

Pyrochlore: Radiation-damage and thermally induced structural reorganization

Tobias Beirau¹, Norbert Huber^{2,3}, Claudia E. Reissner¹, Herbert Pöllmann¹, Ulrich Bismayer⁴

¹Institute of Geosciences and Geography, Mineralogy/Geochemistry, Martin Luther University Halle-Wittenberg, 06120 Halle, Germany, ²Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany, ³Institute of Materials Physics and Technology, Hamburg University of Technology (TUHH), 21073 Hamburg, Germany, ⁴Department of Earth Sciences, University of Hamburg, Grindelallee 48, 20146 Hamburg, Germany

Materials with pyrochlore structure ($A_2B_2O_7$) have been considered as host phases for long-term nuclear waste disposal. Cubic pyrochlore ($A_2B_2X_6Y$) with space group $Fd-3m$ comprises eightfold coordinated A cations that build A_2Y chains and corner-sharing BX_6 octahedra. The mineral can incorporate a large variety of different cations on the A and B positions, including rare earth and radioactive elements (e.g., up to 9wt. % ThO_2 and 30wt. % UO_2). The decay of the incorporated actinides leads to damage in the initially ordered structure. The effect of step-wise thermally induced annealing on the mechanical properties (i.e., E Modulus and hardness), as well as on the short range order, determined by Raman and photoluminescence spectroscopy, will be presented [1]. While, the structural amorphization and subsequent reorganization process can be described by means of percolation theory [2], the latter shows avalanche behavior [3].

- [1] Reissner CE, Roddatis V, Bismayer U, Schreiber A, Pöllmann H, Beirau T. Mechanical and structural response of radiation-damaged pyrochlore to thermal annealing. *Materialia*, 14, 100950 (2020).
- [2] Beirau T, Huber N. Percolation transitions in pyrochlore: Radiation-damage and thermally induced structural reorganization. *Applied Physics Letters*, 119, 131905 (2021).
- [3] Beirau T, Shelyug A, Navrotsky A, Pöllmann H, Salje EKH. Avalanches during recrystallization in radiation-damaged pyrochlore and allanite: Statistical similarity to phase transitions in functional materials. *Applied Physics Letters*, 115, 231904 (2019).

This research was funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation), No. BE 5456/2-1 (T.B.).