DIPARTIMENTO DI GEOSCIENZE
DEPARTMENT OF GEOSCIENCES

Seminario - *Arduino Lecture*

# He and Ne diffusion in minerals view at microscopic to macroscopic scale : implication for (U-Th)/He and Ne thermochronometers

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Aula Arduino

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**Abstract:**

The (U-Th)/He dating method can be applied to different minerals such as apatite, zircon, calcite, iron oxides, and age interpretation requires a good understanding of He 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 diffusion in minerals, we propose a combination of methodologies from the atomic to mineralogical scales. At atomic scale, the Density Functional Theory (DSF) 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 helium diffusion in 3D for anisotropic crystals and for different chemical compositions. The obtained He diffusion coefficients in apatite and hematite 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. Diffusion experiments on artificially damaged crystals using Elastic Recoil Diffusion Analysis (ERDA), can in addition illustrate the damage impact on diffusion. All these data allow to build a helium diffusion model taking into account the damage content, based on a physical model. Finally, the study of He diffusion at geological time and temperature scales enables to identify damage and annealing parameters and calibrate a realistic helium diffusion model.

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