Predictive molecular-dynamics models for investigation of U, U-Mo and U-Mo-Xe systems

Daria Smirnova, Alexey Kuksin, Sergey Starikov, Vladimir Stegailov

Joint Institute for High Temperatures of Russian Academy of Sciences

Uranium alloys are now under active investigation as possible fuels for future fast and research reactors. Understanding the radiation damage effects on the fuel stability is one of the major challenges to be solved on the way to effective and safe fuel design. A description of radiation damage requires knowledge of the atomistic mechanisms of defect generation in solids. In case of uranium the radiation defect properties still have not been sufficiently studied either for pure U or for metallic uranium compounds, including uranium-molybdenum (U–Mo). Therefore reliable models of radiation damage in nuclear fuels are required to explain essential physical effects (point defects clustering, interaction with dislocation loops, grain boundaries etc) and make predictions about the materials characteristics. In this work the atomistic and molecular-dynamics models of pure U and prospective high density U-Mo fuel alloys are proposed. Also a set of new many-body interatomic potentials created especially for predictive modelling and simulation of these nuclear fuels is introduced and discussed [1,2]. The potential functions are fitted to the values of *ab initio* interatomic forces, energies and stresses. The models proposed are validated to be applicable for study of the following issues:

1) Structure of orthorhombic α-U, bcc γ–U, bcc Mo, U_2Mo compound and bcc U-Mo fuel alloys (containing from 7 to 12 wt.% of Mo).
2) Elastic constants, melting temperatures, thermal expansion and room-temperature isotherms of the components of U-Mo system; Grűneisen parameter for liquid and solid U.
3) The point defect (SIA, vacancy) formation energies for pure U and Mo.

The potentials developed are aimed to study the evolution of radiation defects in U and U-Mo fuels. For example, the point defects diffusion mechanisms in U-9Mo are considered and some comparison between the defect diffusivities in pure bcc U and in bcc U-9Mo is made. The potentials also give an opportunity for simulation of fission products (namely Xe) behavior in U, Mo and U-Mo.

1. D.E. Smirnova, S.V. Starikov, V.V. Stegailov Interatomic potential for uranium in a wide range of pressures and temperatures 2012 *J. Phys.: Condens. Matter* **24** 015702

2. D.E. Smirnova, S.V. Starikov, A.Yu. Kuksin, V.V. Stegailov, Z. Insepov, J. Rest, A.M. Yacout. A ternary EAM interatomic potential for U–Mo alloys with xenon. 2013 *Modelling Simul. Mater. Sci. Eng.* **21** 035011