Ab Initio Calculation of Fission Product Gas Dynamics in UO_2 as a Function of Lattice Dilation

t. semi[1], T.M. Lusk

Colorado School of Mines
Golden CO 80401

[1]tsemi@mines.edu

Abstract

The behavior of fission product gases in UO_2 light water fission reactors crucially affects the useful lifetime of the fuel pin. The coupling between elastic stress and gas dynamics is of particular interest since bubbles within the fuel pin are responsible for both fuel swelling and localized stress concentrations. In addition, radially varying thermal profiles generate strain gradients which may facilitate the motion of fission product gases. The precise relationship between gas dynamics and strain has yet to be established. We seek to quantify the energetics of individual and very small clusters of Kr atoms within UO_2 as a function of lattice strain. This is undertaken using Density Functional Theory (DFT) for pure dilations of the lattice. Within this setting, the influence of vacancy defects on the Kr atom dynamics is also considered. The results can be used to predict the tendency of gas atoms to agglomerate as a function of strain and temperature and to quantify the kinetics of individual gas atoms within a strain or temperature gradient. Activation energies and vibrational frequencies, calculated using DFT, can be used to estimate strain-dependent diffusivities of Kr atoms and vacancies.