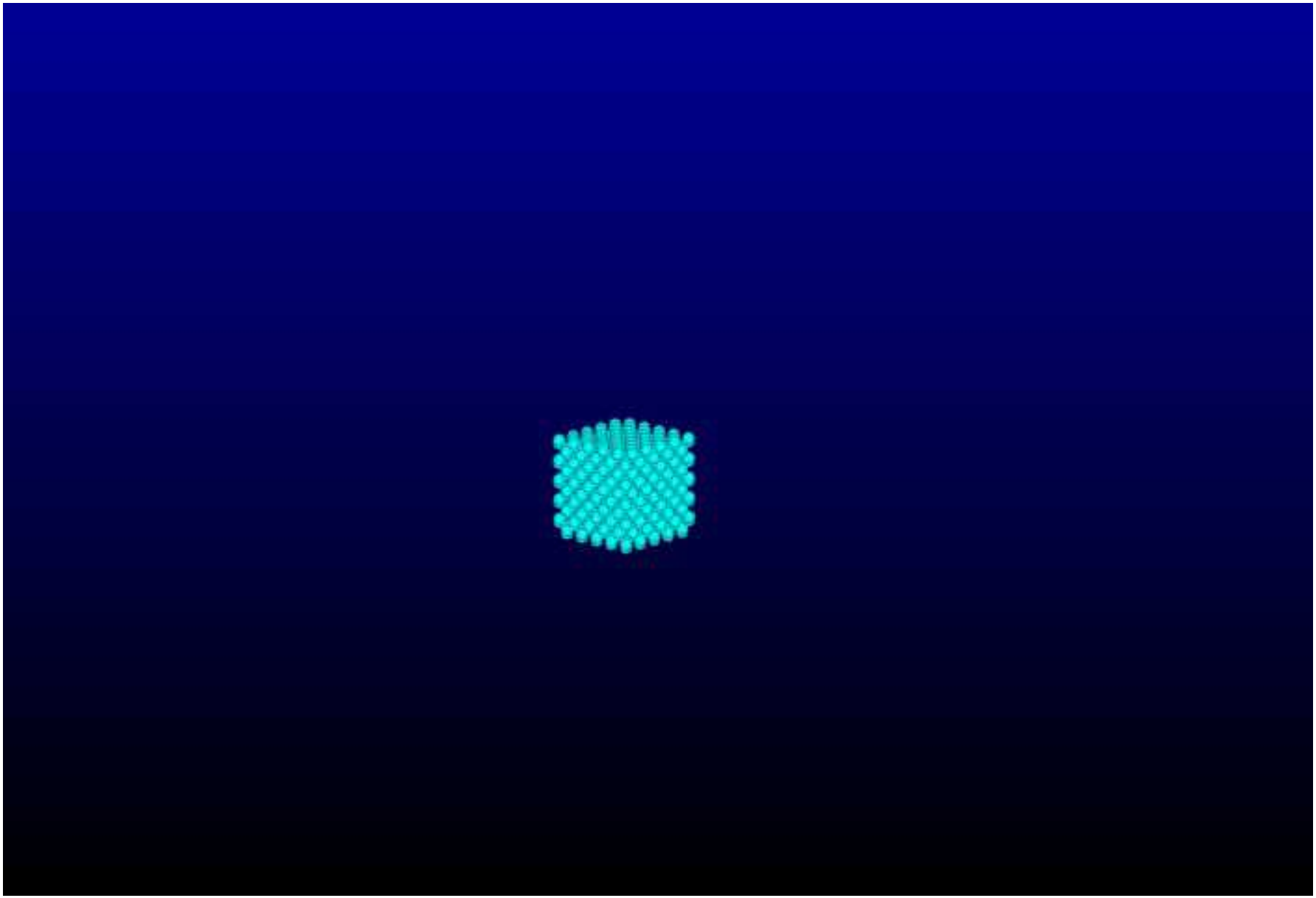
The key is how to write your LAMMPS input file a.i.

LAMMPS Input File

The input file is composed of a sequence of commands, which can be easily accessed by clocking the "commands" button at http://lammps.sandia.gov.



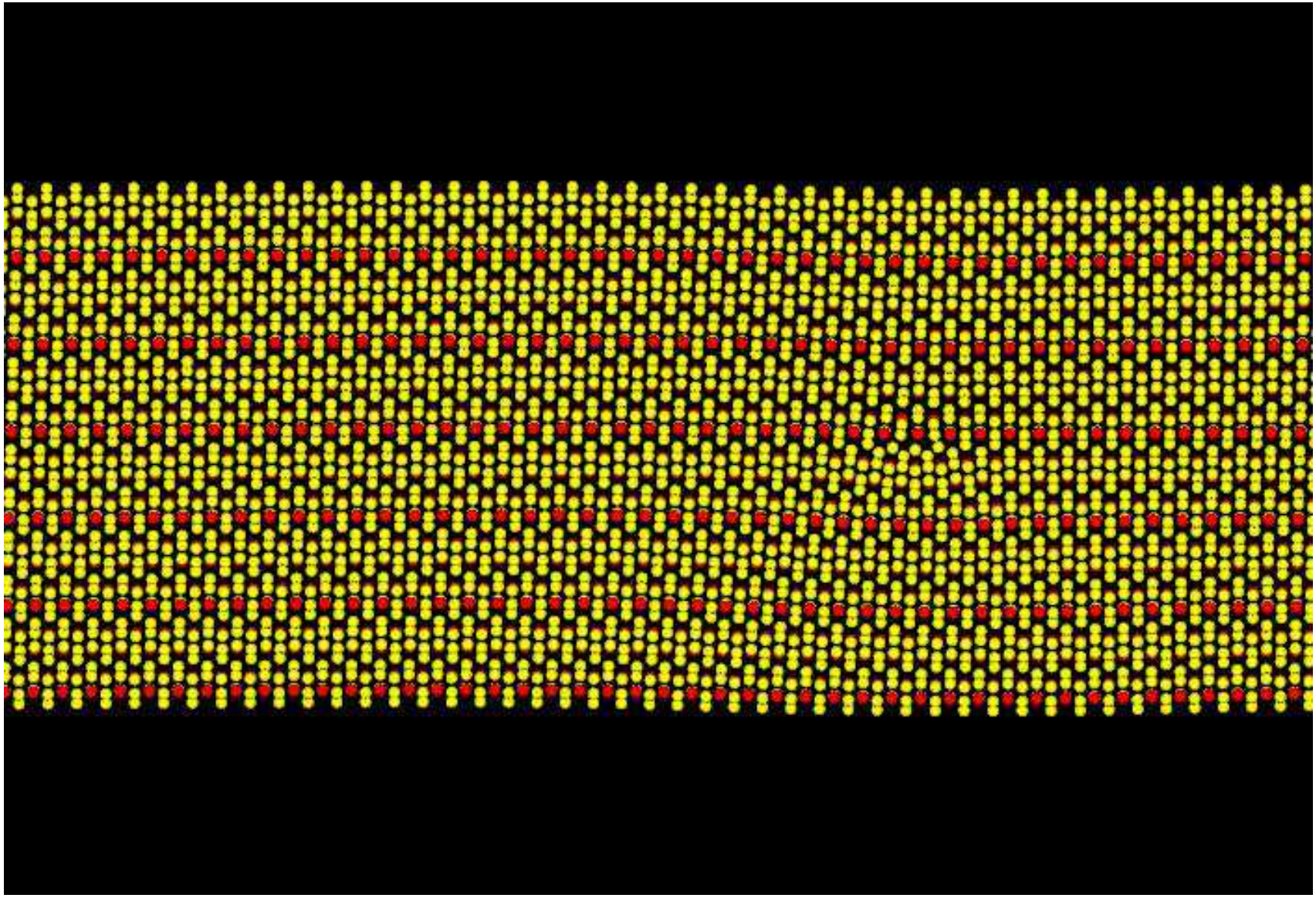
Example 1: $H \rightarrow H_2$ Reaction



Example 1: Input File for $H \rightarrow H_2$ Reaction

```
processors      1 1 1
units           metal
boundary        p p p
atom_style      atomic
lattice         diamond 5.669
read_data       r0.lmp
pair_style      bop save
pair_coeff      * * H_May24.t H
communicate     single cutoff 6.37
neighbor        0.3 bin
neigh_modify    delay 0
timestep        0.0002
thermo_style    custom step etotal pe ke
thermo          10000
velocity        all create 300.0 123 dist gaussian
fix             int all nvt temp 300.0 300.0 0.1
dump            dump all atom 300 r.*
dump_modify     dump format "%d %d %g %g %g" scale no flush yes
run             30000
```

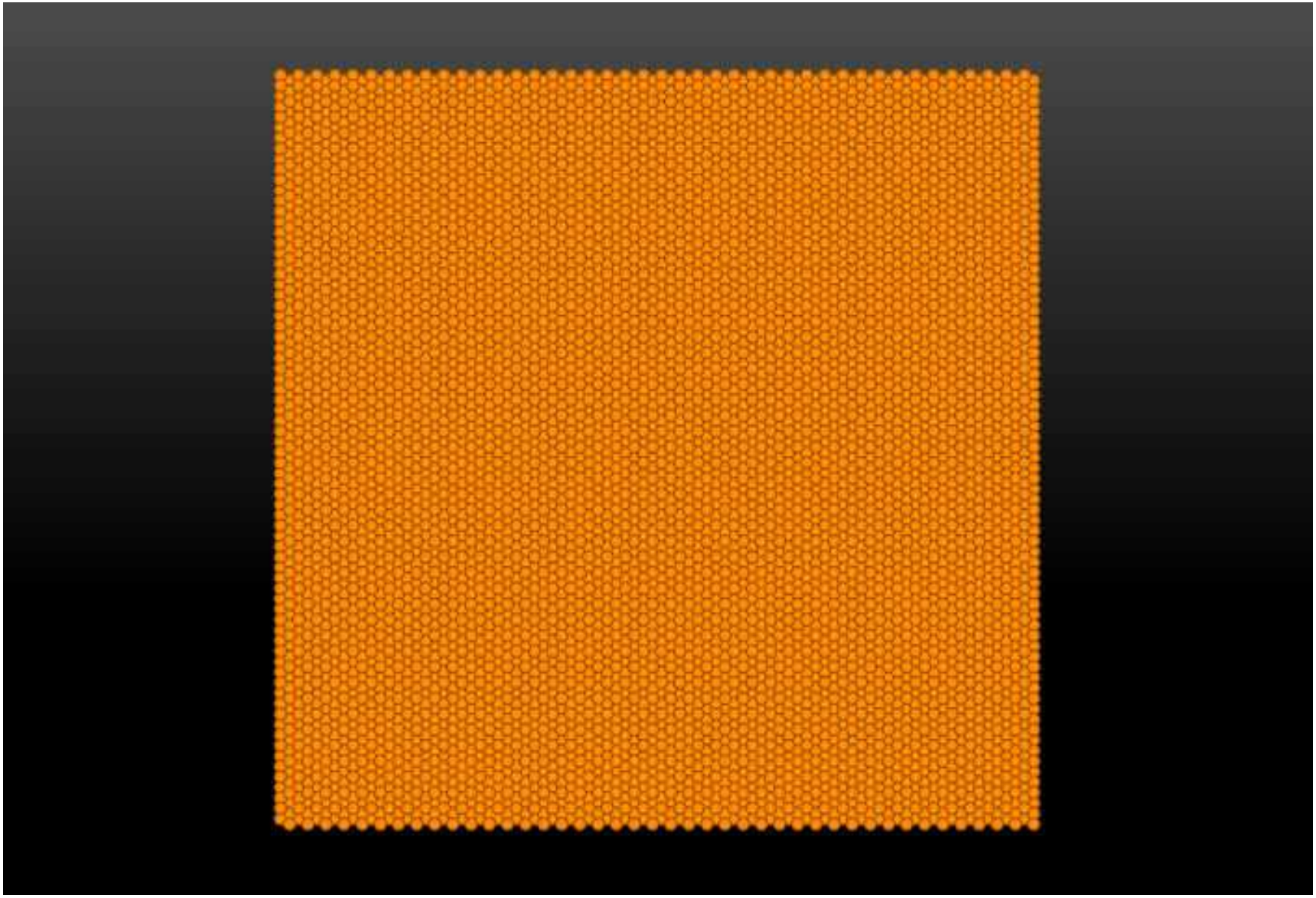
Example 2: Edge Dislocation Motion in $LaBr_3$



Example 2: Input File for Edge Dislocation Motion in $LaBr_3$

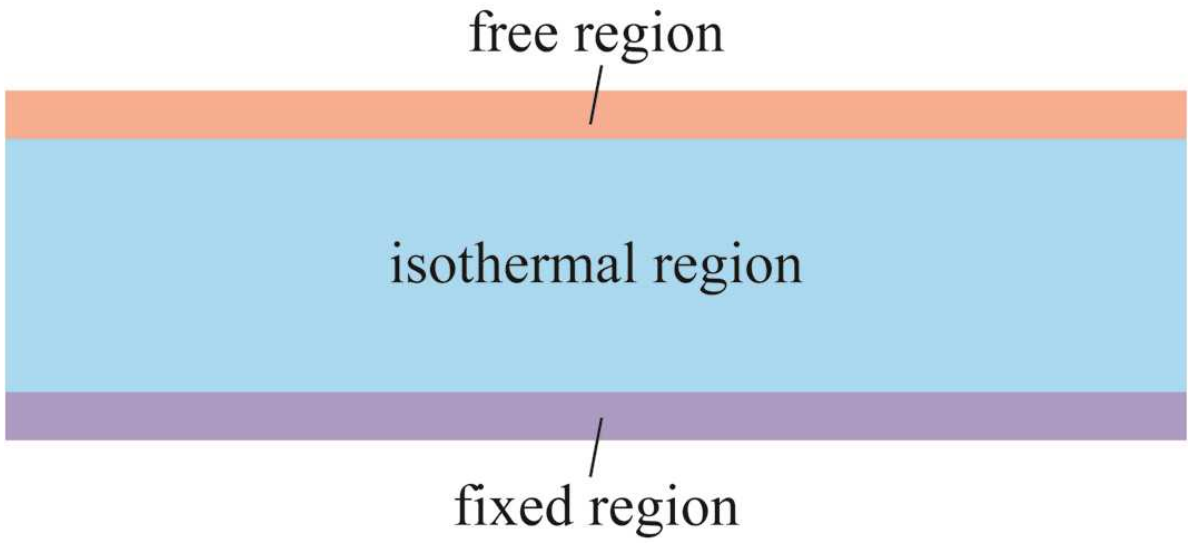
```
units           metal
atom_style      atomic
boundary        p s p
lattice         diamond 5.43095
read_data       r0.lmp
region          top block INF INF 75.8 INF INF INF units box
region          bottom block INF INF INF 6.8 INF INF units box
group           top region top
group           bottom region bottom
group           middle subtract all bottom top
pair_style      eam/alloy
pair_coeff      * *  June5.set La Br
neighbor        0.3 bin
neigh_modify    delay 0
timestep        0.0005
thermo_style    custom step temp pe ke etotal
thermo          10000
velocity        all set 0.0 0.0 0.0 units box
fix             int all nve
fix             temp all temp/rescale 10 0.0 0.0 0.00001 1.0
fix             top2 top addforce 0.114766648 0.0 0.0
fix             bottom2 bottom addforce -0.112471316 0.0 0.0
dump            dump all atom 80000 r.*
dump_modify     dump format "%d %d %g %g %g" scale no flush yes
run             80000000
```

Example 3: Graphene Growth on Cu (111)



Example 3: “Pre-Processing” Deposition Approach

region where
(1) evaporating atoms are first deleted and
(2) depositing atoms are next added



All deposition events are written in lammps input file a.i. This means that a.i is extremely long. A fortran or C++ program can be used to conveniently create a.i.

Example 3: Input File for Graphene Growth

```
Processors      5 1 4
units           metal
boundary        p fm p
atom_style      atomic
lattice         diamond 5.669
read_data       r0
pair_style      bop save
pair_coeff      * * CCu_Oct10_strongCu.t Cu C
communicate     single cutoff 11.208
neighbor        0.3 bin
neigh_modify    delay 0
timestep        0.001
thermo_style    custom step pe temp
thermo          10000
region          fix block INF INF -0.5 3.131 INF INF units box
region          isotherm block INF INF 3.1 9.4 INF INF units box
group           fix region fix
group           isotherm region isotherm
group           free subtract all fix isotherm
group           mobile union isotherm free
velocity        mobile create 1600.0 123 dist gaussian
velocity        fix set 0.0 0.0 0.0
fix             isotherm isotherm nvt temp 1600.0 1600.0 0.1 drag 0.0
fix             free free nve
dump            dump all atom 1600 r.*
dump_modify     dump format "%d %d %g %g %g" scale no flush yes
region          remove block INF INF 20.0 INF INF INF units box
delete_atoms    region remove
region          remove delete
region          isotherm delete
region          isotherm block INF INF 3.1 9.4 INF INF units box
group           isotherm subtract isotherm isotherm
group           isotherm region isotherm
create_atoms    2 single 67.167778 68.659042 63.855309 units box
region          newatom block 67 68 68 69 64 65 units box
group           newatom region newatom
velocity        newatom set 0.0 -8.962803 0.0 units box
group           newatom subtract newatom newatom
region          newatom delete
.....
run             1000
```

In order to deposit thousands of atoms (create new atoms at random locations and delete evaporating atoms), I used a C++ program to write out a long LAMMPS input file.

Topic 5:
Pre- and Post- Processing

Create Embedded Atom Method Potentials for 16 metals[1,2]

Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Fe, Mo, Ta, W, Mg, Co, Ti, Zn

1. Compile create.f and execute a.out < EAM.input will create an EAM .set file for lammps;
2. Users can use the EAM.input file to select elements:

An example of EAM.input:

```
&funccard
atomtype='Al'
&end
&funccard
atomtype='Cu'
&end
&funccard
&end
```


1. X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, Phys. Rev. B, 69, 144113 (2004).
2. X. W. Zhou, H. N. G. Wadley, R. A. Johnson, D. J. Larson, N. Tabat, A. Cerezo, A. K. Petford-Long, G. D. W. Smith, P. H. Clifton, R. L. Martens, and T. F. Kelly, Acta Mater., 49, 4005 (2001).

createAtoms (in LAMMPS Package)

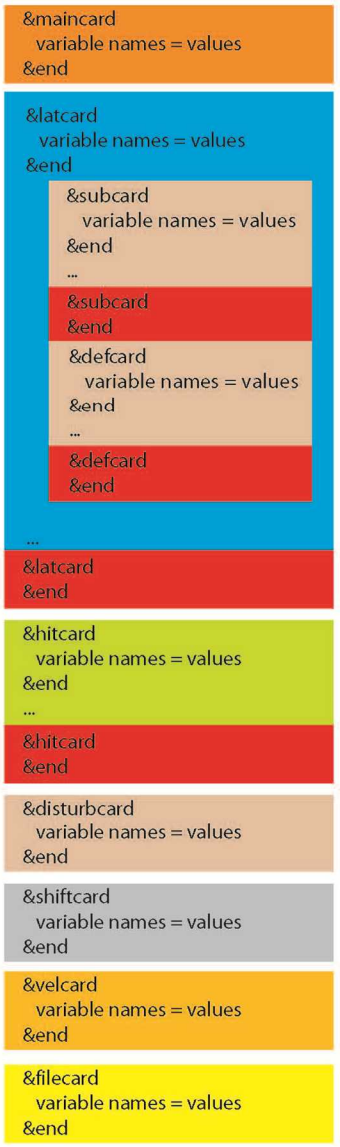


FIG. 1: structure of createAtoms input file.

1. Compile createAtoms.f and execute a.out < create.input will create a configuration;
2. Users needs to write the input file create.input.

```
&maincard
 ntypes=1
 perub=999.5,999.5,999.5
 perlb=-0.5,-0.5,-0.5
 ilatseed=21
amass=1.01,100.0,100.0,100.0,100.0,100.0
ielement=1,100,100,100,100,100
 iseed=212121
&end
&latcard
 lattype='fcc'
 alat=3.138,3.138,3.138
 xrot=1.0,0.0,0.0
 yrot=0.0,1.0,0.0
 zrot=0.0,0.0,1.0
 periodicity=1.0,1.0,1.0
 strain=0.0,0.0,0.0
 delx=0.0,0.0,0.0
 xbound=485.948,511.052
 ybound=485.948,511.052
 zbound=485.948,511.052
&end
&subcard
 rcell=0.0,0.0,0.0
 ccell=1.0,0.0,0.0,0.0,0.0,0.0
&end
&subcard
 rcell=0.25,0.25,0.25
 ccell=1.0,0.0,0.0,0.0,0.0,0.0
&end
&subcard
&end
&defcard
&end
&latcard
&end
&rotatecard
&end
&hitcard
&end
&disturbcard
&end
&shiftcard
 mode=0
&end
&velcard
&end
&filecard
 paradyn="none"
 lammps="rout"
 ensight="yes"
&end
```

Crystal Analysis Tool

Developed by Dr. Alexander Stukowski[1]
Technische Universität Darmstadt, Germany

1. The Crystal Analysis Tool[1] is a computer code that can analyze the output of atomistic simulations of crystals. The code implements algorithms to:
   - identify lattice structures and defect structures formed by atoms,
   - find dislocation lines and determine their Burgers vectors,
   - compute the atomic-level elastic and plastic deformation gradient fields to quantify plastic deformation and elastic lattice strains,
   - generate a geometric representation of the free surfaces of a solid and identify internal voids, measure surface area, porosity, etc.
2. Detailed information can be found at http://dxa.ovito.org/
3. Step by step download and installation instructions are found in the user's manual provided with the source code;
4. The latest source code version can be requested at stukowski@mm.tu-darmstadt.de

1. A. Stukowski, "Crystal Analysis Tool User's Manual," July, 2014.

Crystal Analysis Tool

Example Illustration of dislocation extraction analysis for a dislocation loop:

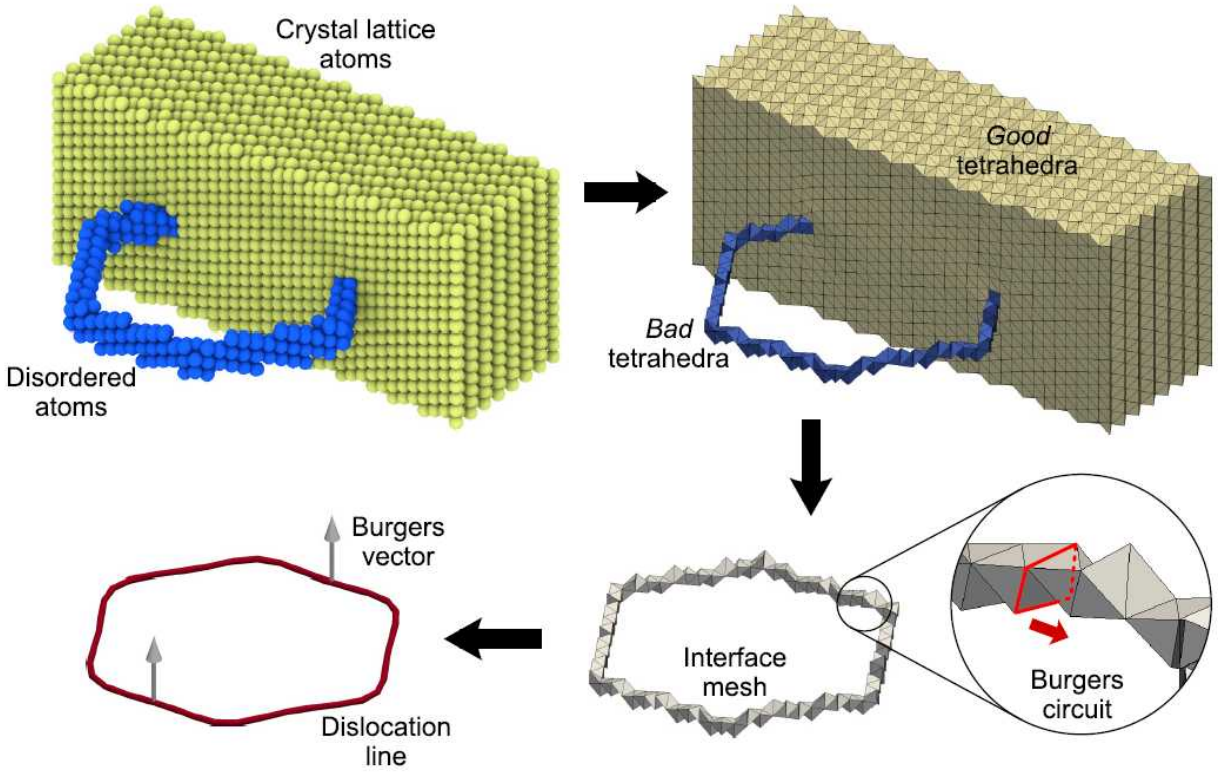
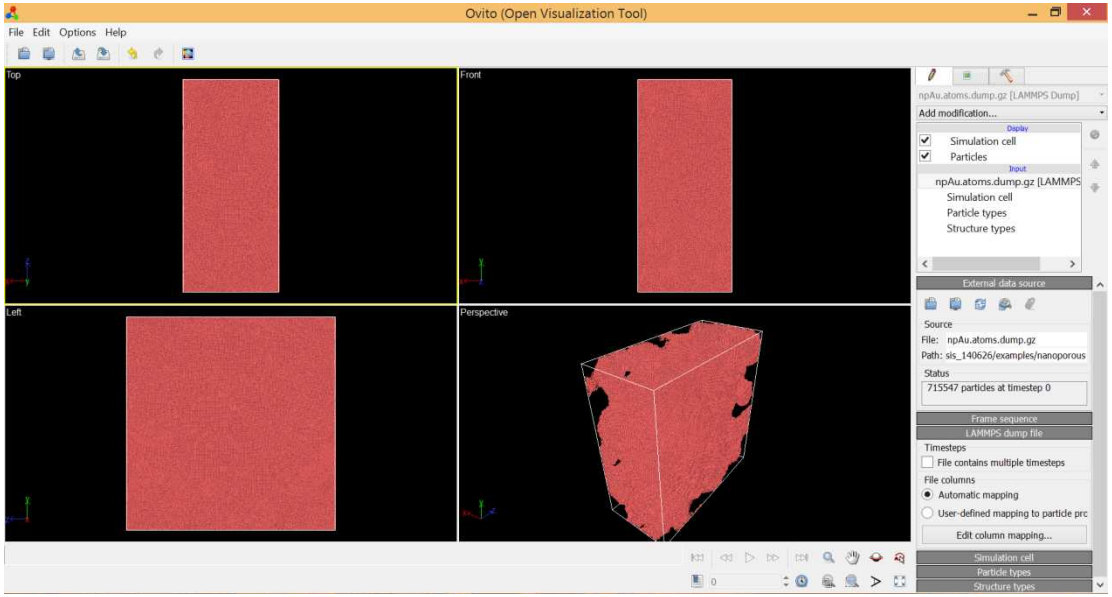


Figure 3: Illustration of the steps of the dislocation extraction algorithm. In this example, a prismatic dislocation loop in a bcc single crystal is identified and converted to a continuous line representation.

*A. Stukowski, V. V. Bulatov and A. Athanasios, "Automated identification and indexing of dislocations in crystal interfaces," *Modelling Simul. Mater. Sci. Eng.,* vol. 20, no. 085007, 2012.

Visualization Tool

1. OVITO (Open Visualization Tool) is also developed by Dr. Stukowski;
2. The visualization software features:
   - Import/export various file formats
   - Particle system rendering
   - Flexible data processing models
   - **Comprehensive analysis of Crystal Analysis Tool output files**
3. Download the code at http://www.ovito.org;
4. Full description of the features can be found at http://www.ovito.org/manual;

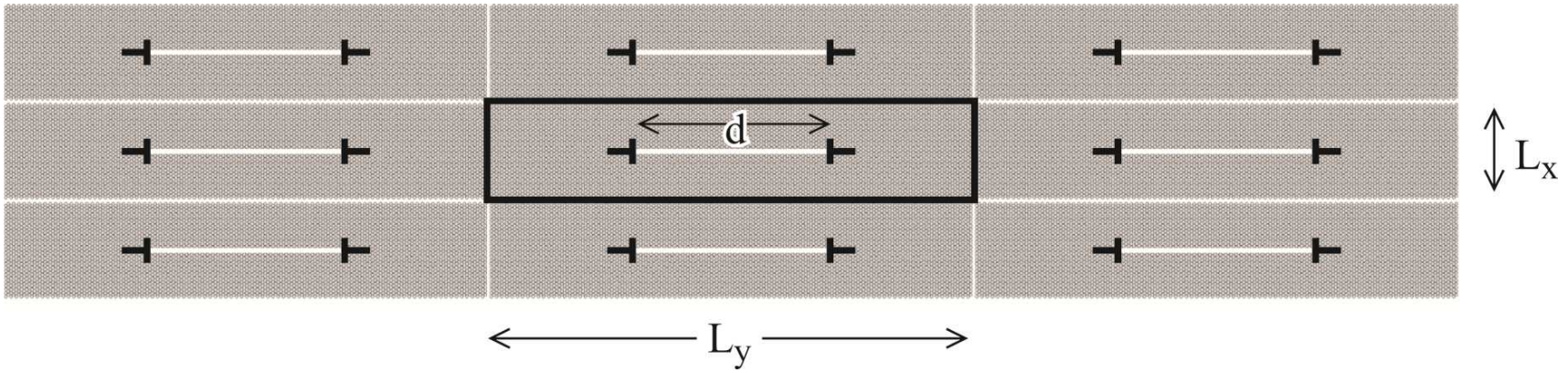


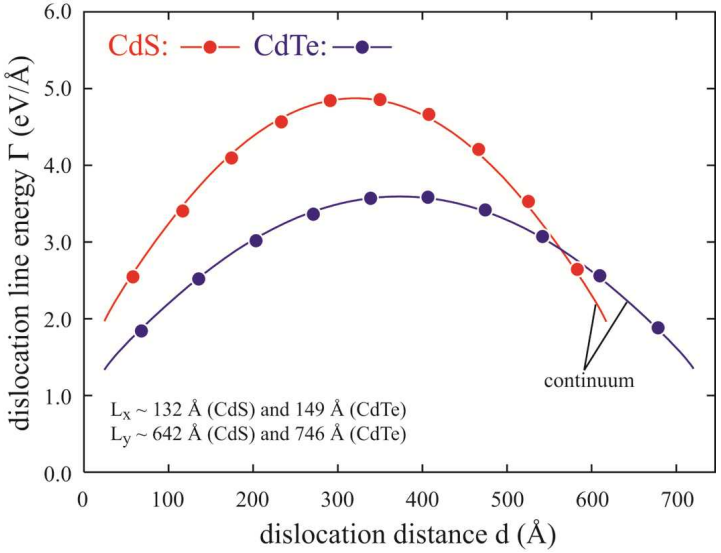
The figure shows OVITO's user interface.

Topic 6:
MD Informed Continuum Models

Dislocation Energy Calculations

Geometry





Quasi-2D Results

1. Continuum energy expression for periodic dislocations can be derived;
2. Fitting continuum expression with MD data leads to

Material	Core energy (eV)	Core radius (Å)	$\frac{Gb^2}{4\pi(1-\nu)}$ (eV)	$\frac{Eb^2}{8\pi} = \frac{Gb^2}{4\pi(1-\nu)}$ (eV)	
				compression	tension
CdS	1.77	18.63	0.46	0.62	0.29
CdTe	1.30	24.92	0.34	0.37	0.23

Topic 7:
Exercises

Exercise: Extracting Dislocations from a Nanoporous Crystal

This exercise combines the Crystal Analysis Tool and OVITO to visualize dislocations detected inside a crystal.

Steps to follow in the Crystal Analysis Tool:

- After installing the source code, copy the nanoporous_analysis bash script provided into the directory ~/{CrystalAnalysis_installation_directory}/examples/nanoporous/
- Run the bash script to perform the analysis

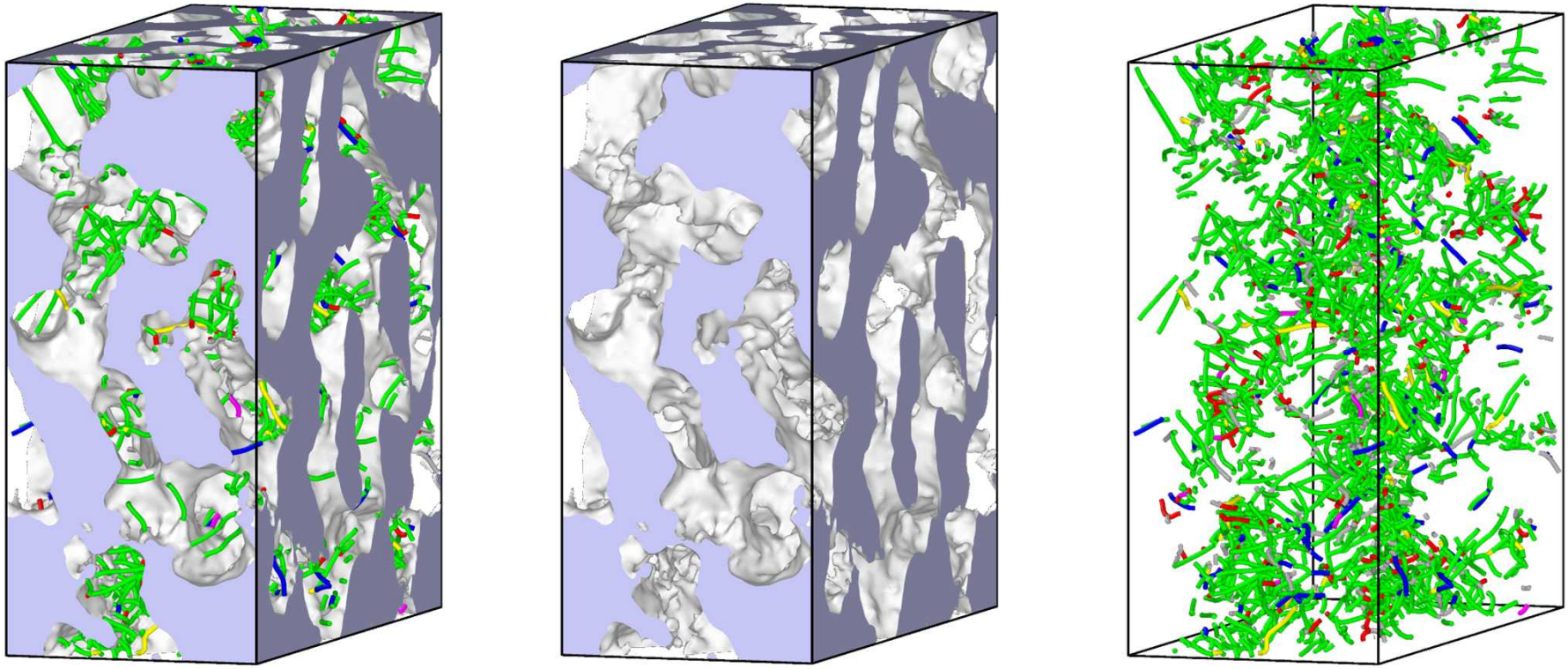
Steps to follow in OVITO:

1. Once downloaded, open OVITO to bring up the user interface
2. Click on Open Local File (top left corner under File) and navigate to the location of the nanoporous directory
3. Open the npAu.ca file

Exercise: Extracting Dislocations from a Nanoporous Crystal (continued)

Steps to follow in OVITO:

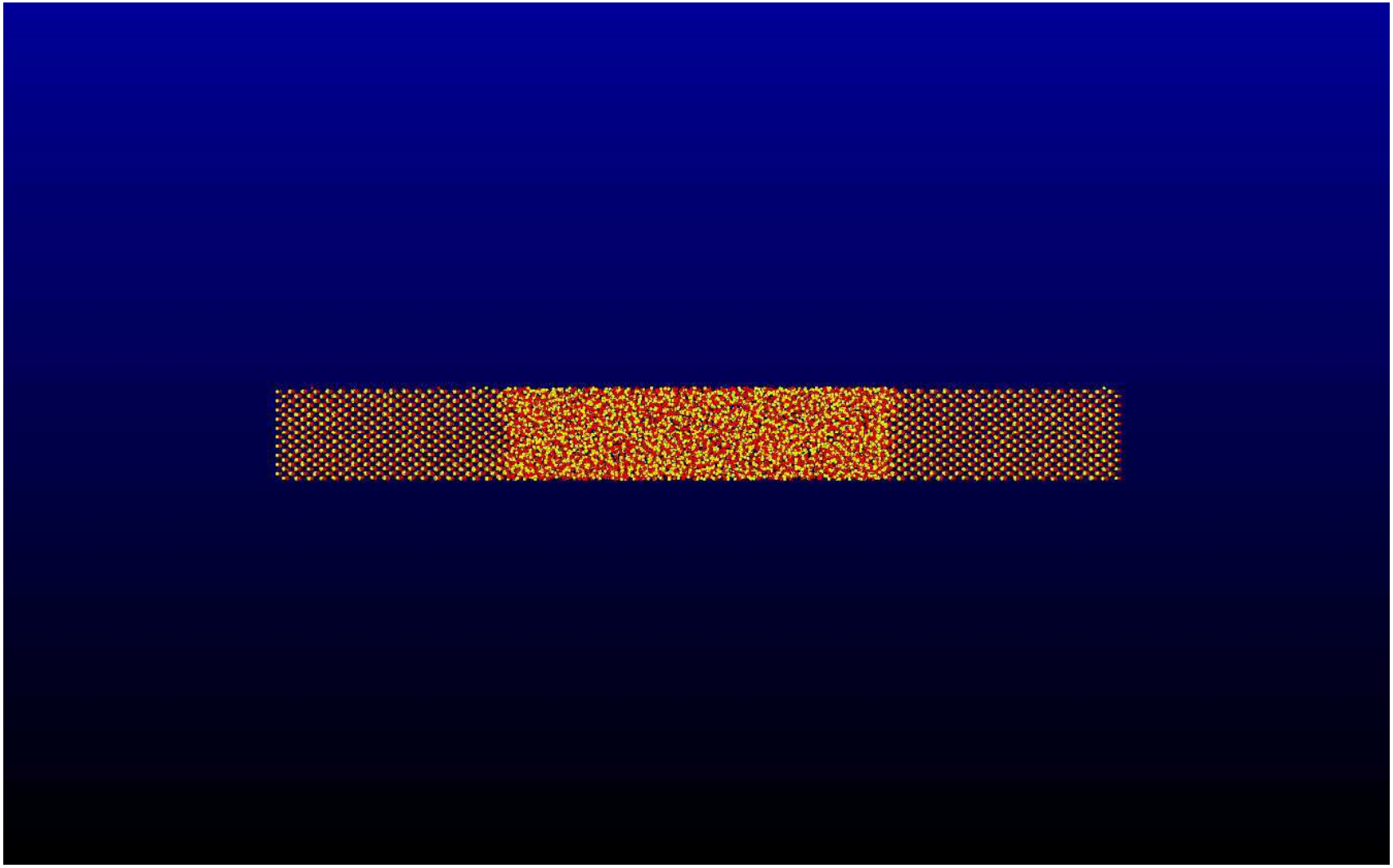
4. The display will show the dislocation segments and the surface mesh (see the rendered figures below)



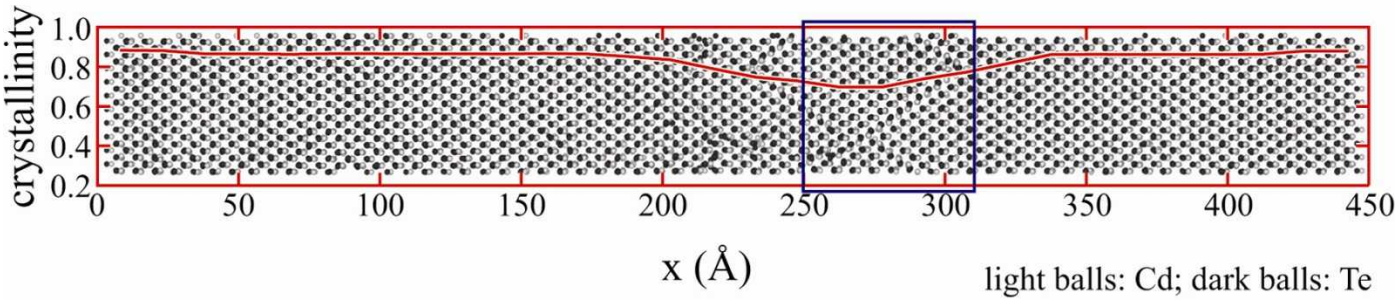
(Left) Surface mesh and dislocations found inside the nanoporous crystal. (middle) Only surface mesh is shown. (right) Only dislocations are shown.

Slides after this are Supplemental

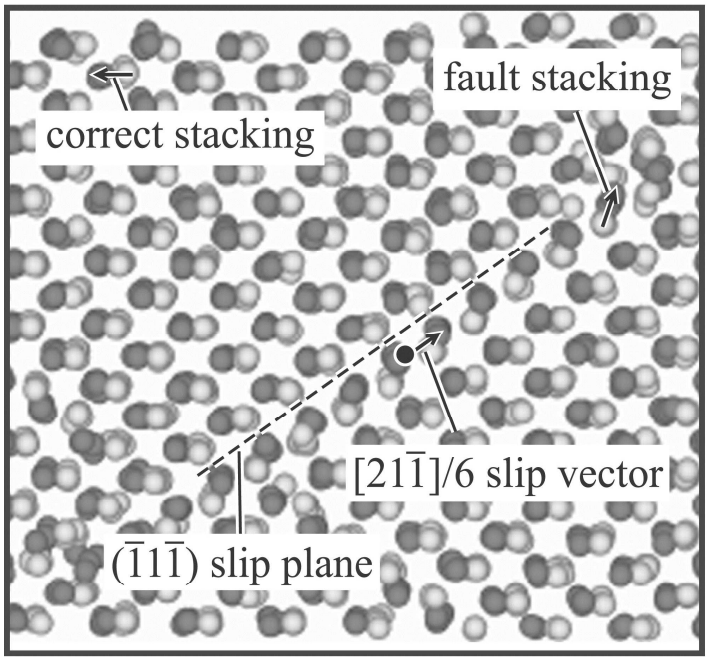
CdTe Melt Growth Simulation



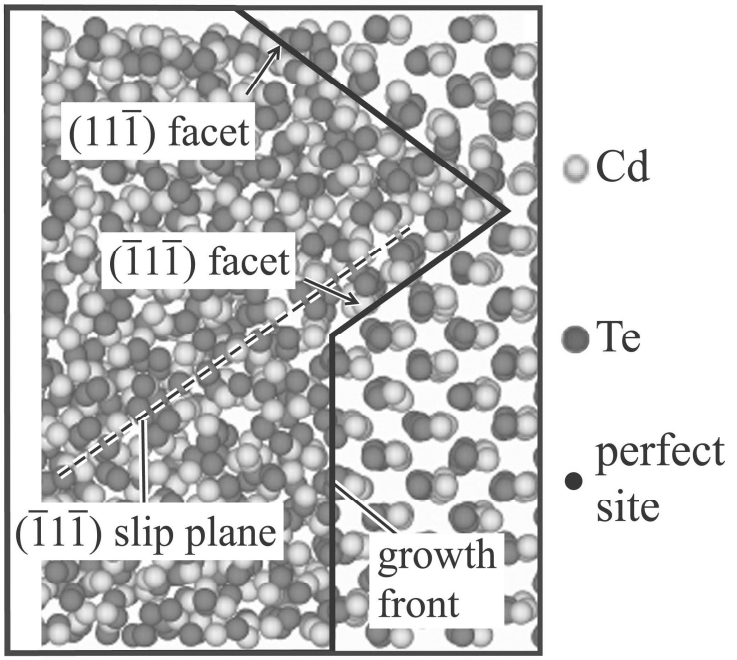
Melt-Growth Defect Formation



(a) framed region in Fig. 4(b)

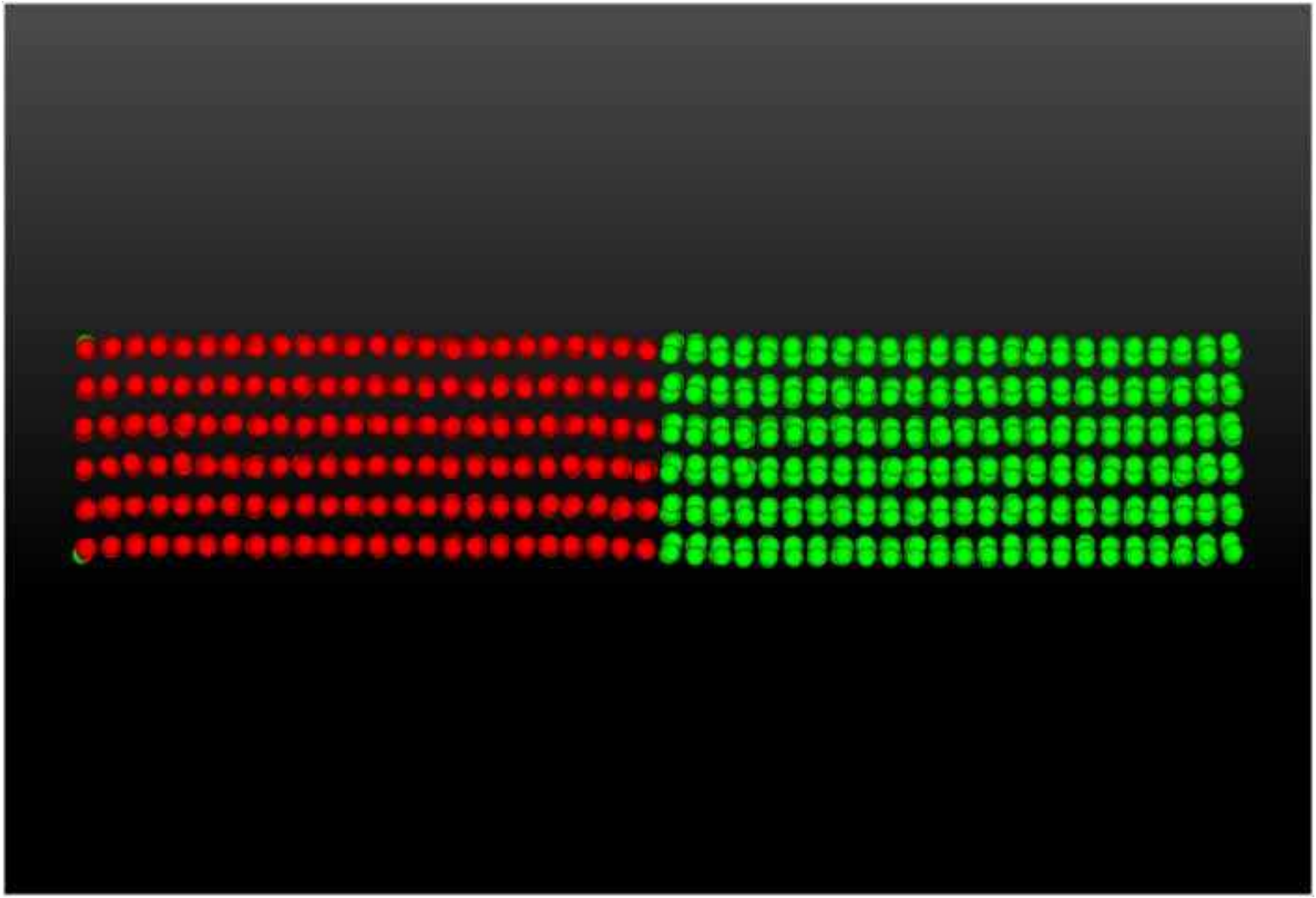


(b) defect nucleation at local facets



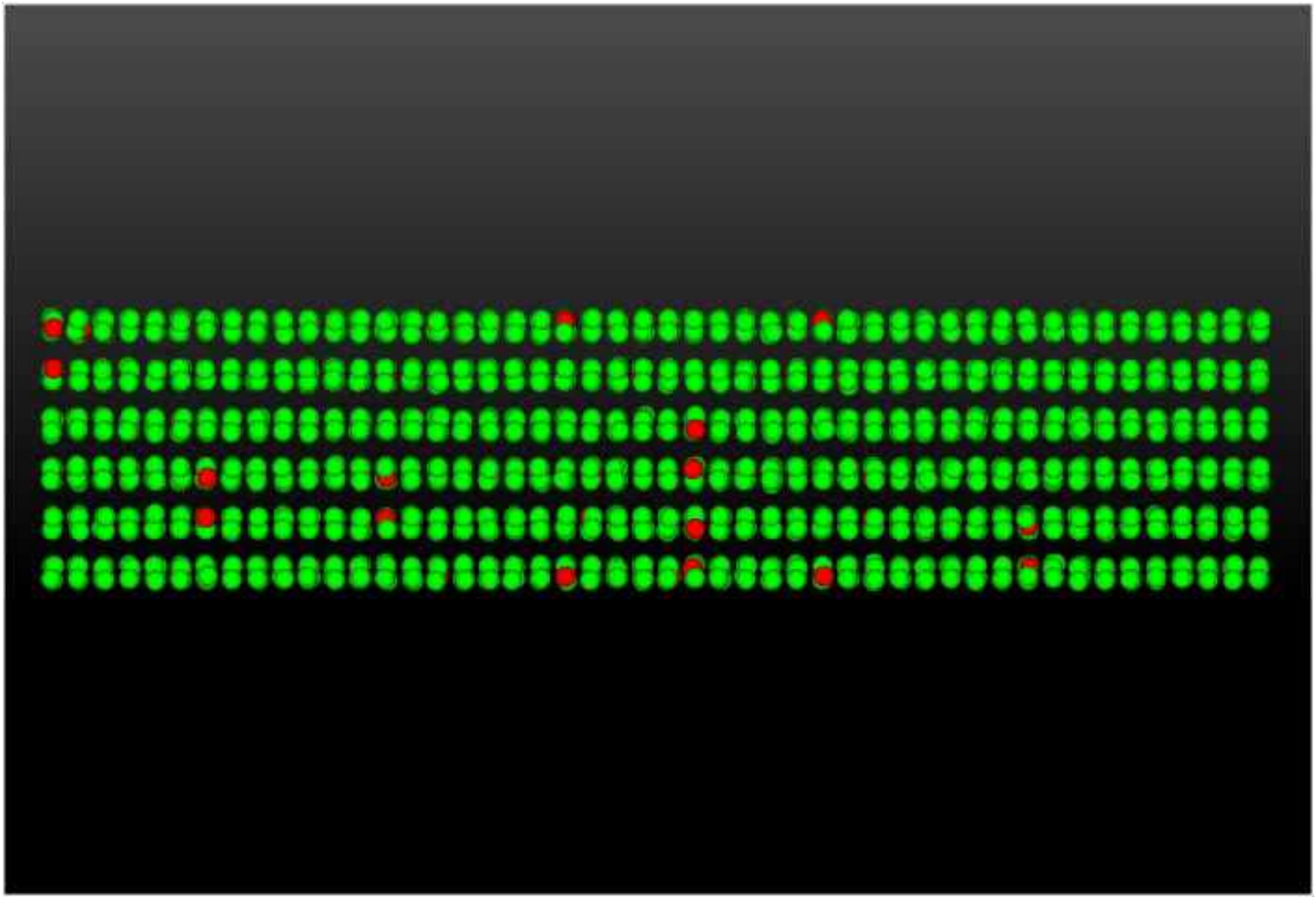
Diamond Formation under High Pressure

T = 2000 K, P = 0.6 Mbars



Graphite Formation under Negative Pressure

T = 1600 K, P = -0.6 Mbars



Graphene Growth