Diffusion under stress of Si impurities in Ni: a first principles study

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Abstract

A first principles study of the effect of strain on the migration of Si atoms in Ni is conducted. For that purpose, migration barriers are computed using the nudged elastic band method and attempt frequencies are computed using the direct force method. A good agreement is found with tracer diffusion experiments. We used the elastic dipole model to calculate effects of strain on migration barriers by performing calculations on unstrained cells, therefore reducing significantly the computing time. We validate this approach by comparing results with migration barriers calculated on strained cells and obtain an excellent agreement up to a strain of 1%. Computing all the jumps frequencies in the neighborhood of Si solutes, the strain dependence appears to be nearly independent from the relative position of the solute atom. A simple elastic model closely predicts the changes in the vacancy jump with strain; this correlates with the changes in geometry for the "cage" of atoms surrounding the hopping atom at the saddle point.

We provide here the results of DFT calculations of strain effect on vacancy diffusion of Si in Ni perfomed using VASP.

These calculations are organized as follow: Folders are organized in two groups, a group of site energy folders and a group of NEB calculation folders. in each site energy folder is provided the relaxed configuration as a POSCAR file, the input INCAR and K-point files and the output as an OUTCAR file. in each NEB calculation folder is provided the initial and final configuration POSCAR file, the final saddle point configuration as a POSCAR file, the input INCAR and K-point files and the output as an OUTCAR file.