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Diffusion in thorium carbide: A first-principles study

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Abstract

The prediction of the behavior of Th compounds under irradiation is an important issue for the upcoming Generation-IV nuclear reactors. The study of self-diffusion and hetero-diffusion is a central key to fulfill this goal. As a first approach, we obtained, by means of first-principles methods, migration and activation energies of Th and C atoms self-diffusion and diffusion of He atoms in ThC. We also calculate diffusion coefficients as a function of temperature.

1. Introduction

The projects behind the future Generation-IV nuclear reactors [1] have boosted research on the possible materials to be used as nuclear fuels, among them thorium and its compounds (carbides and nitrides) [2, 3]. The advantages of these compounds, compared to uranium ones, are: higher melting points, lower thermal expansion coefficients and larger thermal conductivities.

The study of thorium compounds in the context of nuclear fuels involves the prediction of their behavior under irradiation [4]. A first approach to this goal is the estimation of the migration paths, migration energies and diffusion coefficients. In particular, the study of self-diffusion and the diffusion of different incorporated elements.

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