論 文 の 内 容 の 要 旨

論文題目　STUDY ON MICROSCOPIC BEHAVIORS OF HYDROGEN ISOTOPE IN ERBIUM OXIDE FOR TRITIUM PERMEATION BARRIER

(トリチウム透過防止用酸化エルビウム中の水素同位体ミクロ挙動に関する研究)

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The objective of this study is to investigate the microscopic mechanism of hydrogen isotope behaviors in erbium oxide, Er_2O_3, for tritium permeation barrier. These behaviors include H dissociation, H adsorption, H penetration, H diffusion in bulk, grain boundary, and point defects (vacancies). Although we have made a rapid progress in the fabrication of Er_2O_3 coatings, and measure H isotope diffusion and permeation in Er_2O_3 coatings, the detailed mechanism of H isotope diffusion is not clear yet. It can be attributed to complex crystal structures existing in Er_2O_3 coatings. Moreover, the atomic interactions between H and Er_2O_3, they can`t be clarified by experiments. Hence, more effort are required to experiments in terms of H isotope behaviors in Er_2O_3. To better understand H behaviors in Er_2O_3 and conduct experiments efficiently, it is, therefore essential to conduct the corresponding theoretical works.

In this study, we employ *ab initio* calculations based on density-functional theory and classical molecular dynamics to probe H behaviors in conjunction with the corresponding experimental data. Our calculations indicate that the accurate computational simulations have become a valuable tool to precise atomic hydrogen behaviors in Er_2O_3, and complement the experimental data for the interest of tritium permeation barrier, with the considerations of hydrogen isotope effects.