Molecular Dynamics Study of CdSe as Buffer Layer in CdTe/CdS Solar Cell

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Abstract
Cadmium selenide is a II-IV semiconductor compound with properties that are ideal for photovoltaic applications. This project explores the use of CdSe as buffer layer in CdTe/CdS solar cells. A comprehensive study of CdSe was conducted using molecular dynamics simulations. The simulations consisted of the growth of CdSe by homoepitaxy (CdSe/CdSe) and heteroepitaxy (CdSe/CdS). The best growth conditions of CdSe were also used to deposit CdSeTe with varying selenium composition on a CdS substrate. The results show that CdSe has the lowest dislocation density.

Introduction

Over the past years, there has been a resurgence of interest in cadmium telluride (CdTe) based solar cells for their ideal material properties for photovoltaic applications and low manufacturing cost. CdTe/CdS solar cells have a maximum theoretical energy conversion efficiency of approximately 30%. However, this limit has never been achieved in practice due to issues related to the material system. One of them is the considerable strain at the interface between the two layers due to the difference in atomic spacing between the two materials.

Cadmium selenide was explored as a buffer layer to reduce the lattice mismatch between CdTe and CdS. The deposition of CdSe on a (001) substrate plane was simulated using the molecular dynamics method. This method also allows an evaluation of the defects in the film deposited.

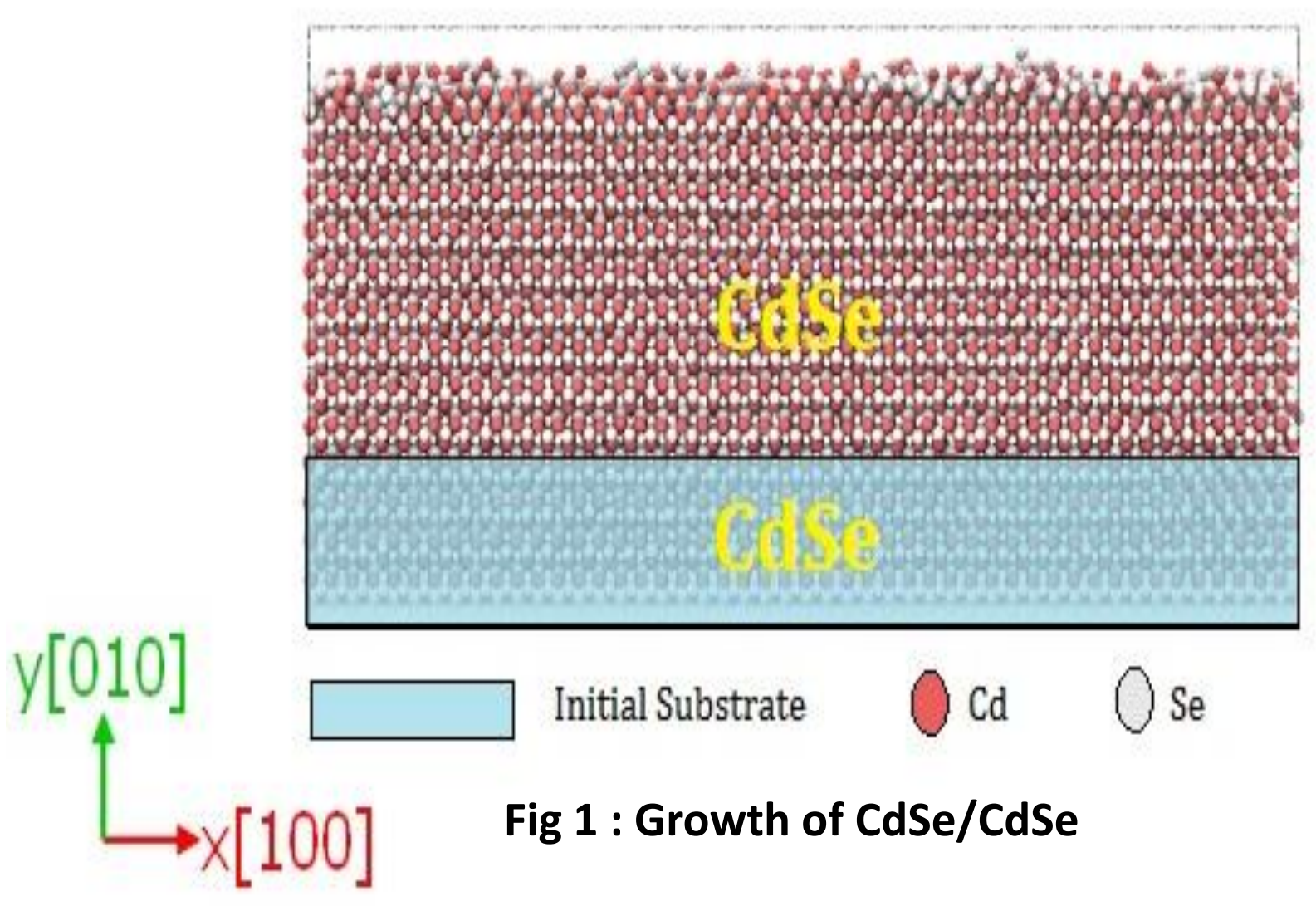
Molecular Dynamics Simulation

Molecular dynamics simulation (MD) is a computational method widely used in materials research. It allows scientists to simulate particle interaction in a system under various conditions over a defined period of time. This simulation was run using a bond order potential that models with high accuracy the interactions between chemical elements of group II and VI. It also serves to predict crystallographic defects in the structure of the film grown.

The MD simulation code used in this project is the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) which is a program designed to run on high performance computers. The LAMMPS allows to simulate large systems of particles.

Results

Homoepitaxial Growth



Conditions
T=1300K
Cd:Se= 1
R=~0.22nm/ns

Fig 1 : Growth of CdSe/CdSe

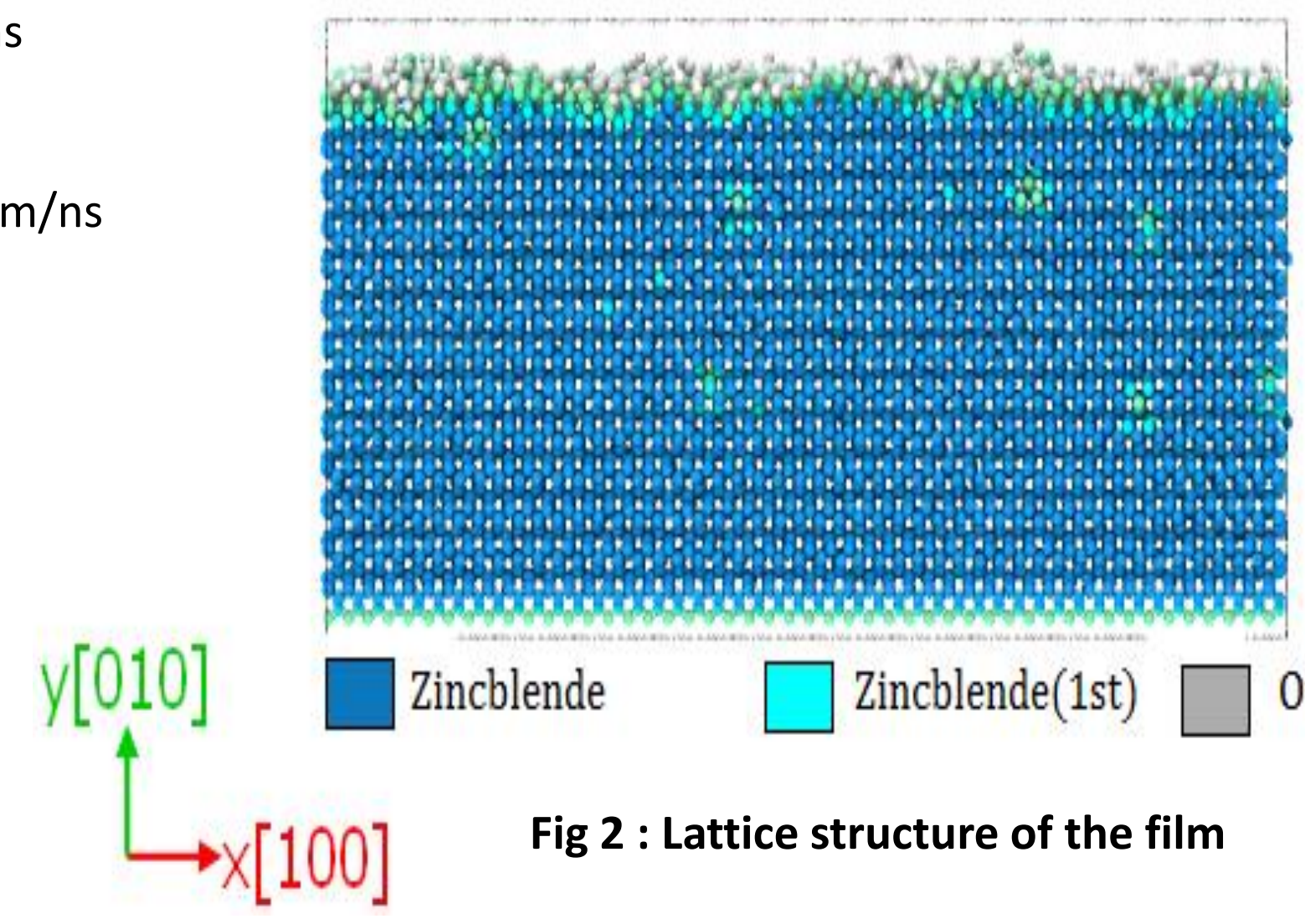
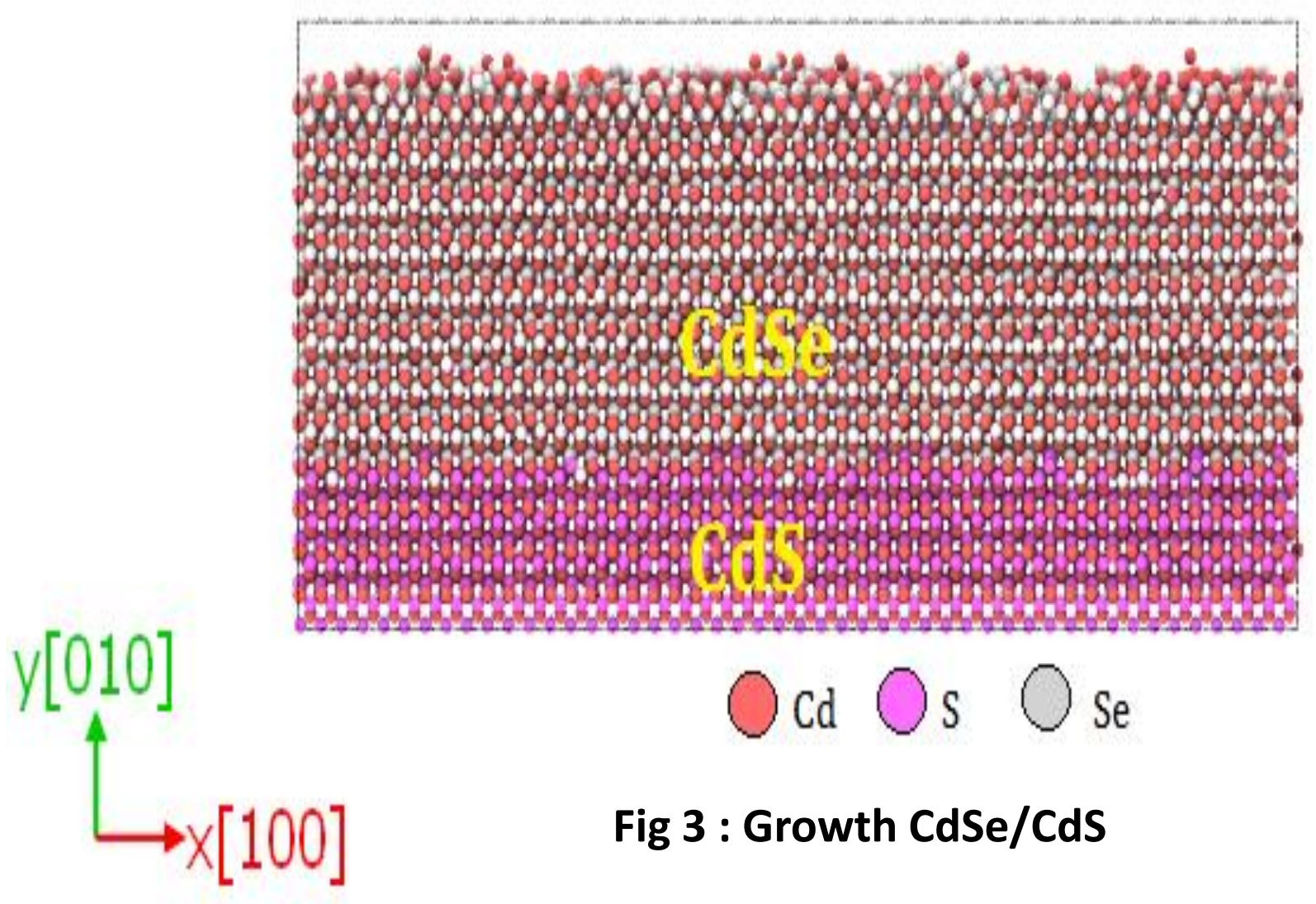


Fig 2 : Lattice structure of the film

Heteroepitaxial Growth



Conditions
T=1300K
Cd:Se= 1
Cd:S=1
R=~0.22nm/ns

Fig 3 : Growth CdSe/CdS

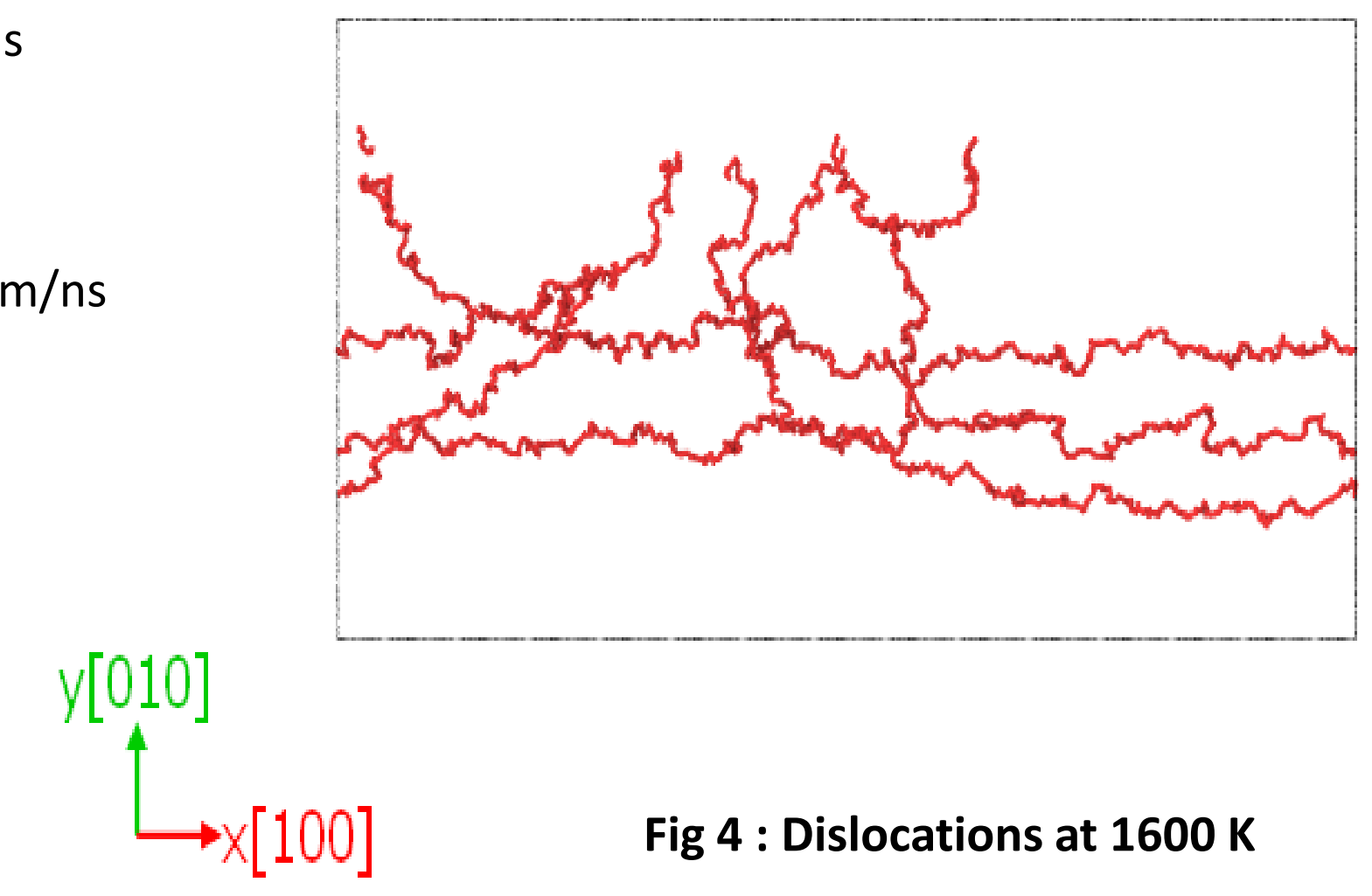
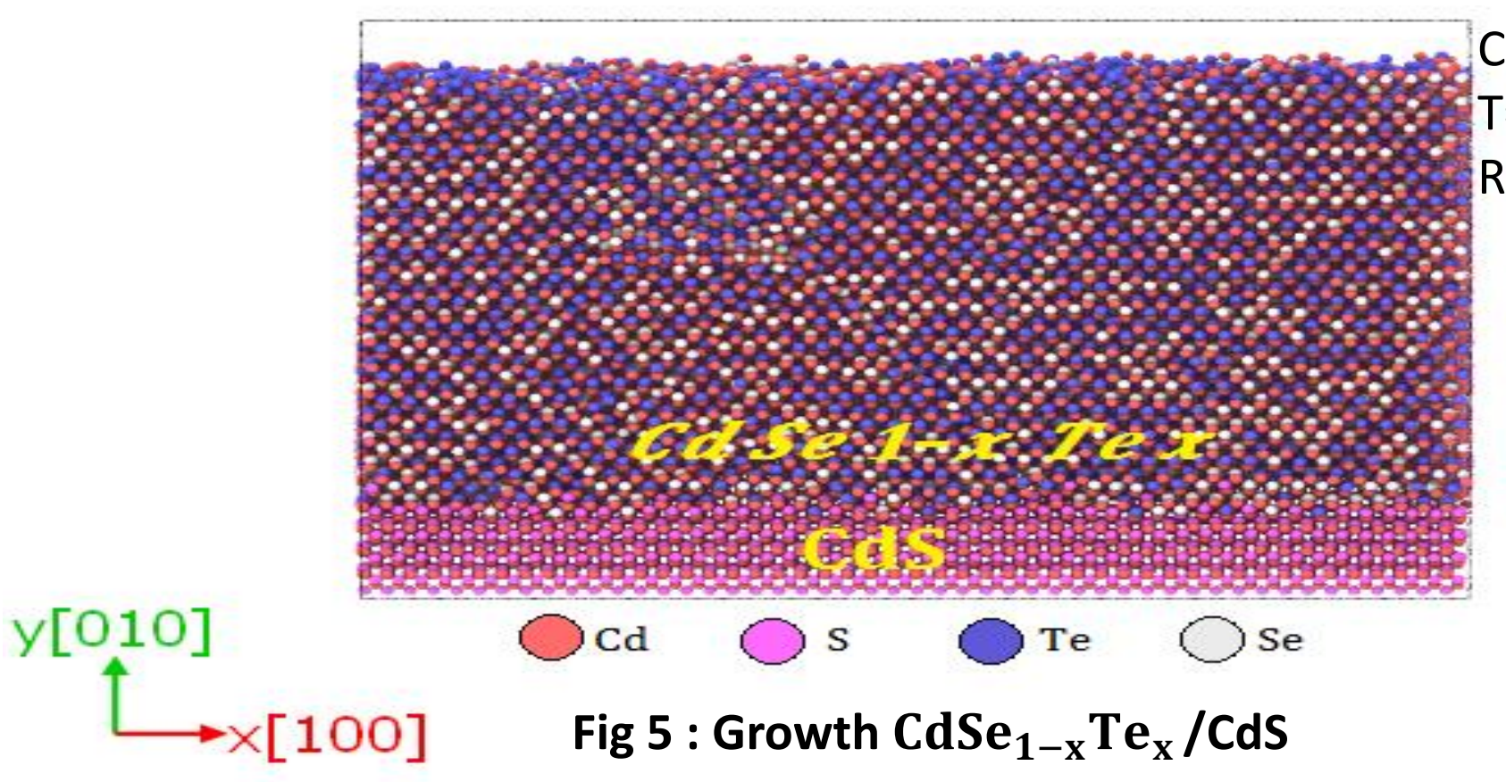


Fig 4 : Dislocations at 1600 K

Alloy $CdSe_{1-x}Te_x$ Growth



Conditions
T=1300K
R=~0.13nm/ns

Fig 5 : Growth $CdSe_{1-x}Te_x$ /CdS

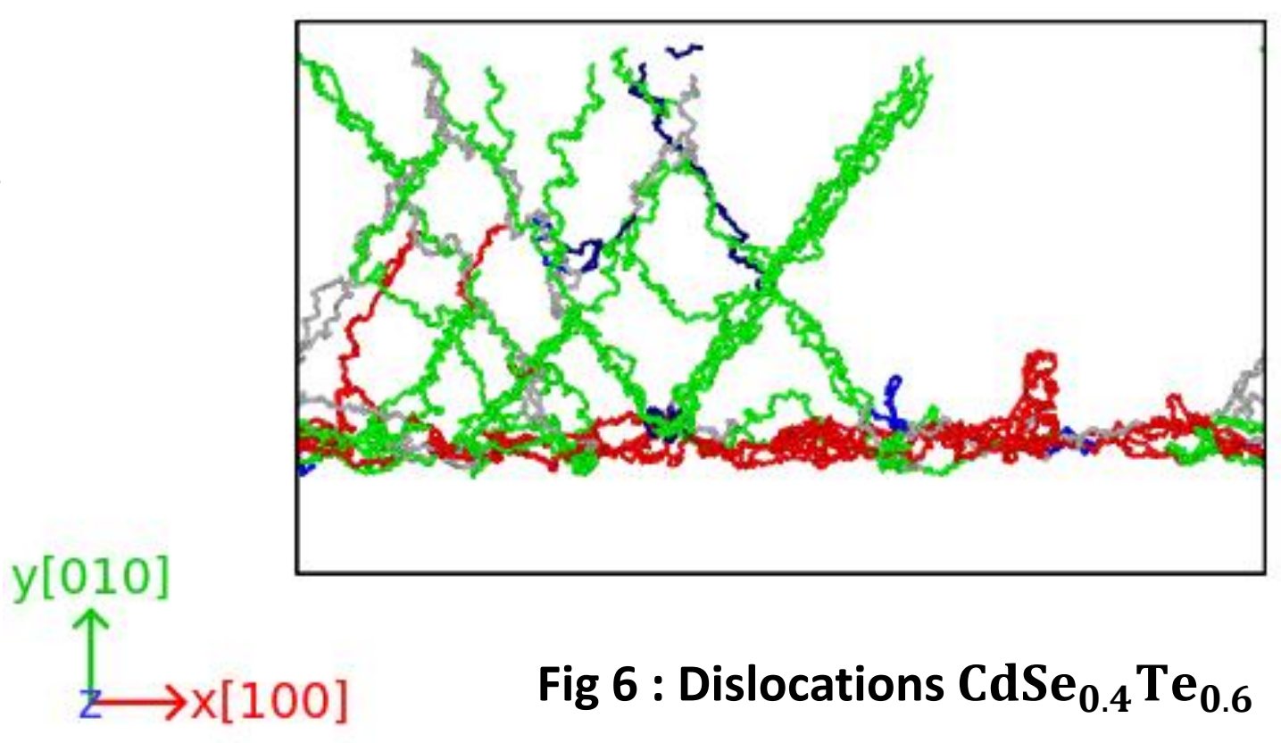


Fig 6 : Dislocations $CdSe_{0.4}Te_{0.6}$

Lattice Structure Analysis

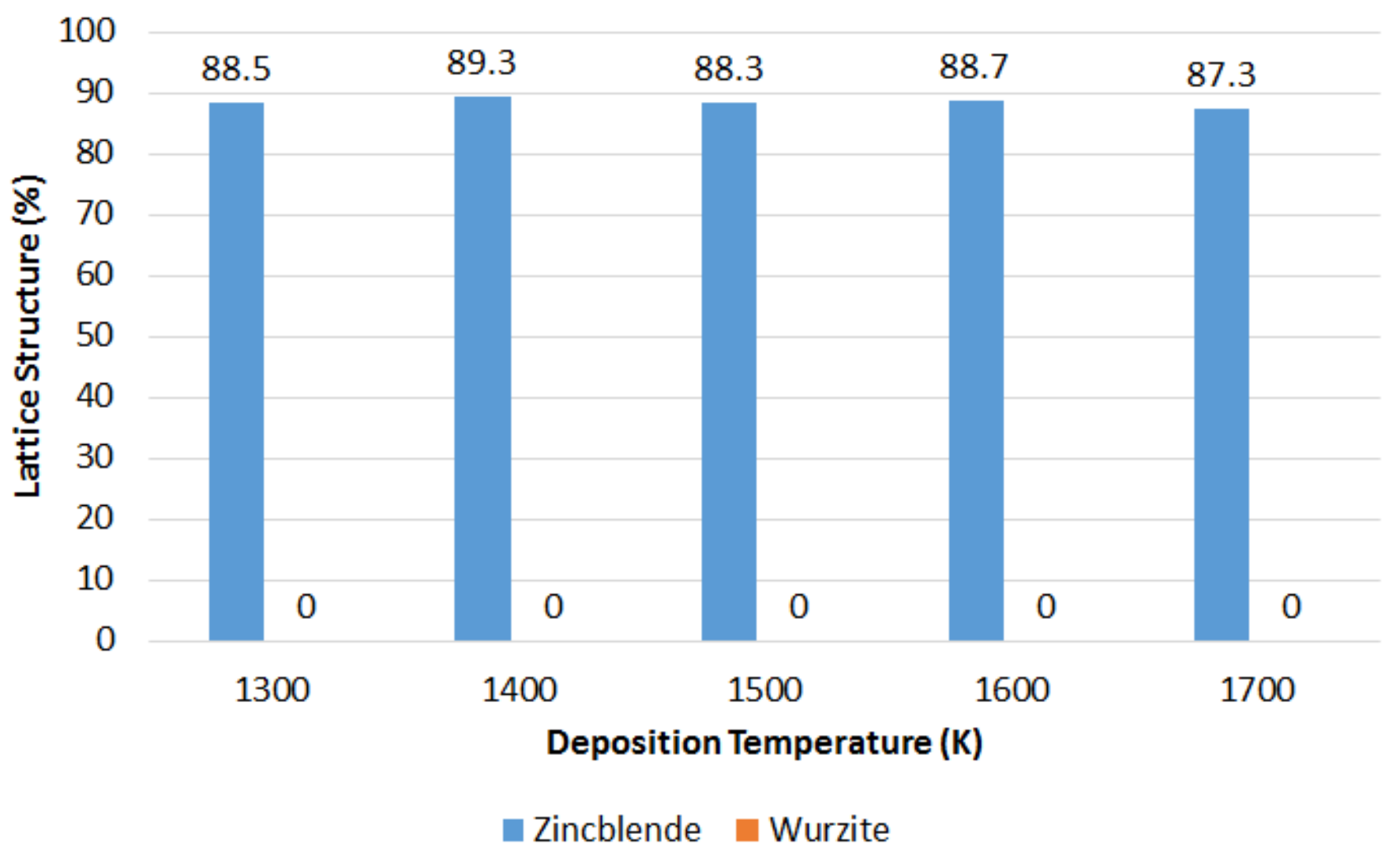


Fig: Plot of temperature versus lattice structure for CdSe/CdSe

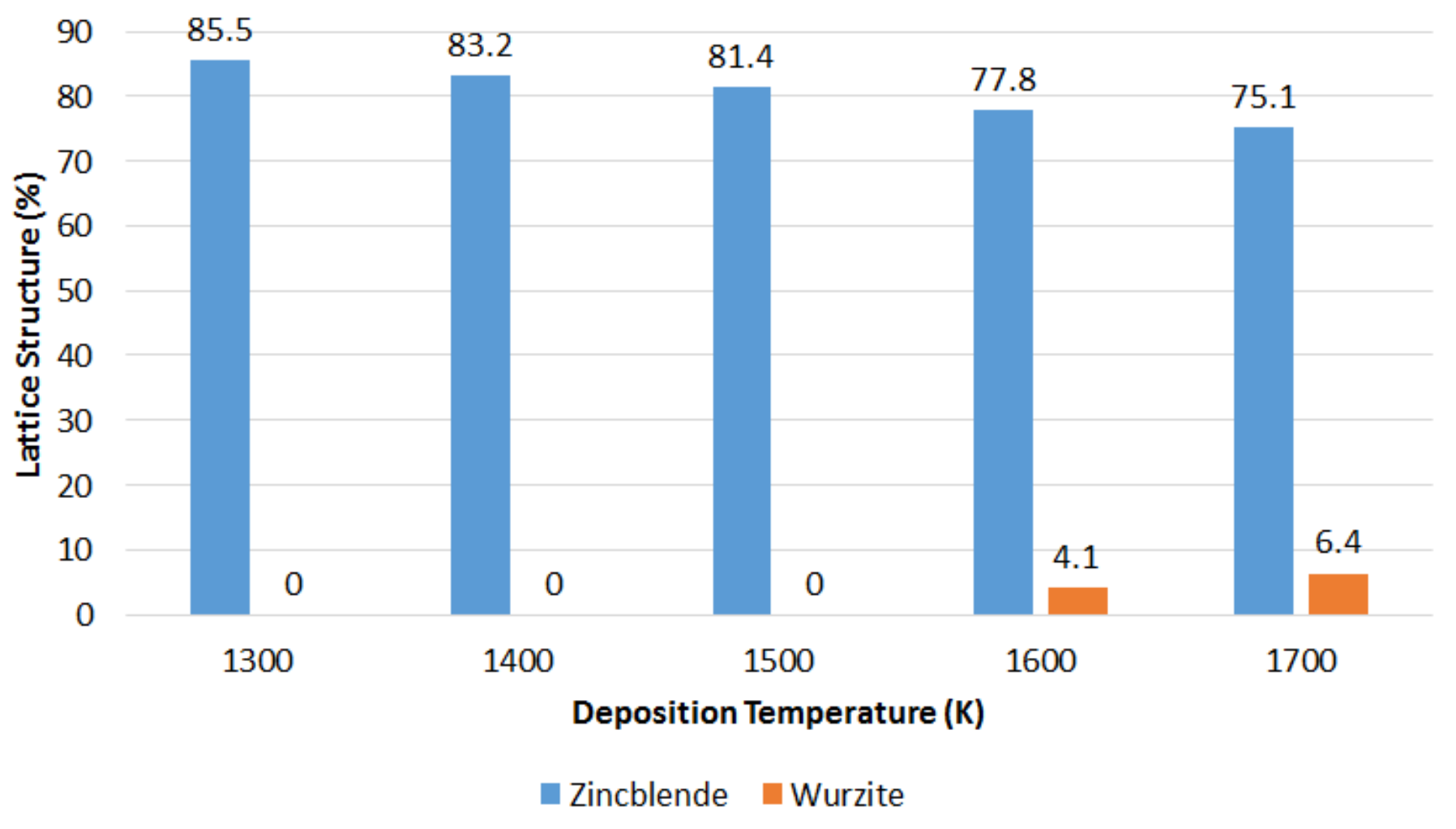


Fig: Plot of temperature versus lattice structure for CdSe/CdS

Defect Analysis

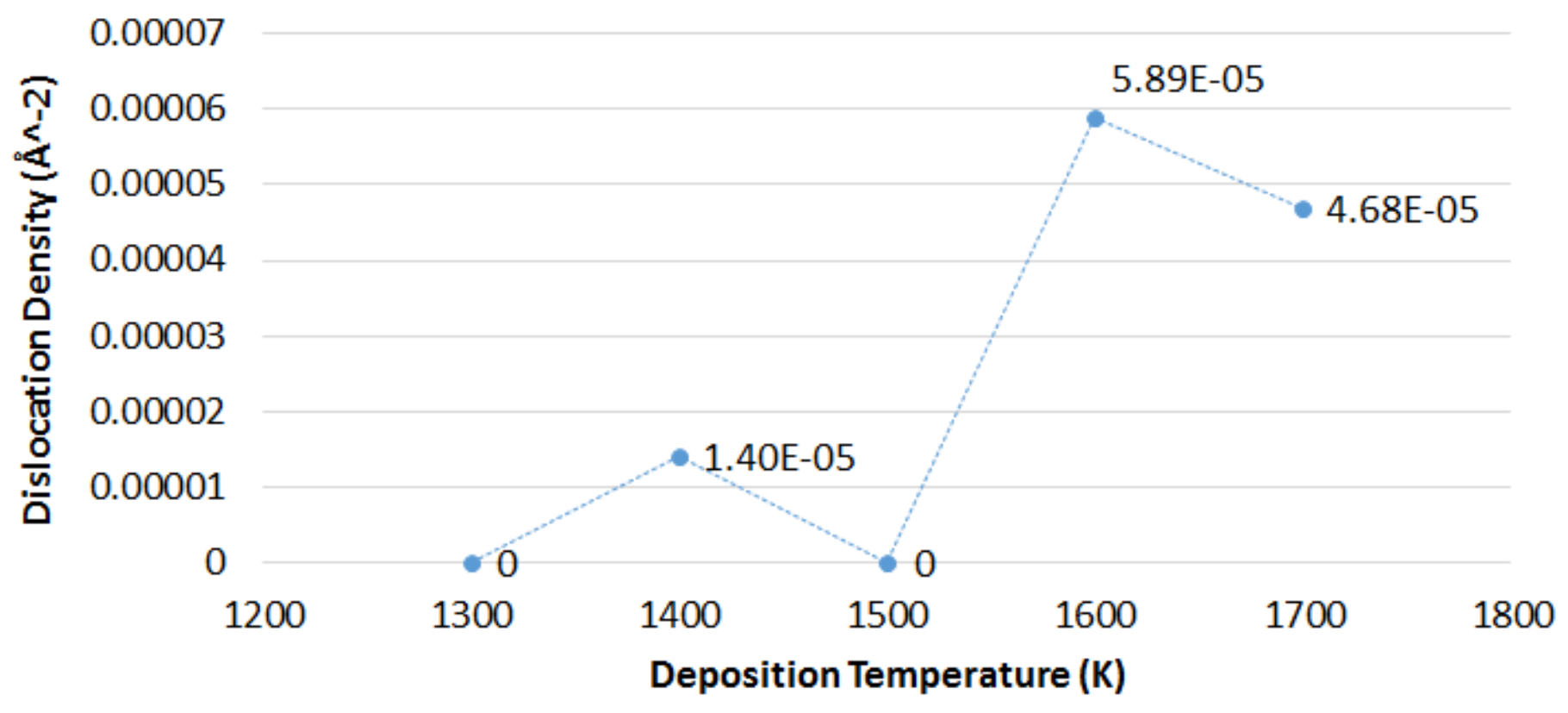


Fig: Plot of temperature versus dislocation density for CdSe/CdS

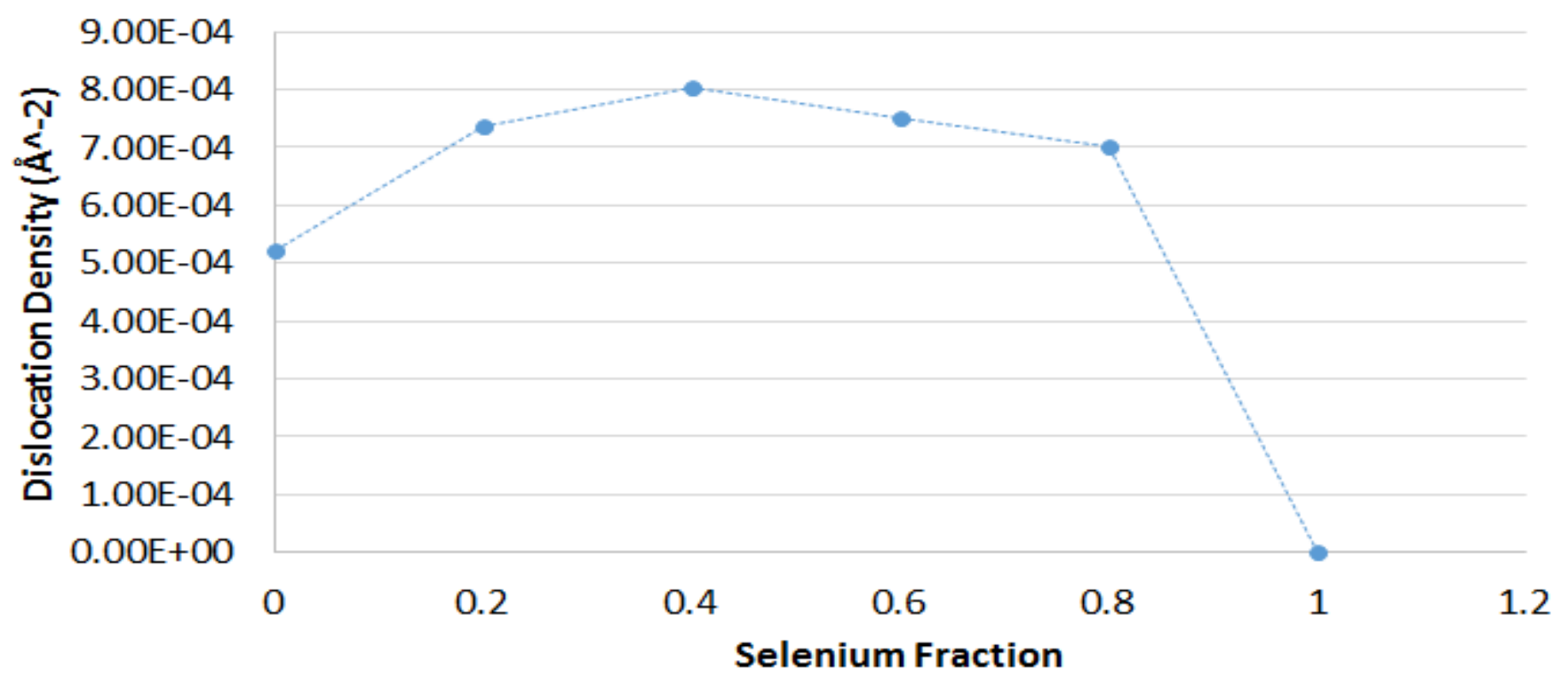


Fig: Plot of selenium fraction versus dislocation density for $CdSe_{1-x}Te_x$ /CdS

Conclusion

- Homoepitaxy
    - Crystal growth was achieved at all temperatures
    - Zinc blende crystal structure was found in all cases
    - Only point defects were found in all cases
- Heteroepitaxy
    - Single-crystal zinc blende at: 1300 K, 1400 K and 1500 K
    - Polytypism (zinc blende and wurtzite) at: 1600 K and 1700 K
    - Point defects observed in all cases – as expected
- Alloy
    - CdSe buffer layer has the lowest defect density
- Future work
    - Grow a cadmium telluride layer on top of CdSe/CdS

References

- W. Cai, J. Li, and S. Yip, "Molecular Dynamics", *Comprehensive Nuclear Materials,* Vol. 1, pp 249-265, 2012.
- X. Zhou, D. Ward, J. Martin, F. van Swol, J. Cruz-Campa, and D. Zubia, "Stillinger-Weber potential for the II-VI elements ZN-Cd-Hg-S-Se-Te", *Physical Review* B88, 085309 (2013).
- G. Brill, Y. Chen, P. Amirtharaj, W. Sarney, D. Chandler-Horowitz, and N. Dhar, "Molecular Beam Epitaxy Growth and Characterization of Cd-Based II-VI Wide-Bandgap Compounds on Si Substrates", *Journal of Electronic Materials*, Vol. 34, 2005.
- S. Plimpton, "Fast Parallel Algorithms for Short-Range Molecular Dynamics", *J Comp Phys*, 117, 1-19 (1995)

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