20th European Mechanics of Materials Conference - EMMC20
Florence, Italy | May 27th-29th, 2026
www.emmc20.unifi.it

Atomistic Investigation of Zr/Nb Interfacial Structure and Energy: From Coherent to Semicoherent Interfaces

Houssam Kharouji[1], Emmanuel Clouet[2], Benoît Appolaire[3], Maeva Cottura[4]

[1] Université de Lorraine, CNRS, IJL, Nancy F-54000, France. houssam.kharouji@univ-lorraine.fr
[2] CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France, France. emmanuel.clouet@cea.fr
[3] Université de Lorraine, IJL, Nancy F-54000, France. benoit.appolaire@univ-lorraine.fr
[4] Université de Lorraine, CNRS, IJL, Nancy F-54000, France. maeva.cottura@univ-lorraine.fr

Paper ID: 504
Symposium S17: Advanced modelling techniques: Mechanics of interfaces and phase transformations

Abstract

Heterophase interfaces play a key role in controlling the mechanical, chemical, and thermodynamic properties of materials. For example, the formation of nano precipitates within a crystalline matrix creates interphase boundaries whose atomic structure and degree of coherency directly influence mechanical properties such as stiffness and strength. In addition, interfacial energy contributes to the thermodynamic barrier for precipitate nucleation and plays a significant role in the kinetics of precipitate growth and coarsening. A fundamental understanding of interface structure and energetics is therefore essential for predicting microstructural evolution. In this work, we investigate the atomic structure and interfacial energy of β-Nb precipitates with a body-centered cubic structure embedded in an α-Zr hexagonal close-packed matrix using atomistic simulations. Both molecular statics simulations based on empirical interatomic potential and ab initio calculations within density functional theory (DFT) framework are employed to provide an accurate description of the optimized interface structures and energies. The study focuses on the Pitsch–Schrader orientation relationship, which has been experimentally observed for β-Nb precipitates formed under irradiation in α-Zr matrix. Infinite coherent interfaces with different orientations, characterized by a significant lattice mismatch between the Nb precipitates and the Zr matrix are first considered. The elastic strain resulting from this mismatch is then relaxed through the introduction of misfit dislocation networks. Molecular

statics simulations are used to determine relaxed atomic configurations and interfacial energies, and to quantify the dependence of interfacial energy over a wide range of lattice misfit. For selected interfaces, the results are then compared with those obtained from DFT calculations to assess the reliability of the empirical interatomic potential.

Keywords:

Interfaces Coherent Semi coherent Atomistic simulations Interfacial energy Misfit dislocation