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Investigation of vacancy damage influence on He diffusion in apatite: implication for the (U-Th)/He thermochronometer

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Helium diffusion in minerals rich in actinides, especially apatite, is considered as strongly impacted by damage, even at low U–Th content. However, no direct evidence exists neither about such an impact nor the damage topology. To better understand the impact of damage on He diffusion, we conducted a study on vacancy damage in apatite, at nanometric to atomic scales, using several methodologies [1]. We investigate the role of vacancy damage that are the one created during alpha decay. Firstly, Transmission Electron Microscopy (TEM) was used to image the damage structure done by He implantation in the first 200 nm below the surface of apatite crystal. TEM images present no visible damage zone at nano-scale, implying that the created damage corresponds well to Frenkel defects (vacancies and interstitials). Secondly, to test the damage impact on diffusion and the trapping efficiency, we conduct both experimental and theoretical studies. Diffusion experiments were performed on He implanted samples by mapping He concentration vs. depth profiles using Elastic Recoil Detection Analysis (ERDA). After measurement of implanted-He profiles and He concentrations, the samples were heated in order to diffuse the implanted profile. The obtained He vs. depth heated profiles and He concentrations reveal the impact of damage on He diffusivity. The results can only be explained by a model where diffusion depends on damage dose, taking into account He trapping in vacancies and damage interconnectivity at higher damage dose. Thirdly, Density Functional Theory (DFT) calculations were performed to simulate a vacancy in a F-apatite crystal, and results are compared with an undamaged apatite cell [2]. The structure becomes slightly deformed by the vacancy and the insertion energy of a He atom in the vacancy is lower than for an usual insertion site. Accordingly, the additional energy for a He atom to jump out of the vacancy is in good agreement with published estimates. This calculation thus shows that small modifications of the structure due to the presence of vacancies efficiently trap He atoms, thus reducing diffusivity. Finally, for an apatite crystal having vacancy-type damage, we propose a He diffusion model able to reproduce well He diffusion data obtained on irradiated samples.

[1] Gerin, C. et al., 2017. Influence of vacancy damage on He diffusion in apatite investigated at atomic to mineralogical scales. Geochim. Cosmoch. Acta, 197: 87-103.
[2] Djimbi, D.M. et al., 2015. Impact of apatite chemical composition on (U-Th)/He thermochronometry: an atomistic point of view. Geochim. Cosmoch. Acta, 167: 162-176.