

## **Abstract**

The role of dislocation nucleation in comprehending material deformation behavior is crucial. The primary aim of this study is to explore dislocation nucleation as a fundamental process, transcending material-specific properties. To examine the various facets of the dislocation nucleation process, we have selected a diverse array of materials, including FCC, alloy steel, and BCC structures. The existing literature on dislocation physics lacks proper insight into the issues involved, and therefore, this study aims to highlight these pertinent aspects for the first time.

Advanced computational techniques, including transition-pathway search, molecular static and dynamic simulations, Monte Carlo simulations, and atomistically informed continuum models, are utilized to comprehensively investigate the fundamentals of dislocation nucleation. The LAMMPS molecular dynamics code is used for all atomistic computations presented in this study, while visualization and analysis of crystalline defects are facilitated by utilizing programs such as AtomsK and OVITO, along with dislocation extraction analyzers. Additionally, this dissertation incorporates in-house MATLAB codes to address specific mathematical aspects relevant to the research.

To begin our study, we focused on a simple FCC crystal to gain insights into the process of dislocation nucleation. Specifically, we explore the homogeneous nucleation of twinning dislocation loops in FCC metals by employing atomistic simulations. The main goal is to understand the mechanism and energetics associated with the formation of twinning dislocation loops, with a specific emphasis on the recently discovered alternate shear mechanism of twin nucleation. This study investigates the nucleation of twinning dislocation loops in FCC metals using atomistic computations and continuum modeling and highlights the importance of twinning partial loop nucleation and growth in FCC materials.

Having investigated the fundamental process of twinning loop nucleation in pure FCC metals, we divert our attention to a new approach of simulating complex alloys. The scope of application and reliability of classical molecular dynamics (MD) simulations depend upon the development of suitable interatomic interaction potentials, which is a major challenge for simulating complex materials like multi-component alloys. The second part examines the suitability of representative-atom approaches like the meta-

atom method for studying the elementary process of loop nucleation. The newly developed meta-atom scheme proposes to replace the elements with meta-atoms of a single variety. In this work, the meta-atom potential has been used to study the dislocation nucleation mechanisms and estimate the energy barriers for dislocation loop formation at various applied shear stresses for both Shockley and twinning dislocations. In particular, we examine the effect of spatial compositional fluctuation on the nucleation mechanism in a complex alloy.

So far, the studies described above have focused on the energetics associated with the mechanisms of nucleation. However, the whole process of nucleation involves the effects of temperature, loading rate, and activation parameters thereby dictating the kinetics of the process. In the third part of our study, we perform statistical analysis of compressive and tensile deformation in BCC Fe nanopillars, obtaining a comprehensive view of the fundamental kinetics of dislocation nucleation and its activation parameters. The BCC systems provide for an interesting case study on account of the tension-compression asymmetry reported in various studies. This study critically examines the existing assumptions regarding the widely employed statistical method of calculating the activation volume and explains the reasons behind exceptionally small activation volumes reported in various experimental and simulation studies. These findings not only challenge existing assumptions but also emphasize the critical significance of adopting a more comprehensive and accurate approach to studying dislocation nucleation.

This work makes a significant contribution to the field of dislocation nucleation, greatly enhancing our understanding of material properties and plastic deformation. The research conducted in this thesis lays a solid foundation for further exploration and extension of studies in these areas.

**Keywords:** Atomistic simulations; Dislocation loop; Nucleation; Deformation twinning; Nudged elastic band; TWIP steel; Meta-atom potential; activation volume; BCC; Fe-nanopillars; Statistical analysis.