ESRF	Experiment title: High-Temperature Mobility of Ce ⁴⁺ ions in Yttrium Stabilized Zirconia Ceramics	Experiment number: 20-01-825
Beamline:	Date of experiment:	Date of report:
BM20 ROBL	from: 13/07/2021 to: 19/07/2021	13/09/2021
Shifts:	Local contact(s):	Received at ESRF:
18	C. Hennig	
Names and affiliations of applicants (* indicates experimentalists):		
*SVITLYK Volodymyr, BM20 HZDR ROBL *HENNIG Christoph, BM20 HZDR ROBL		

Report:

During the 20-01-825 experiment ten samples in the Ce-doped Yttrium Stabilized Zirconia (YSZ) system were studied *in situ* as a function of external temperature. Specifically, powder diffraction patterns the tetragonal $(Ce_{0.000}Y_{0.140}Zr_{0.860}O_{2-x}, Ce_{0.030}Y_{0.136}Zr_{0.834}O_{2-x}, Ce_{0.060}Y_{0.132}Zr_{0.808}O_{2-x}, Ce_{0.090}Y_{0.127}Zr_{0.783}O_{2-x}, Ce_{0.120}Y_{0.123}Zr_{0.757}O_{2-x}) and cubic <math>(Ce_{0.000}Y_{0.250}Zr_{0.750}O_{2-x}, Ce_{0.030}Y_{0.243}Zr_{0.728}O_{2-x}, Ce_{0.060}Y_{0.235}Zr_{0.705}O_{2-x}, Ce_{0.090}Y_{0.228}Zr_{0.683}O_{2-x}, Ce_{0.120}Y_{0.220}Zr_{0.660}O_{2-x}) Ce-YSZ samples were collected in a <math>RT - 1150$ K - RT temperature range. Both Ce-YSZ families have been found to be structurally stable at high temperatures (Fig.1) and no discharge of Ce⁴⁺ ions was observed (Fig. 2, Ce_{0.060}Y_{0.132}Zr_{0.808}O_{2-x} is shown as an example on both figures).

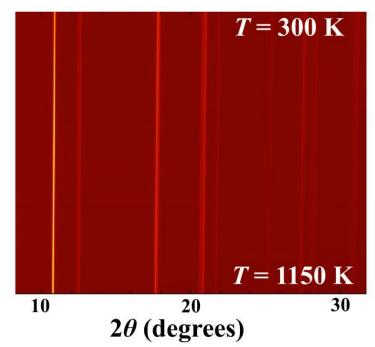


Fig. 1. Evolution of diffraction pattern of tetragonal $Ce_{0.060}Y_{0.132}Zr_{0.808}O_{2-x}$ upon heating indicating absence of any structural transformations

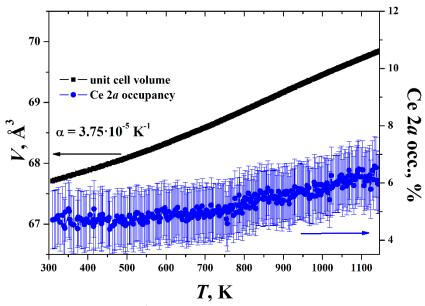


Fig. 2. Evolution of cccupancy of Ce^{4+} (blue) and unit cell volume (black) of $Ce_{0.060}Y_{0.132}Zr_{0.808}O_{2-x}$ upon heating

These results are promising in a context of nuclear waste storage. In these phases Ce^{4+} species have been used as surrogate ions for tetravalent actinide elements like U, Th or Pu. Therefore, incorporated actinide elements in analogous YSZ phases are expected feature similar *T*-dependent behavior, i.e. strong affinity with the parent YSZ matrices. In addition, linear coefficients of thermal expansion have been obtained for all the samples. A corresponding scientific article is currently being written and will be submitted in 2021. Following this successful experiment further experiments as a function of external pressure are planned on these phases.