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Molecular Dynamics Study of Thin Film Growths in Lattice Mismatched Substrates

J. J. Chavez^I, D. Zubia^I, J.L. Cruz-Campa^{II}, G. Nielson^{II}, D.K. Ward^{III}, and X. W. Zhou^{III}

^IDepartment of Electrical and Computer Engineering, University of Texas at El Paso, El Paso TX 79902

^{II}Sandia National Laboratories, Albuquerque NM 87185, ^{III}Sandia National Laboratories, Livermore CA 94550

Abstract

Molecular dynamics simulations were employed to explore the effect in quality of deposition conditions during thin film epitaxy. Current results show that films grown on lattice mismatched substrates form misfit dislocations. Patterned substrate epitaxy suppressed misfit dislocation formation at lower deposition temperatures.

Introduction

Multilayered device fabrication is common in many areas such as photovoltaics and VLSI. The interlayer lattice mismatch strains the materials, creating undesired lattice defects such as dislocations. Nanoengineering techniques such as patterned growth can help suppress these defects and improve device performance.

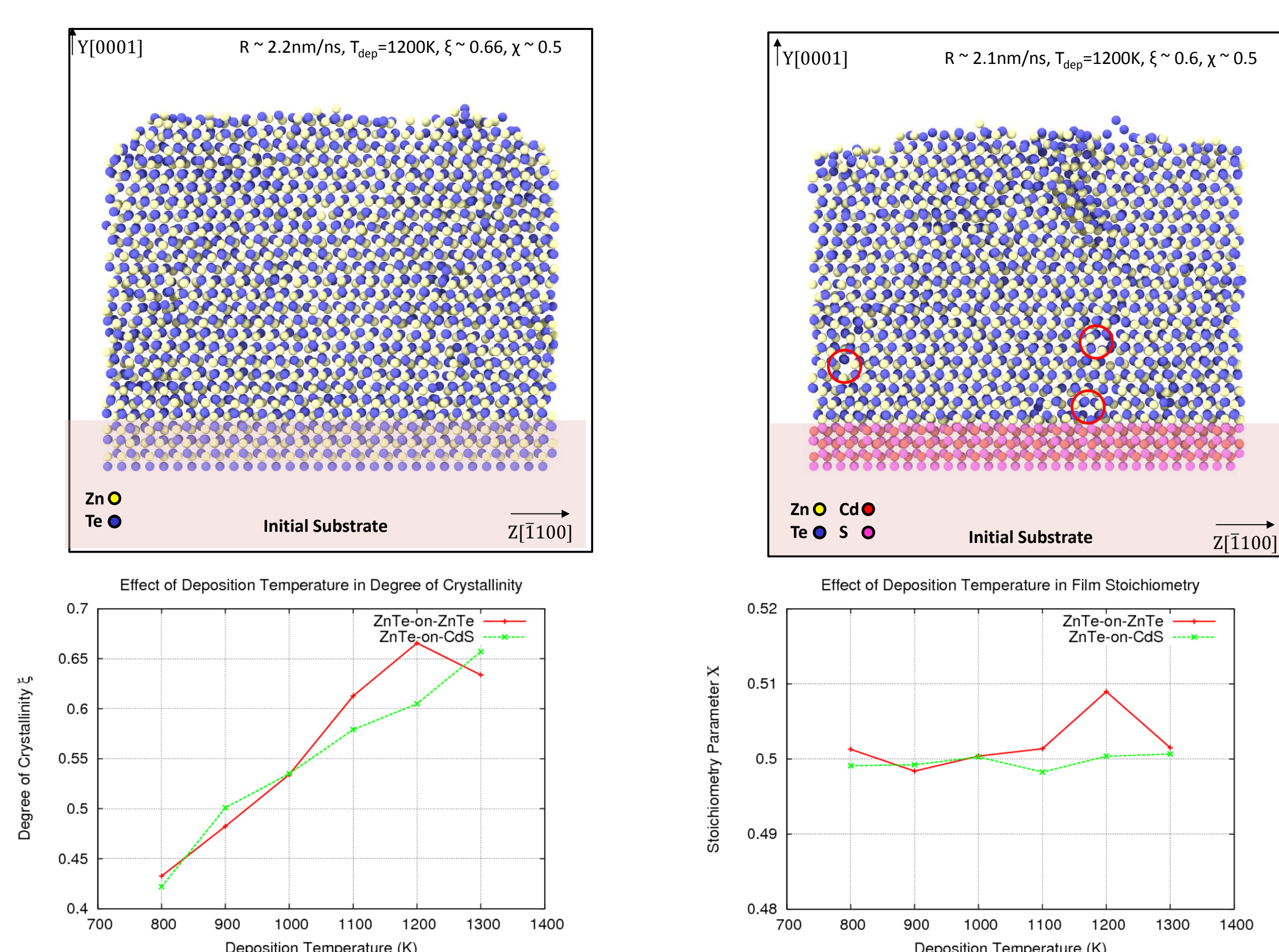
Methods

High fidelity simulations were achieved by employing a carefully parameterized Stillinger-Webber potential¹.

Defects caused by lattice mismatch were studied by comparing matched and mismatched substrate epitaxy. Lattice matched ZnTe homoepitaxy thin films were grown on (0001) substrates. Lattice mismatched ZnTe heteroepitaxy films were grown on CdS (0001) substrates. The effect of pattern growth was observed by comparing lattice matched and mismatched epitaxy on patterned substrates.

A wide range of deposition temperatures was used. Film quality was evaluated by the number dislocations observed and calculating crystallinity and stoichiometry.

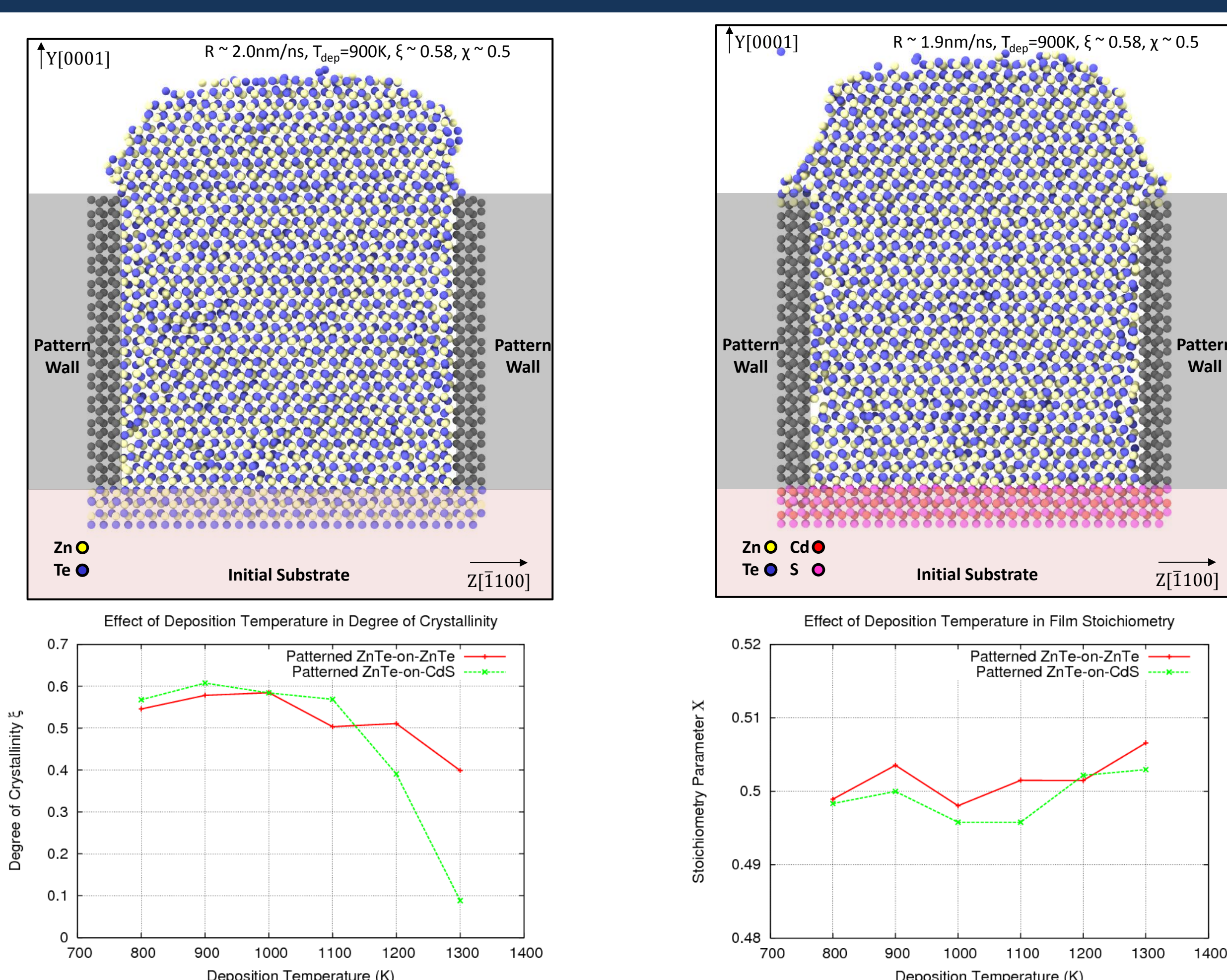
Results



Misfit dislocations were observed in lattice mismatched substrates. Film crystallinity increased with deposition temperature².

Conclusions

Molecular dynamics simulations allowed the study of thin film ZnTe epitaxy. Current results show that lattice mismatch caused misfit dislocations to form. Film crystallinity improves with increased deposition temperature during planar growths. Patterned substrate epitaxy suppressed misfit dislocation formation, but film crystallinity dropped at high deposition temperatures. Future work will consist of quantifying and comparing misfit dislocations in each case.



Pattern substrates helped suppressed dislocation formation. Film crystallinity dropped at high deposition temperatures².

References

- [1] X.W. Zhou, et al. Unpublished.
- [2] A. Stukowski. Visualization and analysis of atomistic simulation data with OVITO - the Open Visualization Tool Modelling Simul. Mater. Sci. Eng. 18 (2010), 015012. <<http://www.ovito.org/>>.