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Helium and neon diffusion in pure hematite (α-Fe_2O_3) crystal lattice

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Hematite (α-Fe_2O_3) has the corundum-type structure and is relatively present on Earth and Mars surface associated to ore mineral precipitation or as a weathering phase. He and Ne retention in such mineral has been intensively investigated experimentally because of the potential use of (U−Th−Sm)/(He−Ne) chronometer and thermochronometer. Therefore, the He/Ne diffusion in hematite crystal is an important issue for the interpretation of (U−Th)/(He−Ne) thermochronometric ages.

For this purpose an accurate investigation of helium and neon diffusion in hematite crystal lattice has been achieved by computational multi-scale approach. Different insertion sites and diffusion pathways are first characterized where the spin polarized density functional theory (sp−DFT) approach coupled to the nudged elastic band (NEB) method is used to determine the migration energies between the insertion sites. Then, a statistical method, based on transition state theory (TST), is used to compute the jump probability between sites. The previous results are used as input data in a $3D$ random walk simulation, which permits to determine the effective activation energy and diffusion coefficient.

Using the He/Ne diffusion coefficients, the closure temperature T_c has been calculated. For typical grain size of 100 microns, T_c will be of 116° C and 297° C for He and Ne atoms, respectively. These results Show that He and Ne atoms are highly retained in the crystal lattice at surface temperature.

The obtained diffusion coefficients confirm that He/Ne retentively power in hematite lattice is very important, allowing a large range of different geological applications such the measurement of hematite crystallization ages on Earth and Mars.