
Atomic-scale to Meso-scale Simulation Studies of Thermal Ageing and Irradiation Effects in Fe-Cr Alloys

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ABSTRACT

Fe-Cr alloys with 9-12% Cr content are expected to have superior properties under high temperature and irradiation, and against corrosion, and therefore are considered the base matrix for advanced ferritic/martensitic steels envisaged as fuel cladding and structural components in Gen-IV reactors and fusion reactors. However, prolonged exposure to fast neutron fluxes and aggressive coolants in operation will unavoidably reduce their capability of withstanding the applied loads. Because thermal and neutron irradiation experiments are expensive both in terms of time and resources, predictive multi-scale simulation tools are needed to foresee the structural and mechanical properties of these steels.

Among all multi-scale simulations, meso-scale approaches (e. g. Phase Field) have emerged as powerful computational tools to simulate microstructures and microstructure evolution kinetics under thermal ageing and excessive irradiation. However, the quantitative Phase Field (PF) approach requires the accurate thermodynamic and kinetic properties developed from atomistic simulations and experiments; therefore atomic-level data and mechanisms will provide key input parameters for the development of accurate PF models. An atomic-scale approach, the Molecular Dynamics (MD) method, provides a route from atomic processes and mechanisms to phenomena at the continuum-level. It can be used to obtain significantly quantitative inputs to the models used for meso-scale phenomena, such as the PF studies of microstructure evolution.

Currently, even though we are able to carry out MD simulations at atomic-scale, we lack the capability to translate the results to meso-scale simulations. Therefore, our study focuses on the development of an integrated modeling platform for MD and PF simulations of the thermal ageing and excessive irradiation of Fe-Cr alloys, with the potential to extend to other alloys.

In this proposal, we target at three primary objectives: (1) MD code development for Fe-Cr alloys which can be utilized to provide thermodynamic and kinetic properties as inputs in meso-scale PF simulations; (2) validation and implementation of the MD code to explain thermal ageing and radiation damage; and (3) an integrated modeling platform for MD and PF simulations. These two simulation tools, MD and PF, will ultimately be merged to understand and quantify the kinetics and mechanisms of microstructure and property evolution of Fe-Cr alloys under various thermal and irradiation environments.