Using Molecular Dynamics to study polycrystalline interfaces and grain boundaries in CdTe Heterostructures

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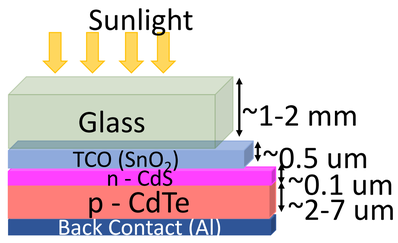
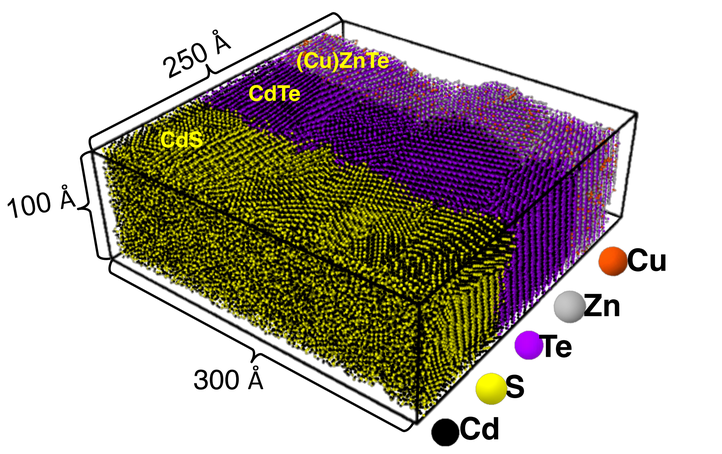
Motivation

- Defects such as interfaces and grain boundaries impact the efficiency of the CdTe solar cells [1].
- Studying the nature of these defects at the atomic scale is difficult using experiments.

Solar Panel [2]



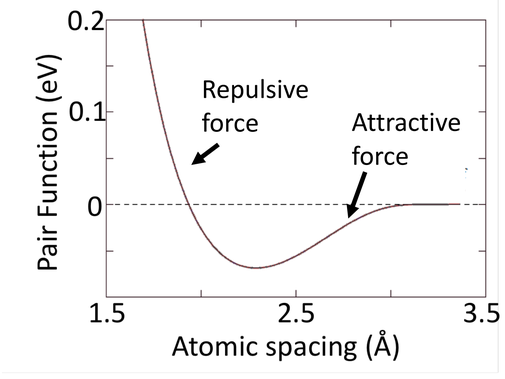
CdTe cell structure



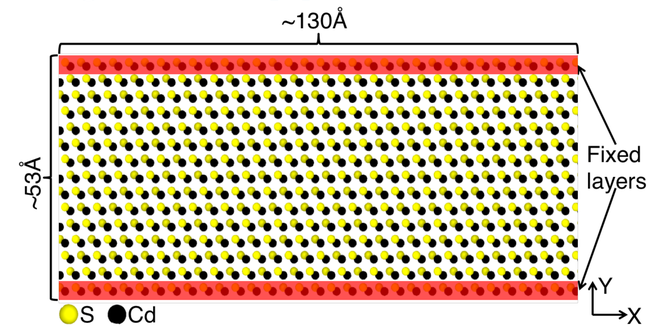
Atomistic simulation of polycrystalline CdTe/CdS interface

Methodology

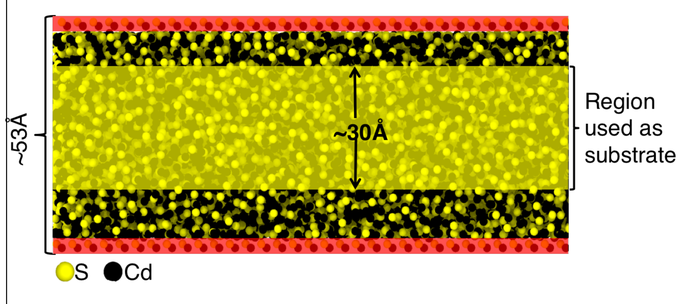
Classical Molecular Dynamics (MD) using LAMMPS [3]



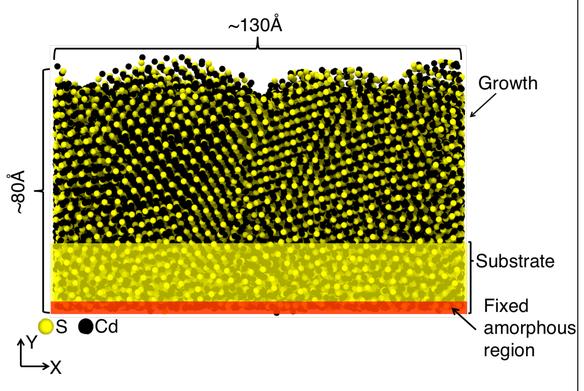
Stillinger-Weber Potential [4] is used for MD simulations



High temperature is applied in between the red regions of the single crystal CdS



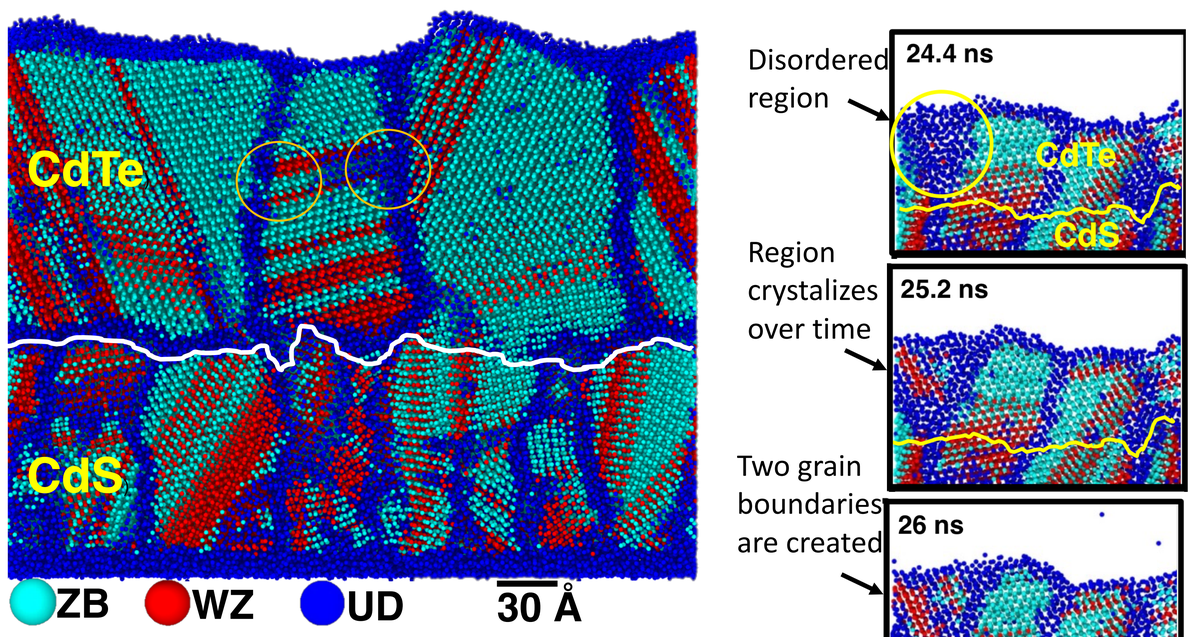
The region in yellow is then extracted and set as a substrate



Initial stages of polycrystalline CdS growth. Yellow region is fixed

Results

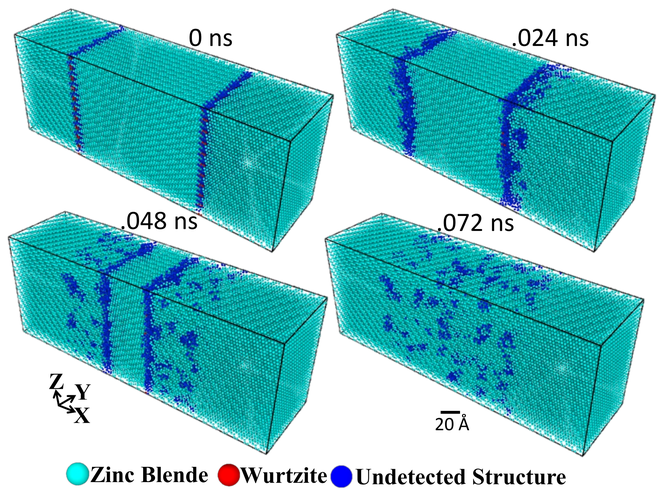
Polycrystalline growth and evolution of CdS/CdTe interface



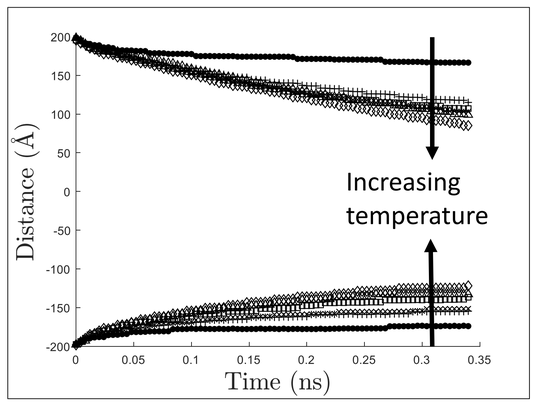
Structural visualization of the polycrystalline growth of CdTe/CdS interface (left). Evolution of the CdTe layer over time (right).

Results

CdTe Grain boundary mobility simulations

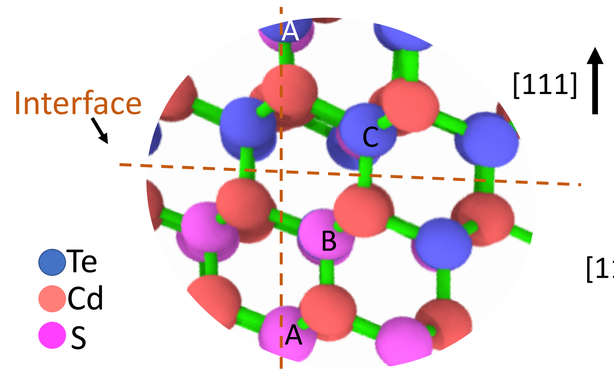


GB motion in CdTe bicrystals [5].

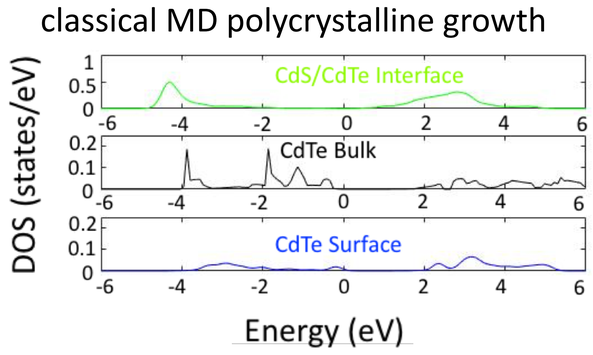


Distance vs time plots of Σ7 grain boundary motion at different temperatures.

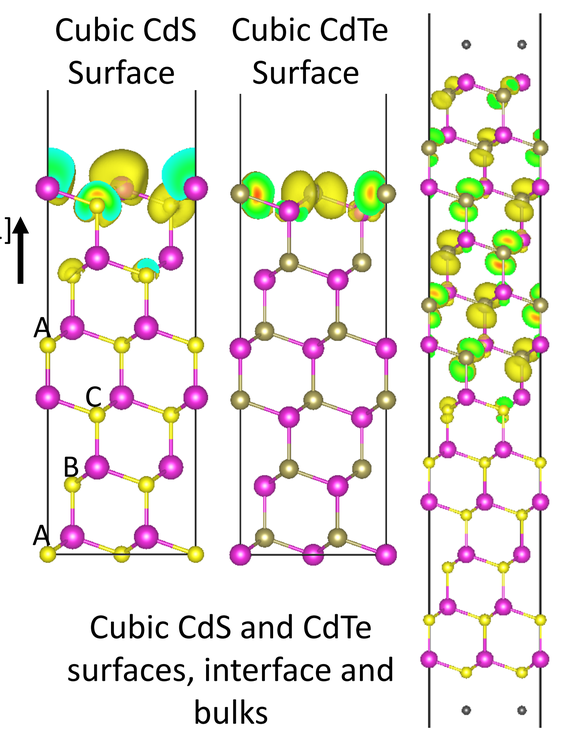
Preliminary Density Functional Theory calculations of grain boundaries and interfaces found on Molecular Dynamics simulations



New CdS/CdTe interface found in classical MD polycrystalline growth



CdS/CdTe interface



Cubic CdS and CdTe surfaces, interface and bulks

Conclusion

- Molecular dynamics can be used to simulate the growth of polycrystalline material at the atomic scale.
- Results show that the structures grown resemble experimental findings very closely.
- Analytical tools can be used to find properties such as grain boundary mobility and atom diffusivity.
- MD together with DFT is a powerful combination to study defects in polycrystalline material.

Acknowledgement

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References

[1] Yan, Y., et. al., Understanding of defect physics in polycrystalline photovoltaic materials. IEEE Photovoltaic Specialist Conference 37, 2011.
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