Fundamental Understanding of Ambient and High-Temperature Plasticity Phenomena in Structural Materials in Advanced Reactors

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Abstract

The goal of this research project is to develop the methods and tools necessary to link unit processes analyzed using atomistic simulations involving interaction of vacancies and interstitials with dislocations, as well as dislocation mediation at sessile junctions and interfaces as affected by radiation, with cooperative influence on higher-length scale behavior of polycrystals. These tools and methods are necessary to design and enhance radiation-induced damage-tolerant alloys. The project will achieve this goal by applying atomistic simulations to characterize unit processes of:

- Dislocation nucleation, absorption, and desorption at interfaces
- Vacancy production, radiation-induced segregation of substitutional Cr at defect clusters (point defect sinks) in BCC Fe-Cr ferritic/martensitic steels
- Investigation of interaction of interstitials and vacancies with impurities (V, Nb, Ta, Mo, W, Al, Si, P, S)
- Time evolution of swelling (cluster growth) phenomena of irradiated materials
- Energetics and kinetics of dislocation bypass of defects formed by interstitial clustering and formation of prismatic loops, informing statistical models of continuum character with regard to processes of dislocation glide, vacancy agglomeration and swelling, climb and cross slip

This project will consider the Fe, Fe-C, and Fe-Cr ferritic/martensitic material system, accounting for magnetism by choosing appropriate interatomic potentials and validating with first principles calculations. For these alloys, the rate of swelling and creep enhancement is considerably lower than that of face-centered cubic (FCC) alloys and of austenitic Fe-Cr-Mo alloys. The team will confirm mechanisms, validate simulations at various time and length scales, and improve the veracity of computational models. The proposed research's feasibility is supported by recent modeling of radiation effects in metals and alloys, interfacial dislocation transfer reactions in nano-twinned copper, and dislocation reactions at general boundaries, along with extensive modeling cooperative effects of dislocation interactions and migration in crystals and polycrystals using continuum models.