He and Ne diffusion modeling in minerals: insight from atomic to mineralogical scale

CÉCILE GAUTHERON[1], JEROME ROQUES[2], LAURENT TASSAN-GOT[2]

[1]GEOPS, Université Paris Sud. 91405 Orsay, France, cecile.gautheron@u-psud.fr
[2]IPN, Université Paris Sud, 91405 Orsay, France, roques@ipno.in2p3.fr; tassango@ipno.in2p3.fr

(U-Th)/He and (U-Th)/Ne dating methods have been applied to different minerals such as apatite, zircon and iron oxides, and their age interpretation requires a good understanding of He and Ne retention through possible diffusion. Several parameters including damage, chemical composition and polycrystalline structure have been proposed to explain the range of He diffusion in crystals. Debates are still ongoing about the blocking effect of damage on He diffusion in minerals, mostly due to their small sizes (nanometer scale). In order to better characterize He and Ne diffusion in minerals, we propose a combination of methodologies from the atomic to mineralogical scales. At atomic scale, the Density Functional Theory (DFT) associated with Kinetic Monte Carlo (KMC) codes allows characterizing He diffusion in 3D in pure crystal lattice. At macroscopic scale, these methods permit to take care of He and Ne diffusion in 3D for anisotropic crystals and for different chemical compositions. In this contribution, we will give particular examples of He and Ne diffusion behavior in apatite, zircon and hematite. The obtained He diffusion coefficients in apatite and hematite (Djimbi et al., 2015; Balout et al., 2017) demonstrate the robustness of these methods. In addition, the impact of damage on He diffusion can also be investigated by using DFT to calculate point-defect energetics, leading to a trapping phenomenon as in larger scale damage. The developed methodology allows us to characterize the different parameters influencing He and Ne retiention in minerals.

Balout et al. 2017. Helium diffusion in pure hematite (α-Fe_2O_3) for thermochronometric applications : a theoretical multi-scale study. Computational and Theoritical Chemistry. 1099, 21-28.

Djimbi et al. 2015. Impact of apatite chemical composition on (U-Th)/He thermochronometry: an atomistic point of view. Geochim. Cosmochim. Acta. 167, 162-176.