Gas bubble evolution in UO_2 - A phase field study

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ABSTRACT

The fission gases xenon and krypton are unceasingly generated in irradiated nuclear fuel, which is a sintered compact of granular uranium dioxide in the current commercial light water reactors (LWRs). Because of their low solubility in UO_2, fission gases tend either to precipitate into bubbles or to be released to the free volume in the fuel rod. Fission gas release and gas bubble swelling are critical issues for the fuel performance of LWRs. Released fission gas can reduce the thermal conductivity of the fuel-cladding gap and cause temperature and pressure increases in the fuel pellet, whereas gas bubble swelling can increase the contact pressure between the fuel and cladding, and lead to cladding failure. Due to the large formation energy of vacancies and Xenon gas atoms at interstitial and/or substitutional sites in nuclear fuel crystals(UO_2), the thermodynamic equilibrium concentrations of these species are very low in the nuclear fuel matrix even at very high temperatures, which imposes difficulties upon the quantitative study of gas bubbles evolution via the phase-field method. In our study, a quantitative phase-field model is put forward to deal with this problem. The free energy density of the system is derived according to the principles of thermodynamics, with consideration of the elastic interaction and with the use of material parameters from experiments. The model enables one to study the kinetics of gas bubble growth with very dilute concentrations of vacancy and gas atoms in the matrix. With this model, the growth of a single bubble and multiple bubbles were simulated under different concentrations of vacancy and gas atoms and at different temperatures. Besides, this model was used to study the gas bubble migration in nuclear fuel. Because of the large temperature gradient in the UO_2 fuel pellet, gas bubbles prefer migrating to the high-temperature zones in nuclear fuels. During the migration, the morphology of gas bubbles changes due to the difference of migration velocities in different zones in nuclear fuel. In this study, we considered the bulk diffusion and vapor transport process, the bulk diffusion mechanism is used for nano-sized gas bubbles and for micron-sized gas bubbles, the vapor transport was considered. Near the center of the nuclear fuel pellets, the gas bubbles have lenticular shape, with distance far from the center area, the gas bubbles are elongated. The gas bubbles tend to migrate to the high-temperature zones and form a hole in the center of the nuclear fuel pellets which is confirmed by the experimental results.

REFERENCES

[1] Garcia, P., et al, "Nucleation and growth of intragranular defect and insoluble atom clusters in nuclear oxide fuels", *Nucl Instrum Methods Phys Res B*, Vol. **277**, pp. 98–108, (2012).

[2] Li, Y., et al, "Phase-field simulations of intragranular fission gas bubble evolution in UO2 under post-irradiation thermal annealing", *Nucl Instrum Methods Phys Res B*, Vol. **303**, pp. 62–67, (2013).

[3] Zhang, L., et al, "Phase-field modeling of temperature gradient driven pore migration coupling with thermal conduction", *Comput Mater Sci*, Vol. **56**, pp. 161-165, (2012).

[4] Vance, I.W. and P.C. Millett, "Phase-field simulations of pore migration and morphology change in thermal gradients", *J Nucl Mater*, Vol. **490**, pp. 299-304, (2017).

[5] Novascone, S., et al., "Modeling porosity migration in LWR and fast reactor MOX fuel using the finite element method", *J Nucl Mater*, Vol. **508**: pp. 226-236, (2018)