J Astrophys Aerospace Technol 2016, 4:2(Suppl)
http://dx.doi.org/10.4172/2329-6542.C1.003

Iodine atom diffusion in SiC and Zr

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Silicon carbide (SiC) is a promising cladding material in light water reactor. The fuel cladding is an important safety barrier in fission nuclear reactors, as it restrains most of the radioactive fission products within its volume. The ability to keep radioactive fission products within the cladding material determines whether SiC can be used as a safe cladding material. Iodine atom diffusion in SiC is calculated with first-principles calculation and nudged elastic band method (NEB) and compared with that in Zr. Without considering vacancy effect, the diffusion rate of iodine in SiC is slower than that in Zr. Consider the vacancy from the neutron irradiation, divacancy can speed up iodine impurity diffusion in SiC. Even larger vacancies slow down iodine diffusion in SiC. Meanwhile, vacancies slow down the diffusion of iodine atom in Zr.

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Quasi-classical chemisorption study about hydrogen molecule storage on Cu_{13} and Pd_{13} atomic clusters

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Chemisorption of hydrogen on transition metals has proven great significance in many industrial treatments and processes such as hydrogen storage, corrosion monitoring and controlling and clean fuel production. The simplest chemisorbed species and ideal system to study is the chemisorption of H atom on surfaces. Molecular dynamic method reporting a quasiclassical simulation of the interaction of H_2 with Cu_{13} and Pd_{13} clusters was reported in this study. Embedded-atom (EA) mode potential was used to define the geometry of the cluster and LEPS (London-Eyring–Polanyi-Sato) potential energy function describe and the interaction between the molecule and cluster. The dissociation adsorption probability of the molecule on the cluster were considered, the roles of initial rovibrational states of the H_2 molecule, and the effect of the change of clusters temperature on dissociation were also examined. It was very clear that from the monitored and plotted data, the reaction cross section increase monotonically with increase of initial rovibrational v_i, j_i sates in the ranges (v=0, j=0; 3; 5; 10) and (v=1; 3, j=0) and that the vibration effect was exerting more influence than that of the rotational in increasing the reaction cross section. It was also seen that the temperature change in the range (295K-300) did not report a significance change in Hydrogen dissociation. The simplicity of the technique and the applicability to practical make it a powerful study for atomistic studies of dissociation of H_2 in metallic clusters.

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