In-Situ Phase Diagram Determination of the HfO_2-Ta_2O_5 Binary Up to 3000 ˚C

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Abstract

Ceramic equilibrium phase diagrams have proven to be difficult to produce for materials above 1500 ˚C. We demonstrate that in-situ X-ray diffraction on laser-heated, levitated samples can be used to elucidate phase fields. In these experiments, solid spherical samples were suspended and rotated by a gas stream through a conical nozzle levitator, heated by a 400 W CO_2 laser at beamline 6-ID-D of the Advanced Photon Source at Argonne National Laboratory. X-ray diffraction patterns suitable for Rietveld refinement were collected at 100 ˚C temperature intervals and were used to determine the phase fraction of phases present. The temperature of each phase was determined based on thermal expansion data collected by powder diffraction in conjunction with the Quadrupole Lamp Furnace (QLF) at beamline 33-BM-C. The liquidus temperature was determined from recoalescence. The crystal structures of new phases were solved using the charge flipping method from powder diffraction data. The HfO_2-Ta_2O_5 binary was investigated as an example system due to its high melting points and application in refractories and electronics.