Mechanical Behavior of Strained Coherent and Semicoherent Layered Metal Halide Perovskites

Joshua Oxendine, Mechanical Engineering and Engineering Sciences
Dr. Xiang Chen, Mechanical Engineering and Engineering Sciences

UNIVERSITY OF NORTH CAROLINA CHARLOTTE

Introduction

- FAPbI3 is a promising photovoltaic material due to its nearly ideal band gap, but suffers from undesirable phase transformation
- MAPbBr3 is added to stabilize FAPbI3 in its photoactive alpha phase
- This addition introduces an interface, which is prone to fracturing under stress
- This project models the effects of strain on the mechanical properties of coherent and semi-coherent FAPbI3-MAPbBr3 bilayers

Method

Molecular dynamics software (LAMMPS) was used with the university's computing cluster to conduct simulations.

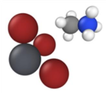

Figure 1: MAPbBr3 Unit Cell

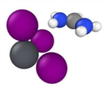

Figure 2: FAPbI3 Unit Cell

Figure 3: Coherent bilayer with Tension parallel to interface

- 50x50x64 unit cell models
- ~2 million atoms
- 5% vacancy concentration
- 2×10^{8} s^{-1} strain rate
- Visualization through Ovito

Results

Models with coherent and semi-coherent interfaces were tested by applying a tensile strain in the x-direction, then recording the resultant stress.

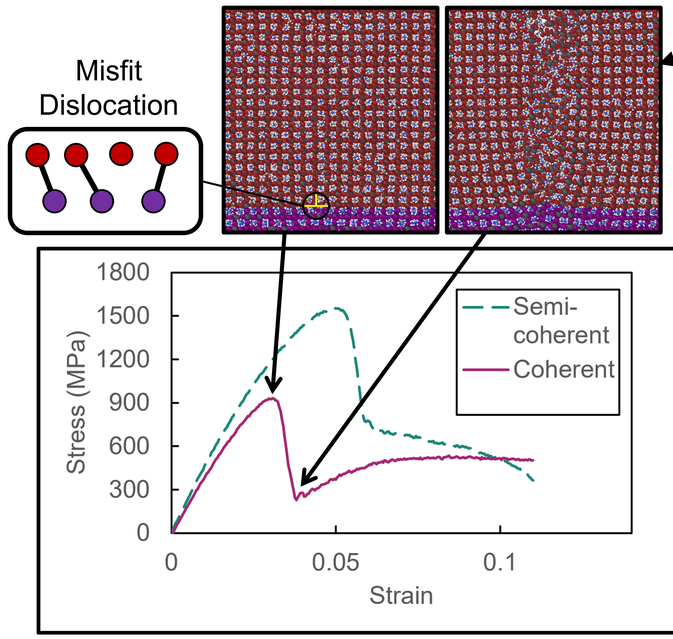

Figure 5: Stress-strain for coherent and semi-coherent interfaces. Fractures form along the misfit dislocation line immediately following peak stress.

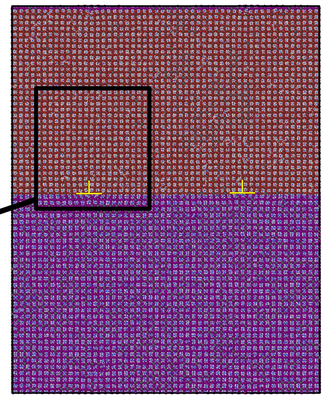

Figure 4: 50x50x32-52x52x32 FAPbI3-MAPbBr3 Bilayer

In both models, fracture occurred first within the MAPbBr3 section of the bilayer.

Due to the significant coherency stress, the coherent interface displayed a lower tolerance for applied strain.

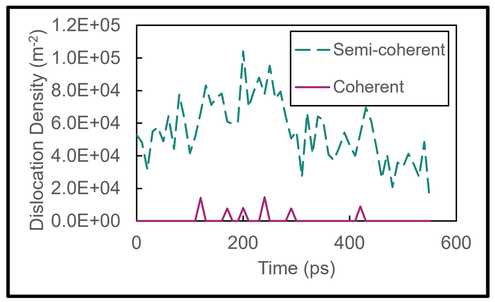

Figure 6: Dislocation density for each interface. Only dislocations located along misfit lines are detected. As a result, the dislocation density is near zero for the coherent model and significantly lower than expected for this material.

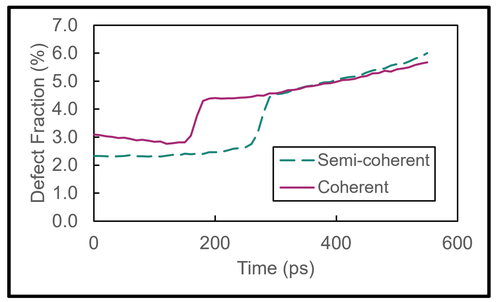

Figure 7: Defect fraction for each interface. Abrupt increases indicate fracture of the MAPbBr3 layer, indicating the point of failure for each model.

The coherency stress suffered by the interface resulted in a weaker interface than the semi-coherent interface with its stress concentrations caused by misfits.

Conclusions

- Forcing a coherent interface was shown to significantly decrease the tensile strength compared to semi-coherent and resulted in earlier fracture
- Due to the high strain rate of the simulation, observed tensile strengths are significantly higher than experimental values
- Limitations of OVITO's Dislocation Analysis (DXA) limited analysis of the material's dislocation behavior
- Additional simulations are required to better analyze dislocation behavior

Future Work

- Implement alternate atomic potentials, including machine learning potentials
- Model non-periodic boundaries to better reflect practical applications
- Observe phase transformations during deformation
- Conduct longer simulations at lower strain rates to better reflect realistic material behavior
- Utilize other visualization software to improve dislocation detection

Acknowledgements

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