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Aggregation and ordering of helium in thoria

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Abstract

The trapping, aggregation and ordering of helium in thoria (ThO₂) was studied by using ion beam irradiation experiments and first principle calculations. Transmission Electron Microscope (TEM) and Grating Incidence X-Ray Diffraction (GIXRD) studies on thoria irradiated with low energy (100 keV) He⁺ ions, showed that the lattice has expanded upto 1.07% in isolated nanometric regions where He ions were implanted. In order to distinguish the role of He atoms and ion irradiation induced damage on the lattice expansion, thoria irradiated with 4 MeV Si⁺ ion was studied, where ion induced damage produced just 0.06% lattice expansion. The observed large lattice expansion in He⁺ ion irradiated sample is due to the implanted helium atoms. First principle calculations showed that energetics prefer aggregation and ordering of He in the octahedral interstitial sites in thoria lattice, and the ordered aggregation eventually results in lattice expansion of 1.25% which is in agreement with experiments. The experiments and calculations confirm that the observed lattice expansion is due to the ordering of He atoms in the octahedral interstitial sites of thoria.

Keywords: Thoria, ion irradiation, DFT calculation, helium aggregation and ordering, lattice expansion.

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