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Editorial: Computational modeling for nuclear materials

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Editorial on the Research Topic
Computational modeling for nuclear materials

With the global development of industrial technology, the increased application for the nuclear energy has driven the widely researches about nuclear materials (Zhou, 2021). Taking account of the unique in-pile irradiation environment, a variety of structural materials will damage and fail under the coupling effect of irradiation, thermal and mechanical loads (Bai et al., 2010). These crucial factors are necessary for assessing the safety of structural components. For investigating the coupling effect under irradiation, the conventional failure analysis approaches and the fracture criterion should be modified and developed. Furthermore, due to the irradiation-induced variation of material toughness, irradiation processing can also be extended to the modification study on special materials. In this Research Topic, the latest research works covering numerical models and analytical methods for the irradiation failure of nuclear materials have been reported.

In reactors, damages and cracks within the fuel elements and the structural components are mainly produced due to the irradiation effect, which is generated by tremendous amounts of thermal energy and extensive fission products diffusion releasing in neutron-induced nuclear chain reaction (Suzuki and Kobayashi, 2008). Electronic components are also affected by irradiation in the extreme service environment (Benton and Benton, 2001). Energetic particles will cause serious ionization or displacement damage in materials, alternating the microstructure and macroscopic properties of nuclear materials (Weeks, 1963; Monnet and Mai, 2019). Therefore, it is significant to investigate the irradiation-induced micro-defects evolution, construct the failure model and assess the safety of materials under irradiation.

Recently, the classical analysis theories, such as the thermodynamically consistent method, the principle of minimum potential energy, the dynamics model, and etc., have been applied in the nuclear material field for taking account of the irradiation effect. The energy corresponding to the irradiation is dissipated for irreversible mechanical strain, heat flow, diffusion of fission products, and forming the new surfaces of damages. Through modifying the conventional analytical theories based on the thermodynamic law, such as the derivation of governing equations, the fracture criterion, the energy release rate for crack propagation, density functional theory, and etc., some effective analytical models and numerical approaches can be developed for studying the effect in terms of irradiation on material performances. For the plane fracture problems in elastoplastic materials, the J-integral possesses clear physical meaning (Rice, 1968; Atluri, 1982), and meanwhile the fracture criteria based on it have been widely used. Applying the J-integral criterion in the analysis of the cracking of ductile materials in reactors has profound engineering prospects (see, for example, Zhang et al.; Dong et al.). Furthermore, according to the article entitled "*Influence of doubly-hydrogenated oxygen vacancy on the TID effect of MOS devices*" by Lu et al., controlling the concentration of doubly-hydrogenated oxygen vacancy in the oxide layer with the value below 10^{14} cm^{-3} are more conducive to the design of anti-irradiation to the total ionizing dose effect.

This Research Topic focuses on the latest advances for the irradiation-dependent analysis of nuclear materials, mainly involving the damage, failure and fracture problems. The Research Topic of four articles provides some creative thoughts and addresses some challenging problems, such as the dynamic model of mobile particles and fixed defects, the energy release rate in irradiated materials, the elastic-plastic three-dimensional J-integral, the effect of residual pores on the tri-isotropic structure, and so forth. These studies promote the understanding for the irradiation effect on nuclear materials failure, and further lay a foundation for designing in-pile components with better safety and reliability.

Author contributions

YD: Writing–original draft. QL: Writing–review and editing.

Conflict of interest

The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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