Hematite and Goethite (U-Th)/He/Ne ages interpretation using crystallographic data and diffusion parameters

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At the Earth's surface, hematite and goethite are common minerals occurring in soils and sediments, including ores. The understanding of the corresponding alteration and weathering processes relies on our ability to perform the dating of formation of these minerals. Two relevant and recent dating methods have been developed, which are related to (U-Th)/He and (U-Th)/Ne geochronometers. They are based on accumulation of 4He and 21Ne associated with the alpha decay of U and Th. Both methods are of particular interest because of possible He and Ne retention over geological ages at surface temperature. However, because of different atomic radius between He and Ne, retention behavior of these two species can be quite different. Moreover, the dating procedure is particularly challenging because of the small crystals size and frequent polycrystalline structure of hematite and goethite. As a matter of fact, some uncertainty exists about He and Ne diffusion parameters, due to the nanometric to micrometric crystal size of natural iron oxide mineral. Accordingly, the determination of (U-Th)/He and (U-Th)/Ne ages requires the understanding of He and Ne production and retention (which may be partial) in iron oxide crystals.

In this study, we theoretically investigate and discuss for the first time the age evolution for pure goethite and hematite crystals with different thermal histories, including reheating to simulate burial. The aim is to quantify the He and/or Ne loss by ejection and diffusion for crystals of different morphology and polycrystalline structures. This will allow one to provide some correction factor for the age. For this purpose, we used new He and Ne diffusion coefficients obtained by multi-scale theoretical approach using Density Functional Theory (DFT) (Balout et al., submitted, a,b), associated with 3D production and diffusion code (Gautheron and Tassan-Got, 2010). The impact of Multi Diffusion Domains simulating polycrystalline structure has been incorporated in this code in order to reproduce realistic crystallographic structure.

Balout, H., Roques, J., Gautheron, C., Tassan-Got, L., Mbongo-Djimbi, D., submitted a. Helium diffusion in pure hematite (α-Fe$_2$O$_3$) for thermochronometric applications: a theoretical multi-scale study.
Balout, H., Roques, J., Gautheron, C., Tassan-Got, L., submitted b. Computational investigation of the interstitial neon diffusion in pure hematite, α-Fe2O$_3$.
Gautheron, C., Tassan-Got, L., 2010. A Monte Carlo approach of diffusion applied to noble gas/helium thermochronology. Chemical Geology, 273: 212-224.