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# Apatite (U-Th)/He thermochronology dataset interpretation: New insights from physical point of view

Cécile Gautheron (1), Duval Mbongo-Djimbi (2), Chloé Gerin (1), Jérôme Roques (2), Cyril Bachelet (3), Erwan Oliviero (), and Laurent Tassan-Got ()

(1) Université Paris Sud, GEOPS, Orsay, France (cecile.gautheron@u-psud.fr), (2) IPN, iN2P3, Université Paris Sud, 91405 Orsay, France, (3) CSNSM, Université Paris sud, 91405 Orsay, France

The apatite (U–Th)/He (AHe) system has rapidly become a very popular thermochronometer to constrain burial and exhumation phases in a variety of geological contexts. However, the interpretation of AHe data depends on a precise knowledge of He diffusion in apatite. Several studies suggest that radiation damage generated by U and Th decay can create traps for He atoms, increasing He retention for irradiated minerals. The radiation damage also anneals with temperature and the amount of damage in an apatite crystal is at any time a balance between production and annealing, controlled by U–Th concentration, grain chemistry and thermal history (Flowers et al., 2009; Gautheron et al., 2009; 2013). However the models are not well constrained and do not fully explain the mechanism of He retention. In order to have a deeper insight on this issue, multidisciplinary studies on apatite combining diffusion experiments by Elastic Recoil Diffusion Analysis (ERDA) with a multi-scale theoretical diffusion calculation based on Density Functional Theory (DFT) and Kinetic Monte Carlo were performed. ERDA experiments were conducted on different macro-crystals, and we probed the shape of a He profile implanted into a planar and polished surface of the crystal. The helium profile evolves with temperature and allows quantifying the He diffusivity and damage impact. Additionally, DFT calculations of a damage-free crystal of apatite with different F and Cl compositions, in similar proportion as natural ones, have been run to find the favored paths of a helium atom between interstitial sites, leading to a computation of the activation energy and the diffusion coefficient. We show that damage free apatite crystals are characterized by low retention behavior and closure temperature range from 33-36°C for pure F-apatite to higher value for Cl riche apatite (up to 12°C higher), for typical grain size and cooling rate (Mbongo-Djimbi et al., in review). Using ERDA and DFT approaches, we demonstrate that in addition to grain chemistry, He diffusivity will be strongly influenced by damage and propose a new physical model. Finally, we propose a new way of interpreting AHe datasets and practical geological examples will be given.

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