Effects of irradiation-induced structural disordering in zirconate pyrochlores at high pressures

<u>Sulgiye Parka</u>, Cameron L. Tracya, Fuxiang Zhangb, Changyong Parkc, Christina Trautmannde, Sarah Finkeldei^f, Maik Lang^g, Wendy L. Maoa, Rodney C. Ewing^{a,*}

^a Department of Geological Sciences, Stanford University, Stanford, CA 94305, USA

^b Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA

^c HPCAT, Carnegie Institute of Washington, Argonne, IL 60439-4803, USA

^d GSI Helmholtzzentrum für Schwerionenforschung, 64291 Darmstadt, Germany

^e Technische Universität Darmstadt, 64287 Darmstadt, Germany

^f Forschungszentrum Jülich, Institute of Energy and Climate Research, IEK-6; Nuclear Waste Management and Reactor Safety, 52425 Jülich, Germany

⁸ Department of Nuclear Engineering, University of Tennessee, TN 37996, USA

Abstract: The effects of swift heavy ion irradiation-induced disordering on zirconate compounds $(A_2Zr_2O_7 \text{ where } A = Sm, Er, \text{ and } Nd)$ at high pressures are investigated using synchrotron X-ray diffraction (XRD). Irradiation experiments were performed at the GSI Helmholtz Center with ¹⁹⁷Au ions accelerated to energy of 2.2 GeV. Angle dispersive synchrotron powder X-ray diffraction measurements were completed at the Advanced Photon Source at Argonne National Laboratory, where samples were pressurized up to ~ 60 GPa using-diamond anvil cells. Analysis of the XRD data demonstrate that: (1) Sm₂Zr₂O₇ and Nd₂Zr₂O₇ undergo a phase transformation from ordered pyrochlore to a disordered defect-fluorite with swift heavy ion irradiation; 2) energetics of disordering lower the pressure transition point in pyrochlores Sm₂Zr₂O₇ and Nd₂Zr₂O₇ and; 3) swift heavy ion irradiation increases the pressure transition point in a defect-fluorite Er₂Zr₂O₇ by introducing more interstitials. The effects of disordering in different zirconate compositions under high pressure are explained in terms of the variation in phase space with A-site cation substitution.