A High-Fidelity Molecular Dynamics Approach for Studying Dislocations in $Cd_{1-x}Zn_xTe$ Crystals

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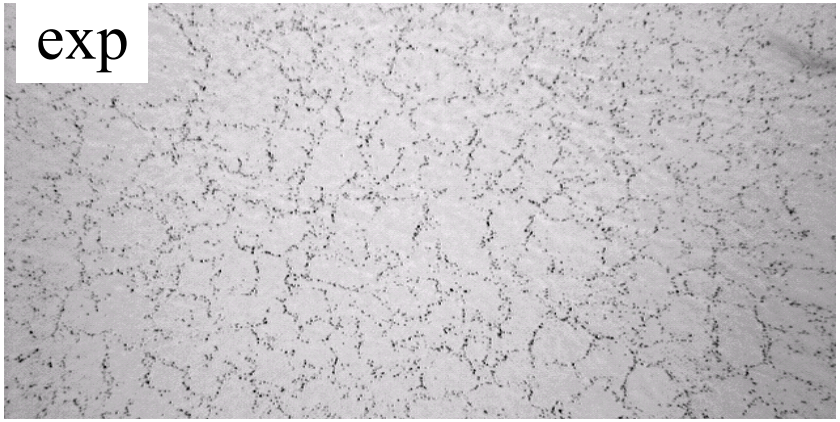
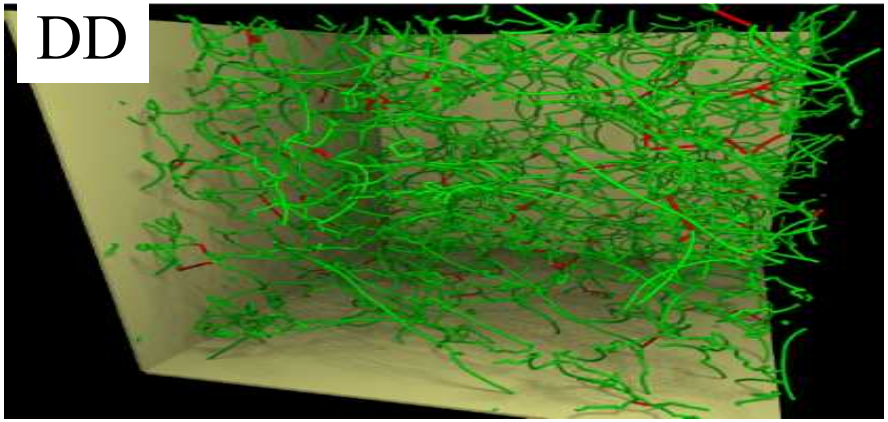
Radiation Detection $Cd_{1-x}Zn_xTe$ Problem

1. Improvement of the leading radiation detection semiconductor $Cd_{1-x}Zn_xTe$ (CZT) has been slow for the past 15+ years;
2. Properties are limited by dislocation cell structures[1], which might be controllable by point defects[2];
3. Dislocation dynamics (DD) simulations can guide experiments;
4. Atomistic simulations are needed to provide inputs for DD;
5. We have developed a high-fidelity CdZnTe bond order potential to enable molecular dynamics simulations of dislocations in CZT.





1. F. P. Doty, X. W. Zhou, J. A. Zimmerman, D. K. Ward, B. M. Wong, and Q. M. Li, SORMA WEST 2012.
2. P. Rudolph, C. Frank-Rotsch, U. Juda, F.-M. Kiessling, Mater. Sci. Eng. A, 400-401, 170 (2005).

Analytical Bond Order Potential (BOP)

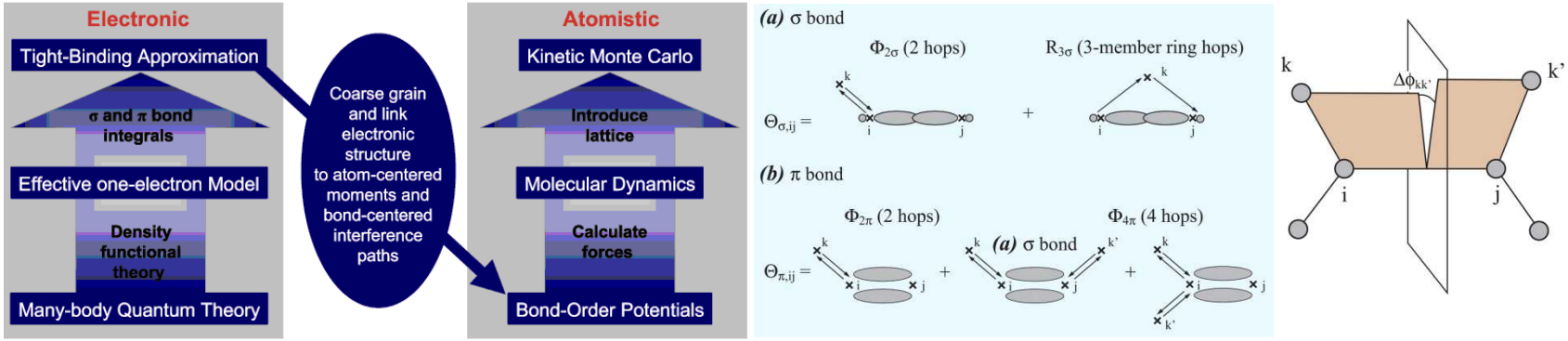
$$E = \frac{1}{2}\sum_i \sum_{j \neq i} \phi_{ij}\left(r_{ij}\right) - \sum_i \sum_{j \neq i} \beta_{\sigma,ij}\left(r_{ij}\right) \cdot \Theta_{\sigma,ij} - \sum_i \sum_{j \neq i} \beta_{\pi,ij}\left(r_{ij}\right) \cdot \Theta_{\pi,ij}$$

$\phi_{ij}(r_{ij})$: core-core repulsion; $\beta_{\sigma,ij}(r_{ij})$ and $\beta_{\pi,ij}(r_{ij})$: σ and π bond integrals describing electron hopping probabilities among different orbital's; $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$: σ and π bond orders describing half of difference in number of electrons in the bonding and anti-bonding states. $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$ are complicated functions of bond length and bond angles.

1. 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).
2. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 59, 8487 (1999).
3. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. Lett., 84, 4124 (2000).
4. D. G. Pettifor, and I. I. Oleinik, Phys. Rev. B, 65, 172103 (2002).
5. R. Drautz, D. Nguyen-Manh, D. A. Murdick, X. W. Zhou, H. N. G. Wadley, and D. G. Pettifor, TMS Lett., 1, 31 (2004).
6. 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).
7. 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).

BOP Origin

Cyrot-Lackmann theorem



1. Derived from quantum mechanics theory through systematic coarse-graining;
2. Separate treatment of σ and π bonding energies (products of bond order* and bond integral#);
3. The first two levels of the expanded Green function retained for the σ and π bond orders;
4. Up to four electron hops are considered, naturally incorporating the 3-member ring term in the σ bonding ($R_{3\sigma}$) and the dihedral angle ($\Delta\phi_{kk'}$) effect in the p bonding;
5. Valence effect is addressed.
6. Accuracy comparable to quantum mechanics and scale comparable to conventional molecular dynamics.

* bond order: half the difference of electrons in the bond and anti-boding states.
\# bond integral: hopping probability of electrons from one orbital to another.

Growth Simulation Enabling Potentials

Our Cd-Zn-Te BOP meets two criteria:

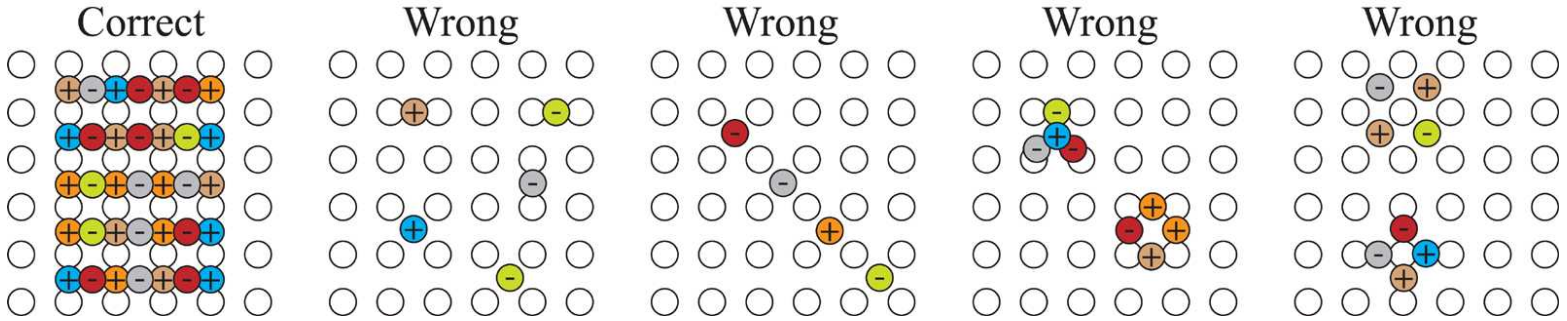
1. Captures property trends of many phases as determined from quantum calculations;
2. Predicts correctly crystalline growth during MD simulations.

Note that:

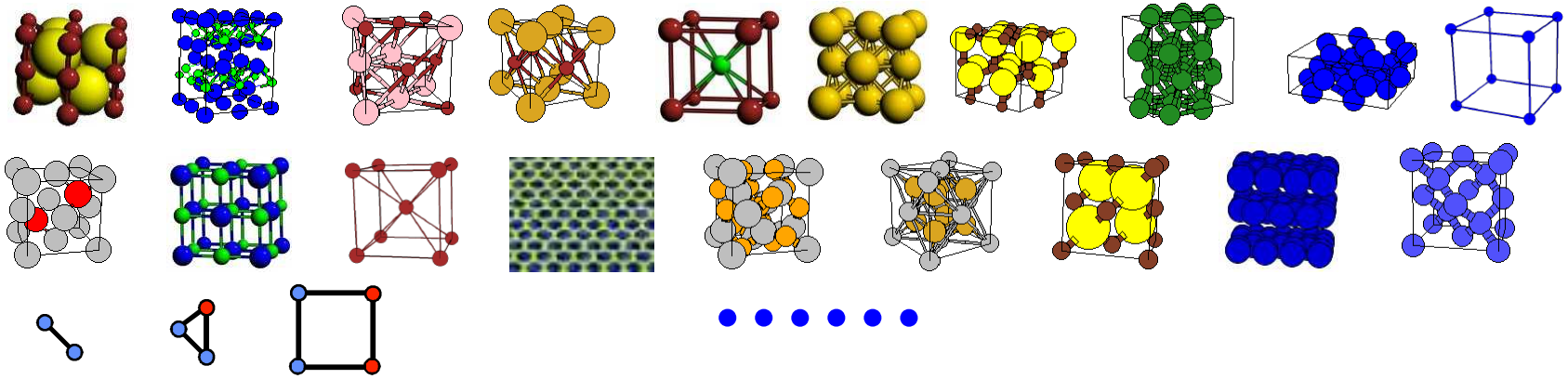
1. Growth simulations test unlimited number of configurations;
2. Most previous methods do not consider growth simulations
   $\Rightarrow$ rare to satisfy both criteria.

Growth Simulations Extremely Challenging

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



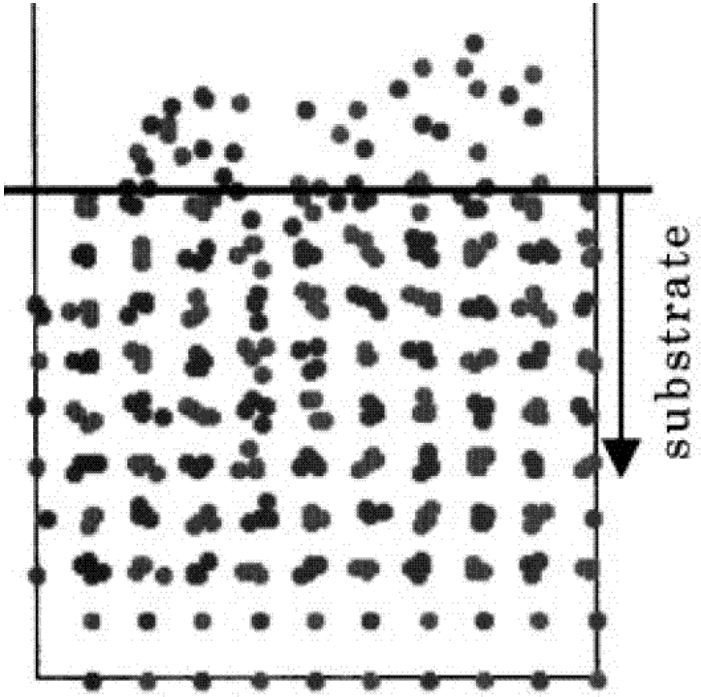
- **Capturing property trends of a large number of clusters, lattices, and defects are necessary, but this alone will not ensure successful growth simulations.**



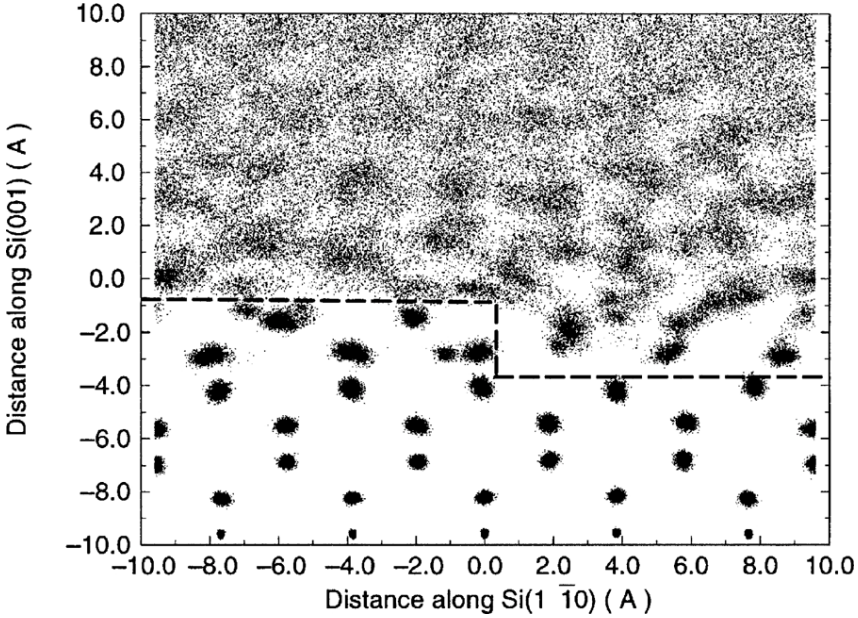
- **Extensive iterations are usually needed to develop an growth-enabling interatomic potential.**

Literature Examples of Growth Simulations

InAs on (110) GaAs[1].



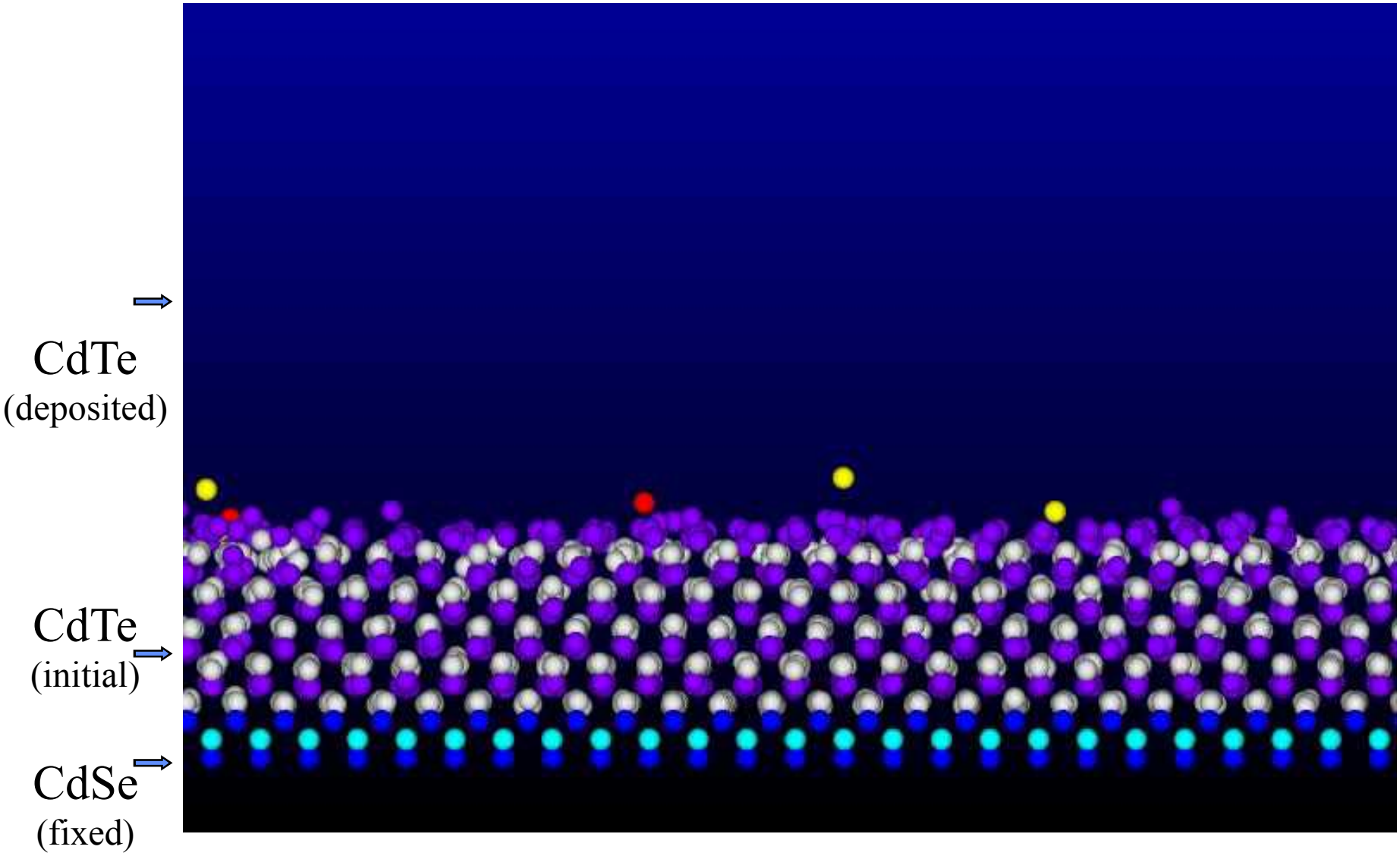
CdTe on (100) Si[5].



None of the potentials listed below predicts the crystalline growth.

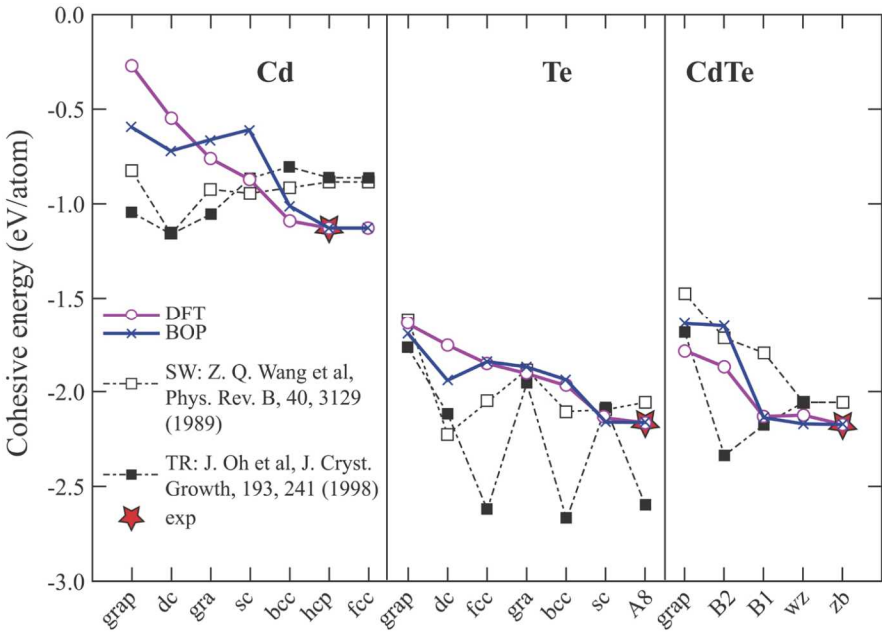
1. M. Nakamura, H. Fujioka, K. Ono, M. Takeuchi, T. Mitsui, and M. Oshima, J. Cryst. Growth, 209, 232(2000).
2. J. Tersoff, Phys. Rev. B, 39, 5566(1989). – for Si (amorphous growth, but can re-crystallize at 2200 K through bulk transformation).
3. P. A. Ashu, J. H. Jefferson, A. G. Cullis, W. E. Hagston, 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).

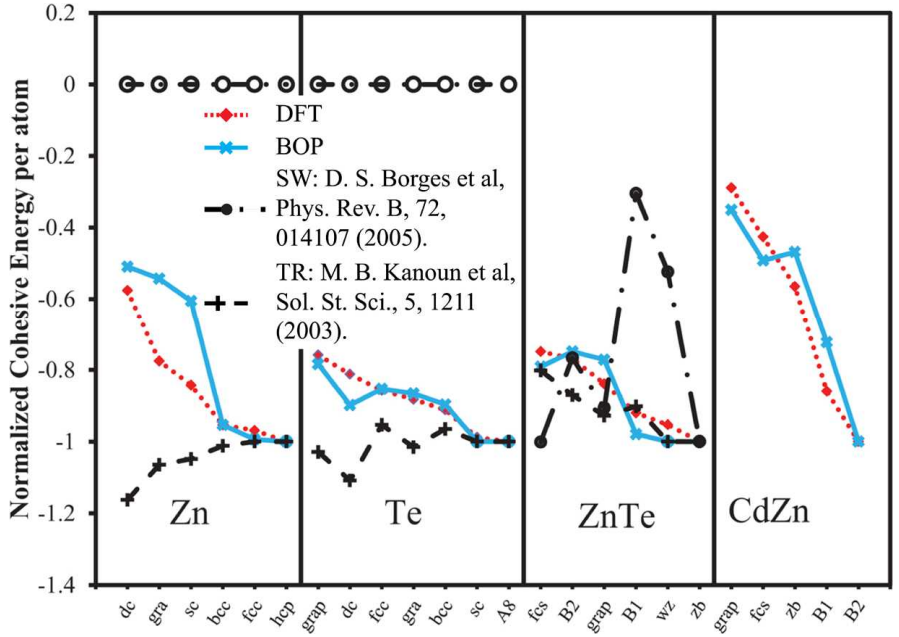
BOP-Based Molecular Dynamics (MD)



BOP Verification

Captures property trends of many phases including clusters, lattices, surfaces, defects, etc.

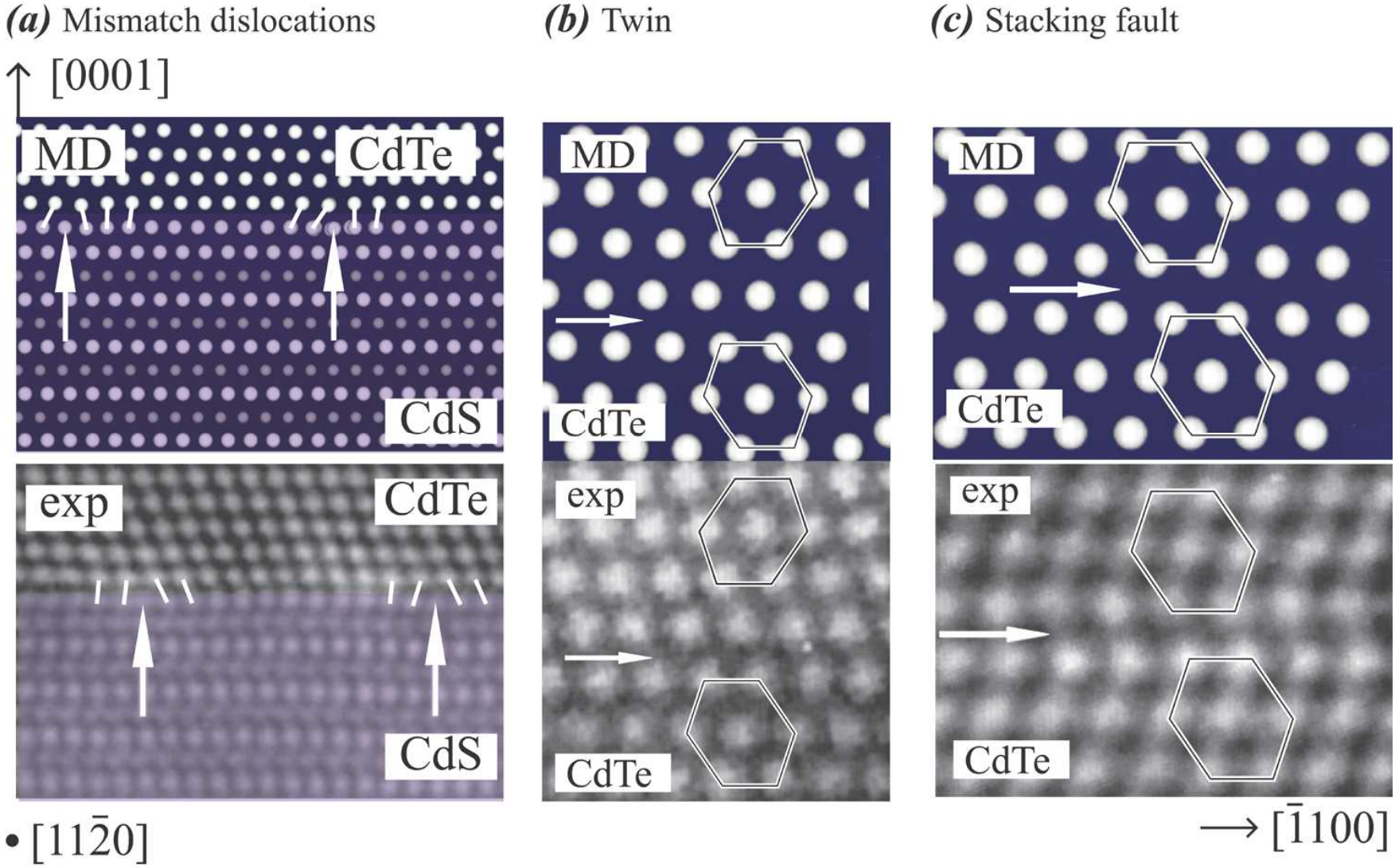




1. D K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 85, 115206 (2012).
2. D. K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 86, 245203 (2012).

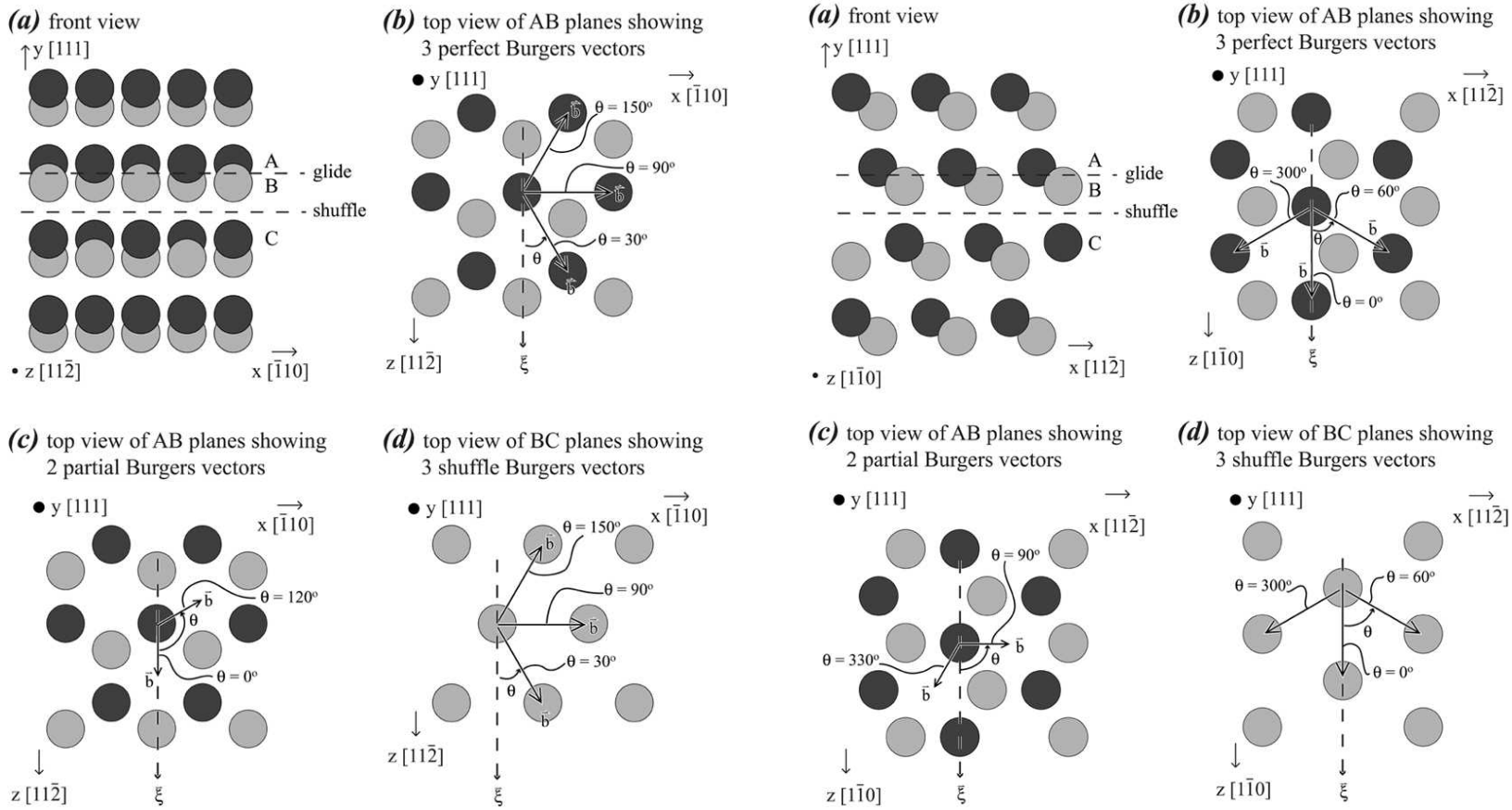
BOP Validation Example

accurately predict CdTe/CdS defects



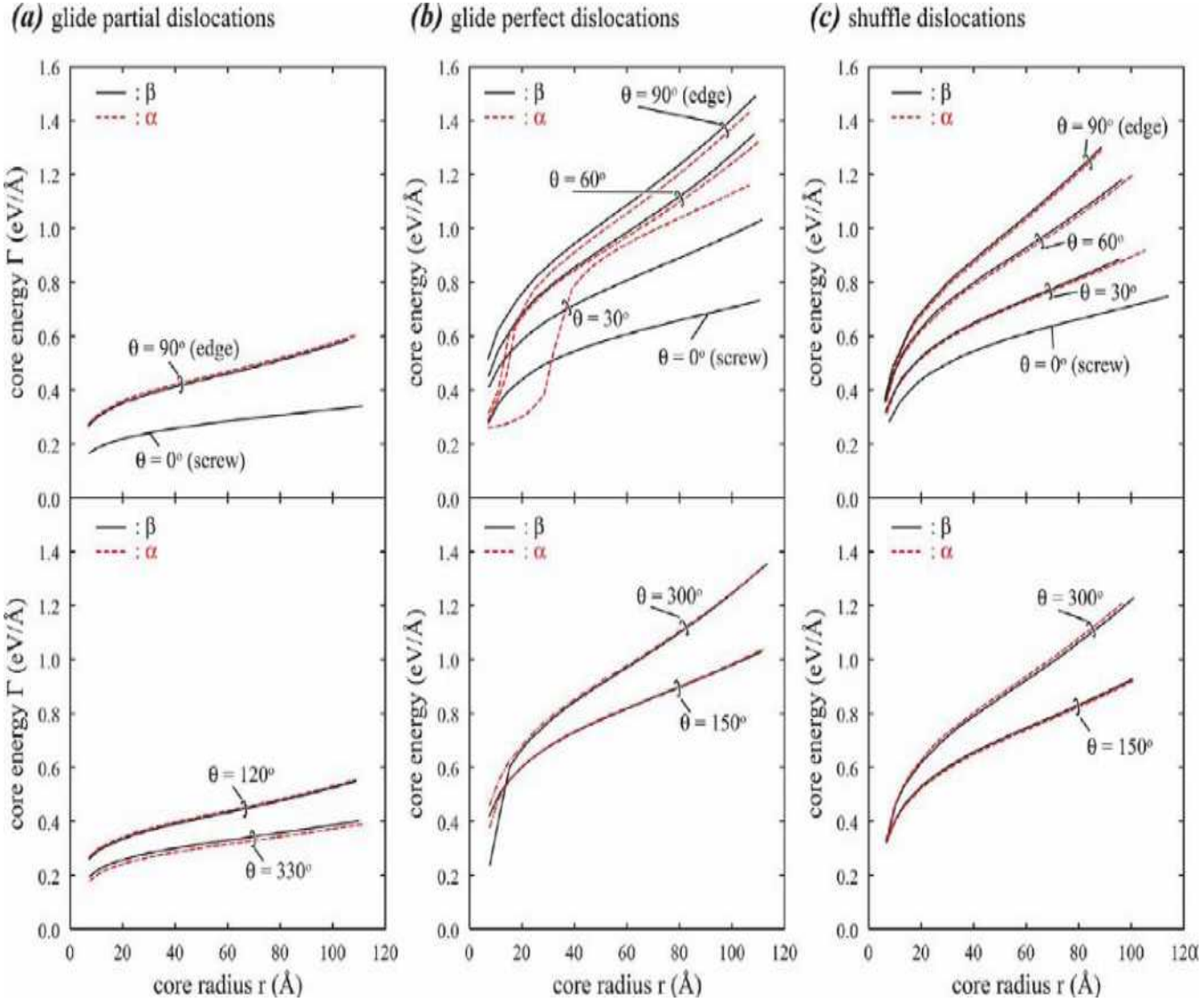
HRTEM from Y. Yan, R. G. Dhere, K. M. Jones, and M. M. Al-Jassim, J. Appl. Phys. 89, 5844 (2001).

Complexity of Dislocations

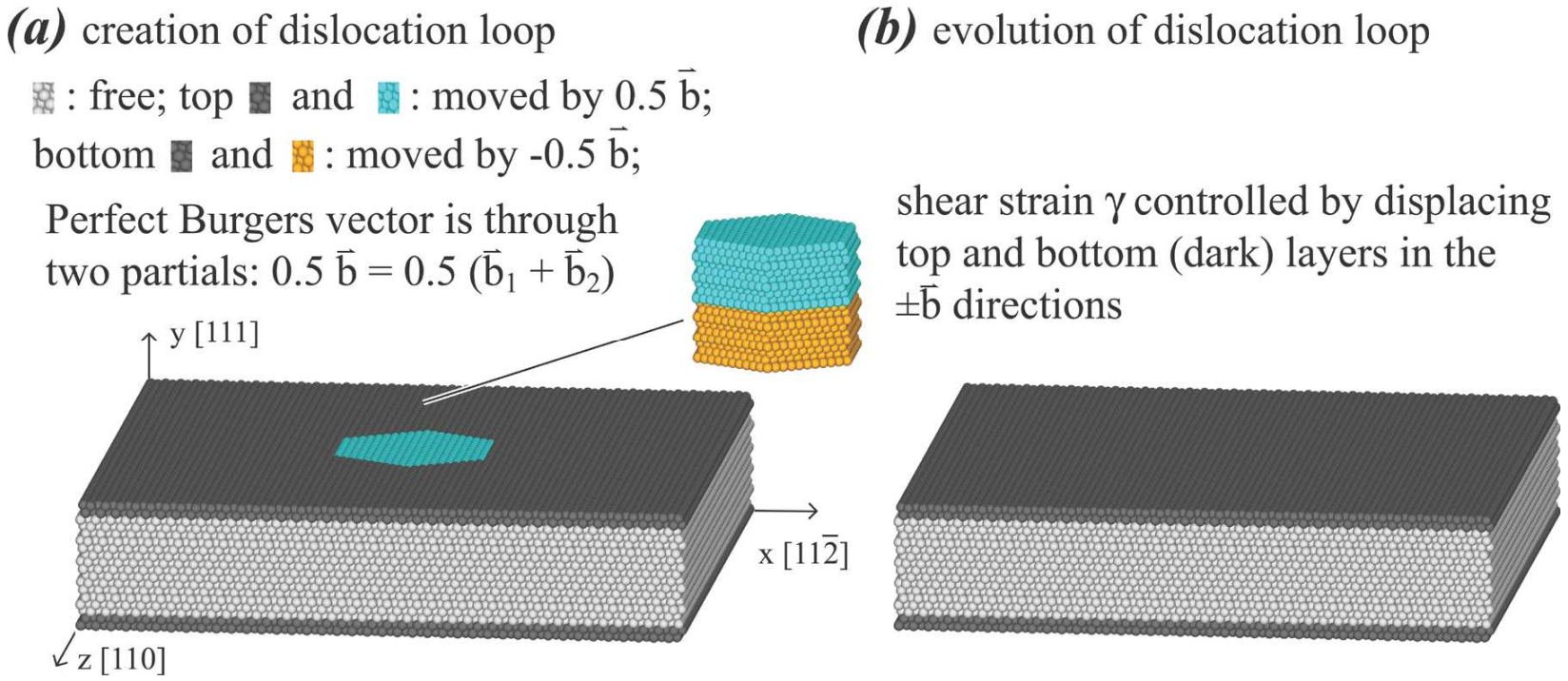


There are 30+ different dislocations (combinations of shuffle, glide, α, β, edge, screw, mixed, partial, perfect) in binary CdZn alone.

Dislocation Line Energies



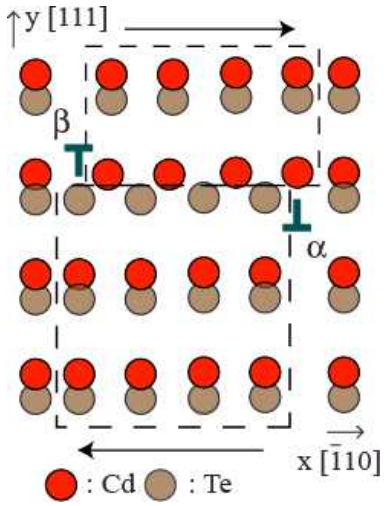
Dislocation Loop Model

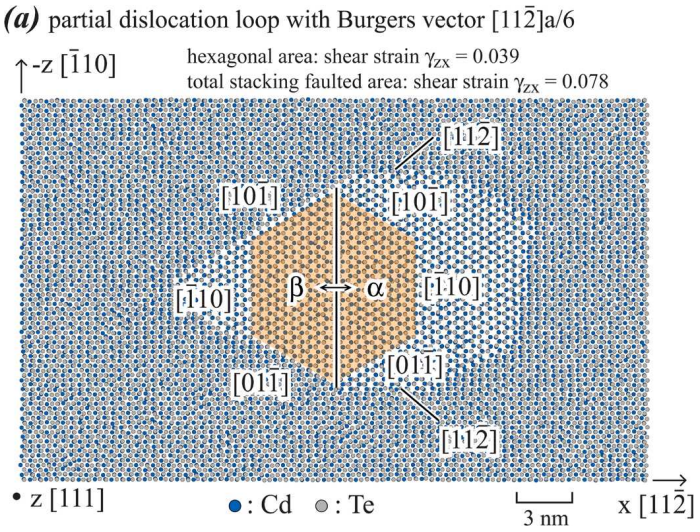


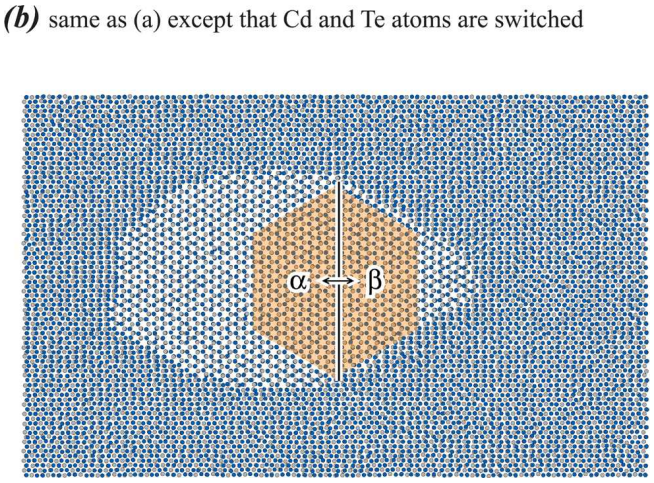
(a) the upper black and blue regions are moved by positive half Burgers vector, and the lower black and orange regions by negative half Burgers vectors;

(b) dislocation motion is simulated by continuously moving the top and bottom black regions in positive and negative Burgers vector directions.

Partial Dislocation Motion

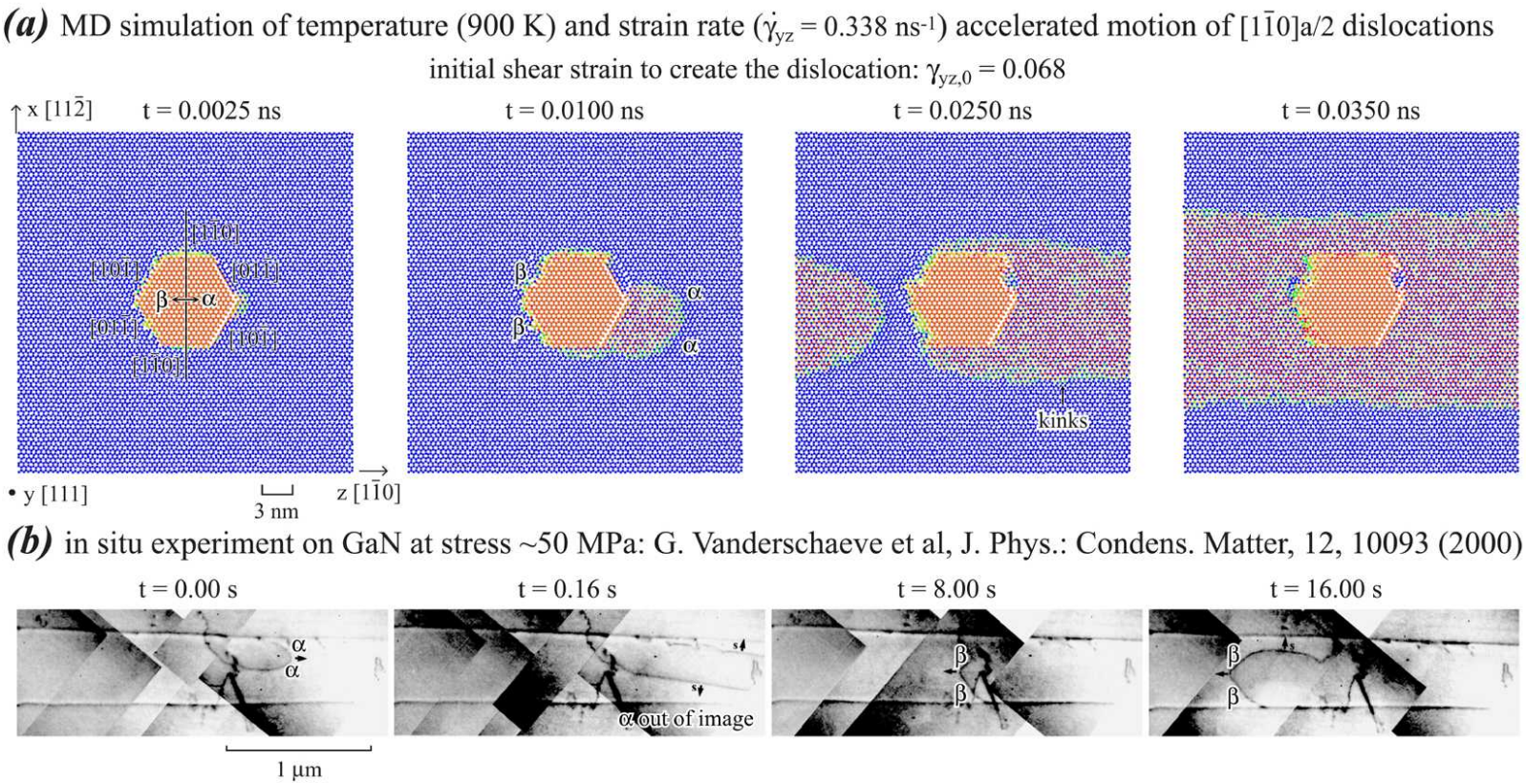






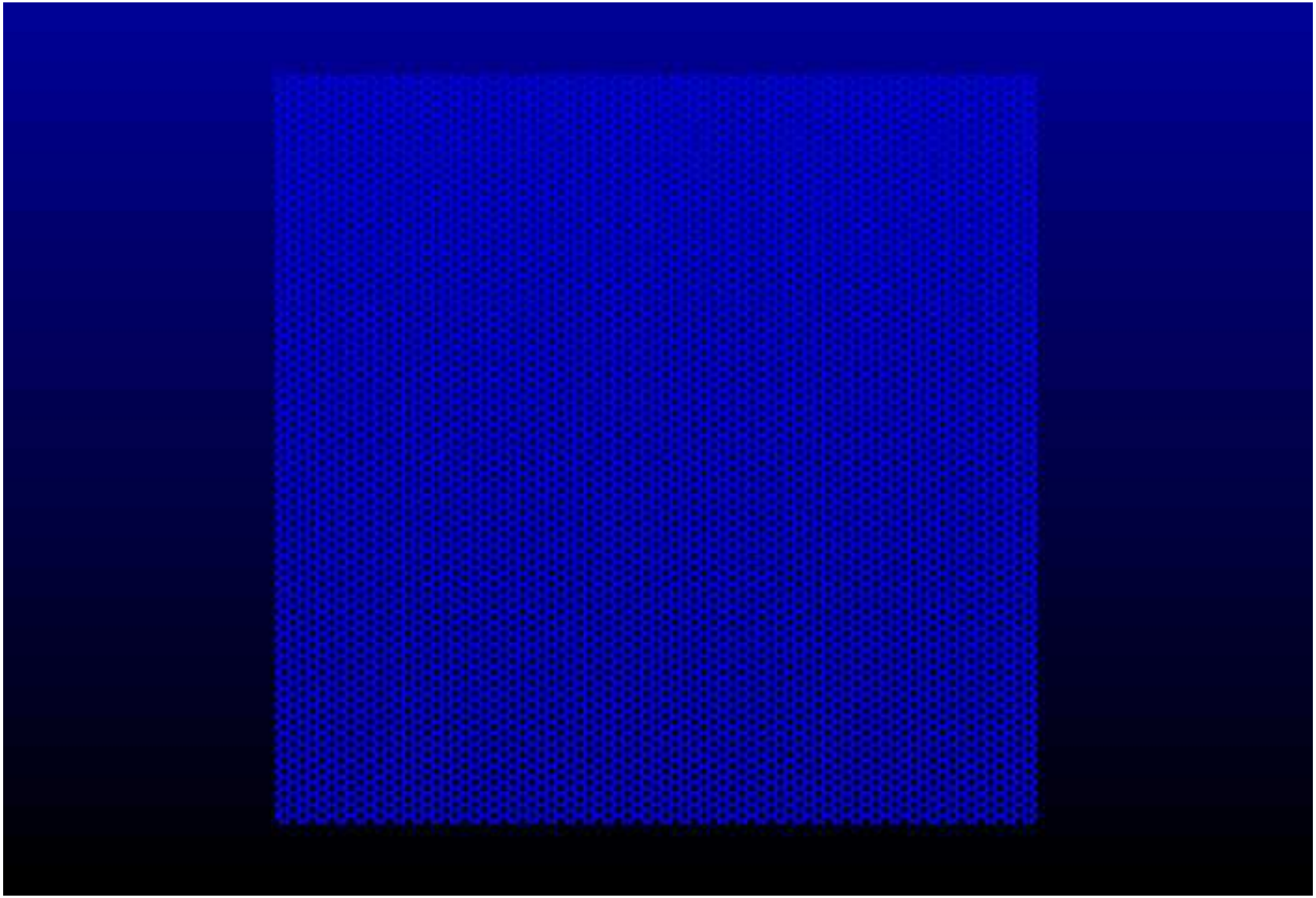
α partial dislocations have a higher mobility than β partial dislocations.

Perfect Dislocation Motion & Validation

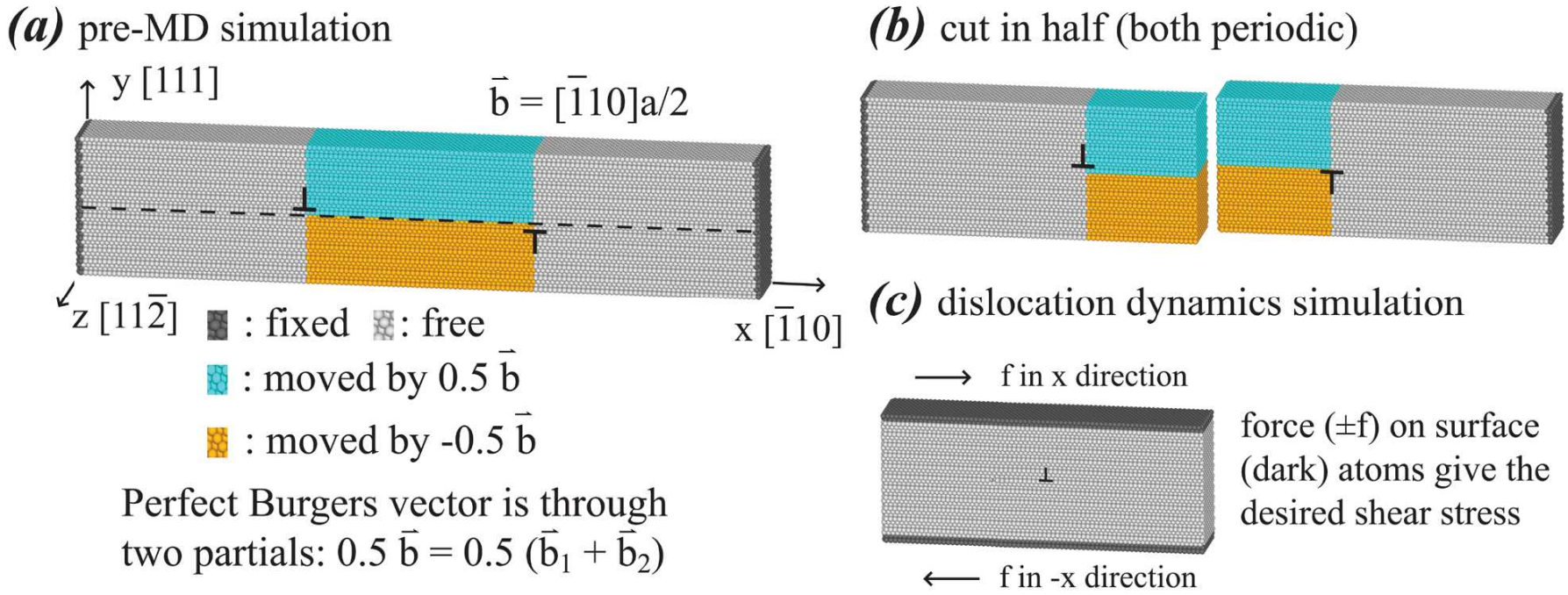


Simulations predict that α perfect dislocations have a higher mobility than β perfect dislocations, in agreement with semiconductor compound TEM experiments.

Perfect Dislocation Loop Dynamics



Edge Dislocation Dynamics Model

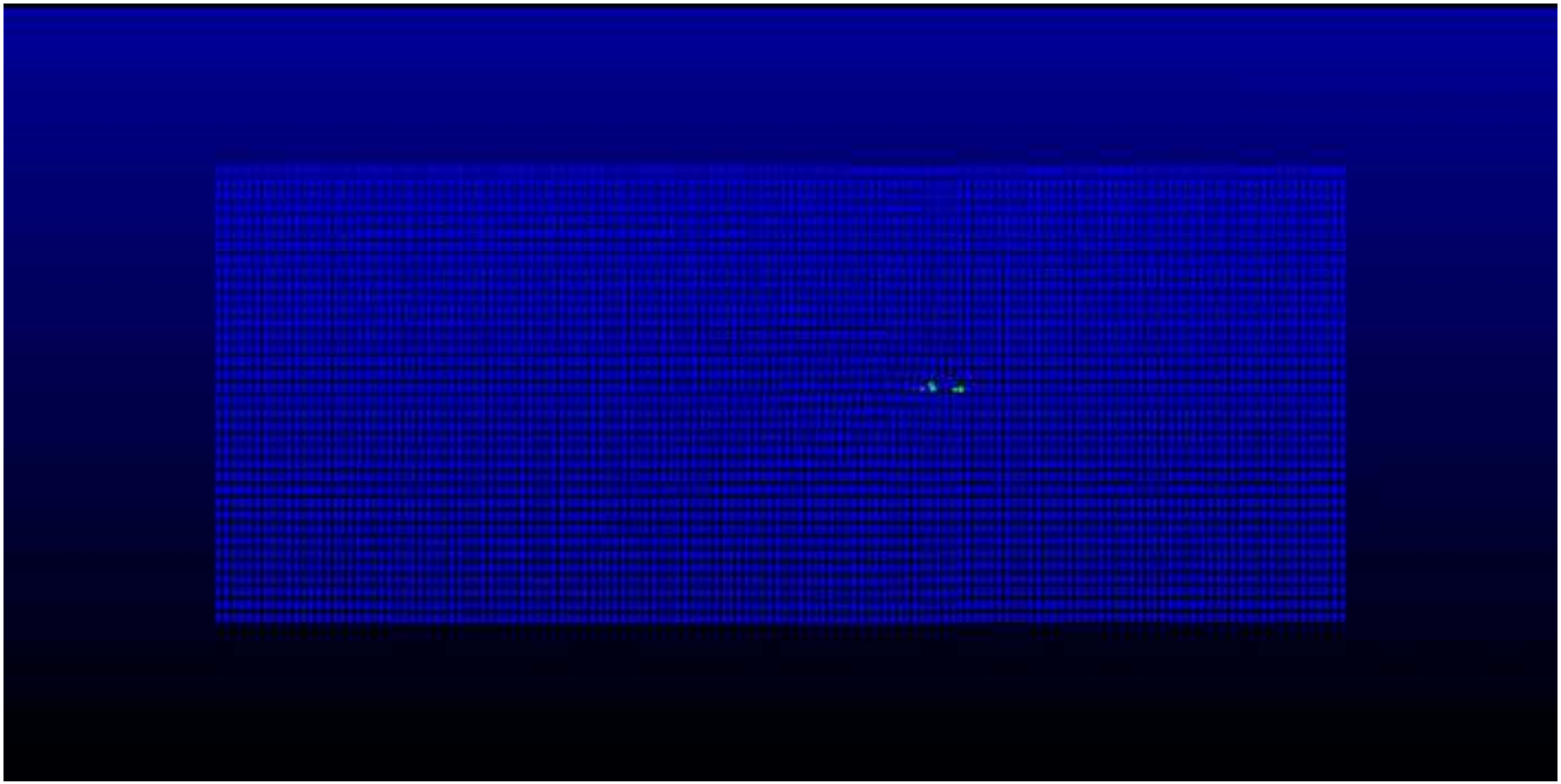


(a) the blue and orange regions are moved by positive and negative half Burgers vectors;

(b) the system is cut into two pieces containing α and β dislocations respectively;

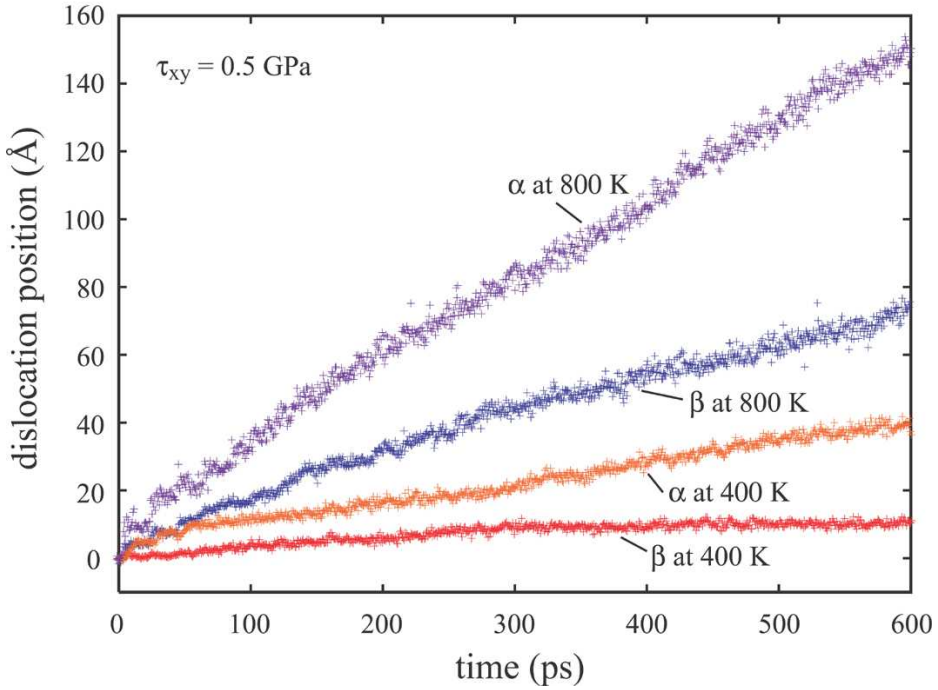
(c) dislocation motion is simulated by applying force to the top and bottom black regions.

Edge Dislocation Dynamics

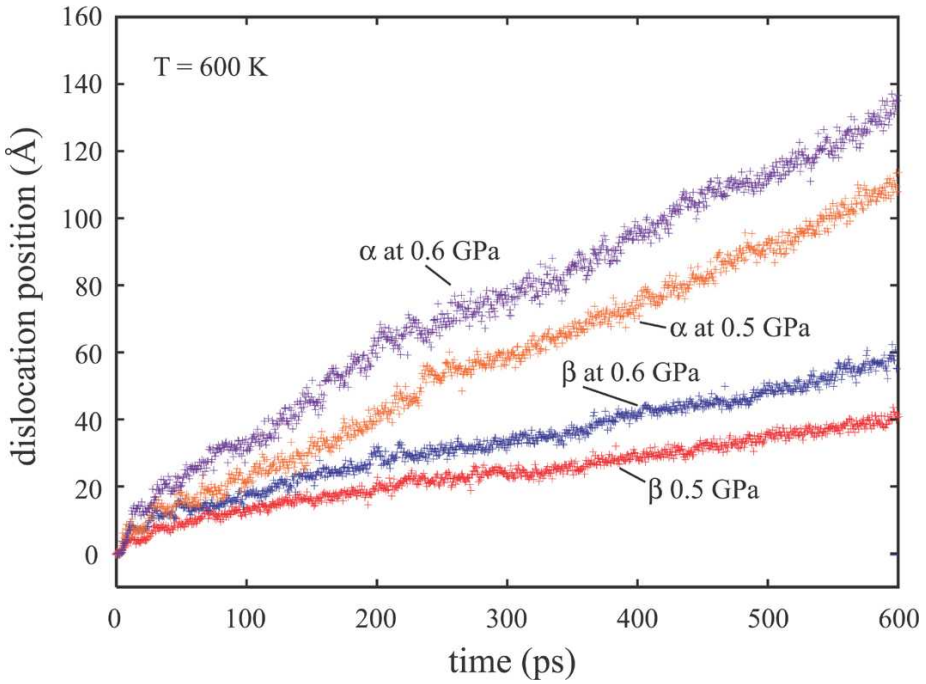


Edge Dislocation Dynamics Curves

(a) effect of temperature at a given stress

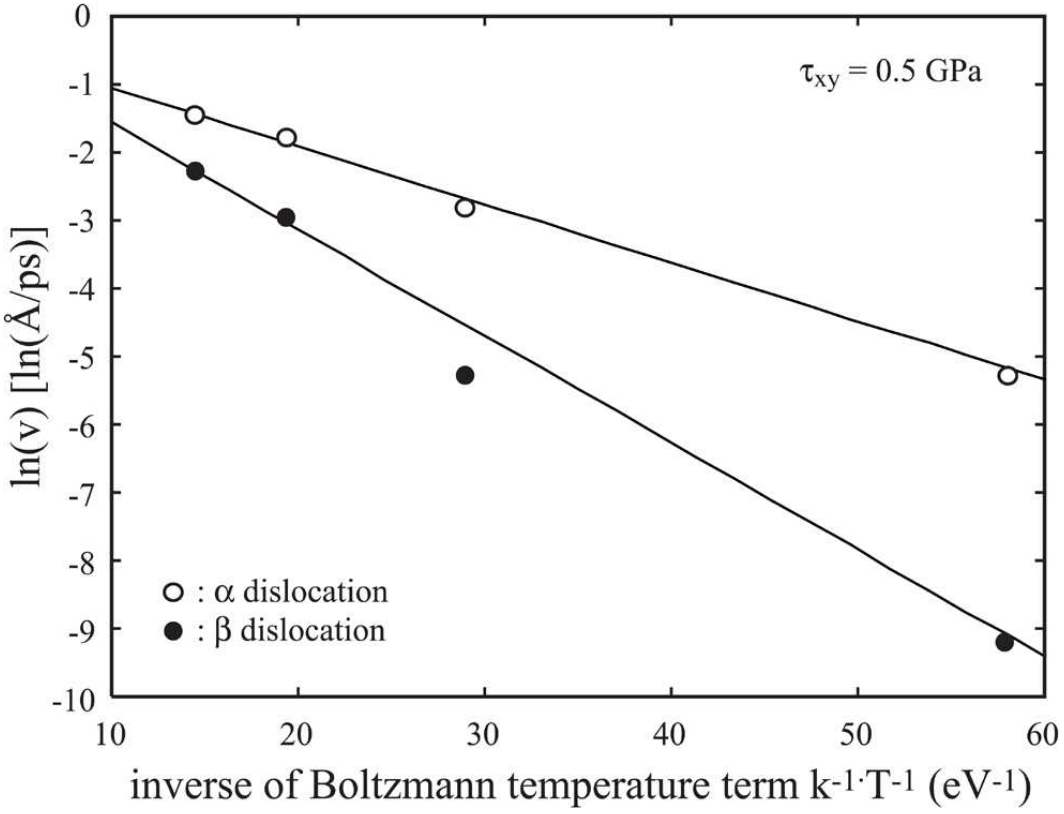


(b) effect of stress at a given temperature



Steady-state dislocation dynamics is achieved in all of our simulations.

Verification from Arrhenius Equation



$$v = v_0 \cdot \exp\left(-\frac{Q - \tau \cdot \Omega}{kT}\right)$$

1. Dislocation velocities at various T and t, as determined from MD, satisfy Arrhenius equation.
2. We found activation energies of 0.14 eV and 0.27 eV and activation volumes of 17 Å3 and 36 Å3, respectively for α and β glide edge dislocations.

Published BOP Potentials

GaAs

1. D. A. Murdick, X. W. Zhou, H. N. G. Wadley, D. Nguyen-Manh, R. Drautz, and D. G. Pettifor, Phys. Rev. B, 73, 045206 (2006).
2. D. A. Murdick, H. N. G. Wadley, and X. W. Zhou, Phys. Rev. B, 125318 (2007).

CdZnTe

1. D K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 85, 115206 (2012).
2. D. K. Ward, X. W. Zhou, B. M. Wong, F. P. Doty, and J. A. Zimmerman, Phys. Rev. B, 86, 245203 (2012).
3. X. W. Zhou, D. K. Ward, B. M. Wong, F. P. Doty, J. A. Zimmerman, G. N. Nielson, J. L. Cruz-Campa, V. P. Gupta, J. E. Granata, J. J. Chavez, and D. Zubia, Phys. Rev. B, 85, 245302 (2012).
4. 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).
5. X.W. Zhou, D. K. Ward, B. M. Wong, and F. P. Doty, Phys. Rev. Lett., 108, 245503 (2012).

Available in LAMMPS

Conclusions

1. BOP approaches DFT fidelity required for growth simulations;
2. BOP reproduces the experimental observation that α dislocations move much faster than β dislocations;
3. Core energies of 30+ dislocations have been derived for CdTe.
4. A robust method has been developed to calculate activation energy Q and activation volume Ω for dislocation motion. We found Q = 0.14 and 0.27 eV, and Ω = 17 and 36 $Å^3$ respectively for α and β edge types of glide dislocations;
5. Our method now enables large scale DD simulations of dislocation cell structures in CZT.