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Diffusion in UAl_4: Calculations Based on the Compound Defect Structure

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ABSTRACT

In a previous work we obtained the structure of point defects for UAl_4 in thermal equilibrium. We identify in the present work the more likely mechanisms for Al mobility in the compound and analyze transition states by NEB method in VASP code. We have calculated the compound total energy variation according to the migration path of aluminum and obtained the minimum migration energy paths. This allowed us to propose two most likely mechanisms for the diffusion of Al atoms in the rich side Al intermetallic: a) antistructural bridge mechanism (ASB) and b) vacancy mechanism between first neighbors aluminum Al1 sites (NN). Based on all results and discussions we propose that the aluminum diffusion mechanism occurs in UAl_4 by means of NN mechanism with activation energy of 1.90 eV which compares relatively well with experimentally observed value 2.06 eV or the value 2.17 eV obtained using a semi-empirical model.