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Dislocation Behavior in $Cd_{1-x}Zn_xTe$ Crystals

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Abstract—$Cd_{1-x}Zn_xTe$ (CZT) crystals are the leading semiconductors for radiation detection, but their properties are sensitive to dislocation network structures. To apply dislocation dynamics methods to simulate the evolution of dislocation network structures under the thermal mechanical conditions imposed during material synthesis, dislocation behavior such as their energies, mobilities, and their interaction with other defects must be understood and used as inputs. Here we use a state-of-the-art Cd-Zn-Te bond order potential to perform extensive molecular dynamics simulations to study configurations, energies, and mobilities of a variety of possible dislocations in $Cd_{1-x}Zn_xTe$ crystals. The activation free energies and activation volumes of thermally activated dislocation motion are also determined for the important dislocations discovered in the studies. Furthermore, our results are found to match the available experimental data very well. Due to the state-of-the-art nature of the bond order potential, and the stringent experimental validation, our results should reliably provide new insight into understanding important dislocations in the material, and guidance toward experimental efforts for improving dislocation network structures in CZT crystals.

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