Equilibrium and Non-Equilibrium Molecular Dynamics Simulations of Heat Conduction in Uranium Oxide and the Solid Solution with Plutonium Oxide

T. Arima[1,C, S], S. Yamasaki[2], Y. Inagaki[1] and K. Idemitsu[1]
[1]*Faculty of Engineering, Department of Applied Quantum Physics and Nuclear Engineering, Kyushu University, Fukuoka, Japan*
arimatne@mbox.nc.kyushu-u.ac.jp

[2]*Department of Applied Quantum Physics and Nuclear Engineering, Faculty of Engineering, Kyushu University, Fukuoka, Japan*

For the nuclear fuel performance, the thermal conductivity is one of the most important properties and is dependent on various fuel parameters, i.e. oxygen stoichiometry, Pu content, temperature, etc. So we have evaluated the thermal conductivity in terms of such parameters by the EMD simulation and have shown the effectiveness to predict thermal behaviors of fuels [1]. However, the EMD simulation needs the more CPU time to obtain the more reliable results. Thus the homogeneous NEMD as the alternative to EMD is expected to perform with reducing the CPU time per run and without the comprehensive change in the algorithm, i.e. periodic condition [2].

In the present study, the thermal conductivity of nuclear fuels, i.e. UO_2, UO_{2-x} and $(U,Pu)O_{2-x}$ has been calculated by EMD and NEMD simulations at temperatures up to 2000 K. The interatomic potential was the Born-Mayer-Huggins type with the partially ionic model [1]. In the EMD simulation, according to the Green-Kubo relationship, the thermal conductivity was determined by the transport coefficient defined as the integration of the correlation function of heat flux. On the other hand, in the homogeneous NEMD algorithm proposed by Evans [2], it was given by the ratio of the time-averaged heat flux to the perturbative external force, F_{ext}, to each particle in the simulated cell.

NEMD showed the almost comparable results to ones from EMD and needed only one tenth of the number of time steps per run for EMD. Then the linear relationship between heat flux and F_{ext} was observed up to ca. 2E8-2E9 m^{-1}. The result obtained by these simulations was that the thermal conductivity decreased with increase of temperature and defects, i.e. oxygen interstitial or vacancy and was rather insensitive to Pu content.

[1] T. Arima, S. Yamasaki, Y. Inagaki, K. Idemitsu, *J. Alloys and Compd.* **43**, 400 (2005).
[2] D.J. Evans, *Phys. Lett.* **91A**, 457 (1982).