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Bond Order Potential Simulations of Dislocations in CdTe

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Introduction

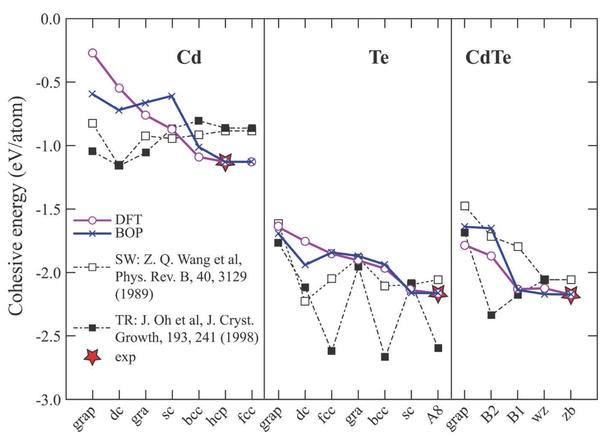
Efforts in the past 15+ years to minimize Te particles has not resulted in an anticipated improvement of the $Cd_{1-x}Zn_xT$ (CZT) crystals for γ-ray detection. Recent evidences suggest that an improvement is likely, but only when dislocation cell structures in CZT crystals are controlled. However, there are a large number (partial, perfect, edge, screw, α, β, shuffle, glide etc.) of combinations of dislocations in CZT, and it is experimentally expensive to optimize the overall dislocation cell structures with so many variables. Here we use a recently developed CZT bond order potential to perform molecular dynamics (MD) simulations to study configurations, energies, and mobilities of 30 different types of possible dislocations in CdTe (i.e., x = 1) crystals. This work is a first step towards understanding important dislocations and guiding experiments to further improve CZT crystals.

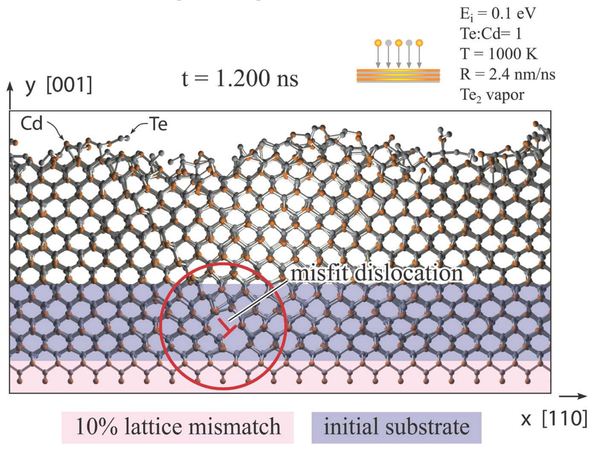
The Leading-Edge Bond Order Potential Approach

Bond order potential (BOP) [Pettifor et al, Phys. Rev. B, 65, 172103 (2002)] is analytically derived from quantum-mechanical theories, captures properties of a large number of phases, and predicts correctly crystalline growth during the most demanding chemical-vapor-deposition simulations (i.e., chemistries of vapor and crystal differ dramatically). None of other potentials are even close to meet these standards.

MD Verifications

Our Cd-Zn-Te BOP captures property trends of an impressive number of 70+ elemental and compound phases as compared with density-function-theory (DFT). As one example, calculated energies for selected phases, as shown in the left figure below, indicate that the BOP significantly improves over the literature Stillinger-Weber (SW) and Tersoff-Rockett (TR) potentials that do not even capture the lowest energies for the equilibrium phases (stars). BOP also successfully predicts the crystalline growth and misfit dislocation formation during MD simulations of CdTe/GaAs multilayer growth, as shown in the right figure below.



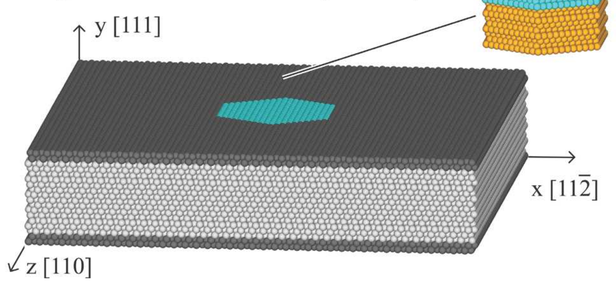


Dislocation Loop Model

(a) creation of dislocation loop

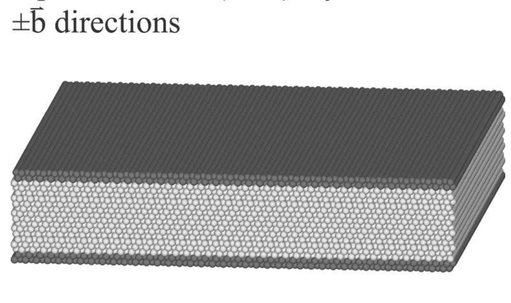
: free; top and : moved by 0.5 $\vec{b}$;
bottom and : moved by -0.5 $\vec{b}$;

Perfect Burgers vector is through two partials: $0.5\,\vec{b} = 0.5\,(\vec{b}_1 + \vec{b}_2)$



(b) evolution of dislocation loop

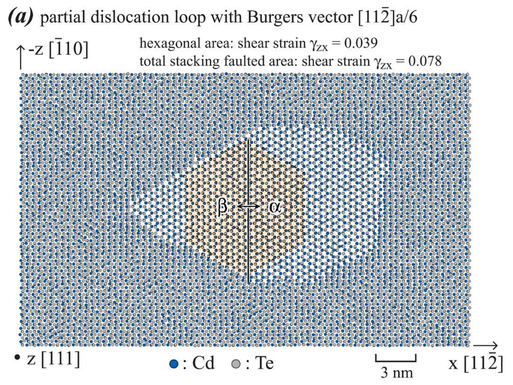
shear strain γ controlled by displacing top and bottom (dark) layers in the $\pm\vec{b}$ directions



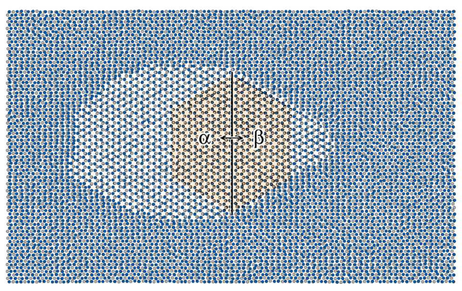
In figure (a) above, a dislocation loop is created by moving the top black and blue regions half of the Burgers vector, and the bottom black and orange regions a negative half of Burgers vector. In figure (b) above, the evolution of the dislocation loop is simulated by continuously moving the top and bottom black regions in the positive and negative Burgers vector directions respectively.

Experimental Validation

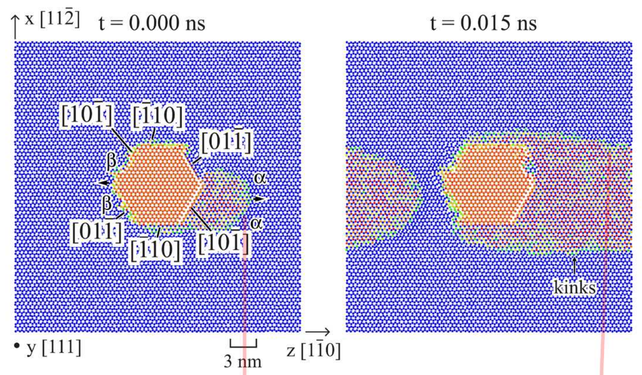
(a) partial dislocation loop with Burgers vector [11$\bar{2}$]a/6



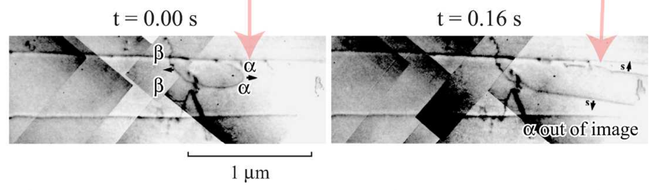
(b) same as (a) except that Cd and Te atoms are switched



(a) MD simulation on CdTe at strain rate ($\dot{\gamma}_{yz}$ = 0.338 ns^{-1})
Burgers vector [1$\bar{1}$0]a/2, temperature 900 K



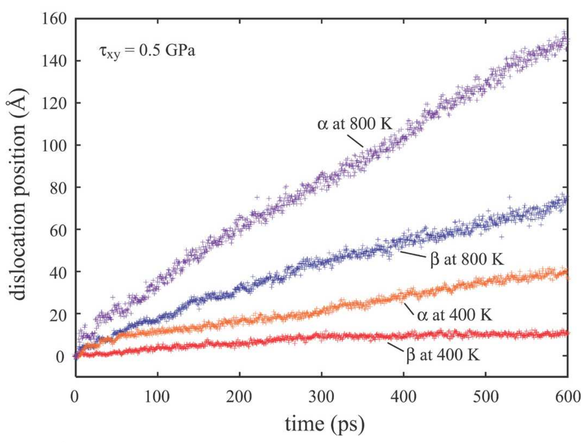
(b) in situ experiment on GaN at stress ~50 MPa
G. Vanderschaeve et al, J. Phys.: 12, 10093 (2000)



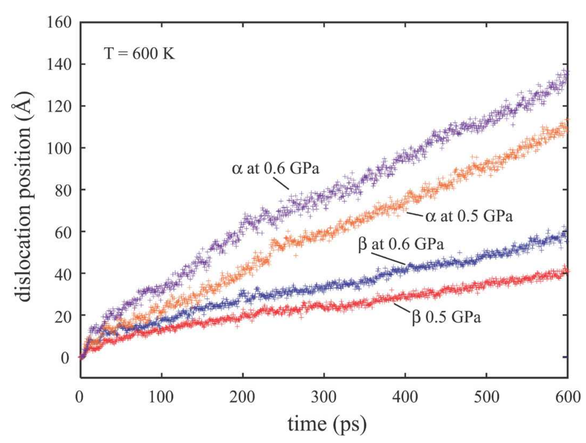
As shown in the left figure above for partial and the right figure above for perfect dislocations, BOP-based MD predicts more mobile α dislocations than β dislocations, in good agreement with experimental observations for semiconductor compounds [e.g., the right figure (b) above].

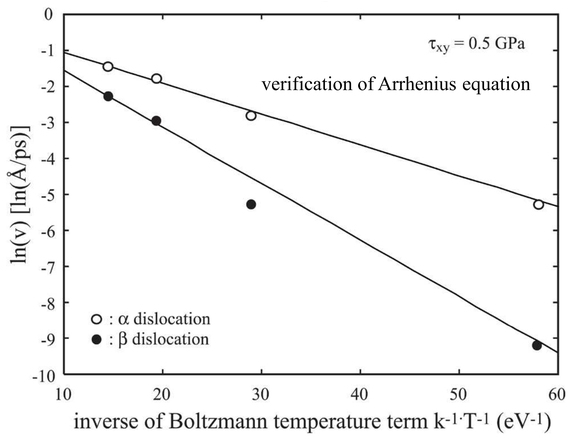
Quantification of Dislocation Mobility

(a) effect of temperature at a given stress



(b) effect of stress at a given temperature





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

In thermal activation regime, dislocation velocity ν at temperature T and stress τ follows the Arrhenius equation. Q: activation energy; Ω: activation volume; k: Boltzmann constant; and ν_0: a constant.

Dislocation velocities at various T and τ can be determined from BOP-based MD simulations, as shown in figures (a) and (b) above. This allows us to verify the Arrhenius equation (i.e., the thermally activated motion), and determine activation energies of 0.14 eV and 0.27 eV and activation volumes of 17 $Å^3$ and 36 $Å^3$, respectively for α and β glide dislocations.

Conclusions

Our work demonstrates the fidelity of the BOP. It reproduces the relative mobilities of α and β dislocations seen in experiments. It produces necessary inputs for large scale dislocation dynamics simulations to explore methods to control dislocation cell structures. In addition to edge dislocations that contribute to the cell structures by their climbing motion, our work also indicate the importance of screw dislocations in CZT because the motion of an α sector of a dislocation loop elongates the screw dislocation sectors.

Acknowledgements

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