Topotactic Motif and Orientation Relation Extraction for Phase Transformations from In-Situ X-ray Powder Diffraction

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In- situ high temperature synchrotron, X-ray powder diffraction was used to extract the topotactic Motif and orientation relationship between orthrohombic $Hf_6Ta_2O_{17}$ (Ima2, S.G. 46) and tetragonal HfO_2 ($P4_2/nmc$, S.G. 137) peritectic reaction at ~2250 ˚C

$$Hf_6Ta_2O_{17} \rightarrow HfO_2 + L$$

The topotactic relationship for the peritectic reaction was established by examining Bragg peaks which were continuous throughout the peritectic transformation. These Bragg peaks described a face-centered, Z=4, pseudo-cell, cation Motif that was present in both the parent (tetragonal HfO_2) and the product (orthorhombic $Hf_6Ta_2O_{17}$) phases. A topotactic orientation relation matrix was determined from continuous, Bragg peaks common to the parent and product phases. The continuous Bragg peaks defined by using reciprocal vectors in terms of the parent (HfO_2) structure were minimized in strain when compared with the product ($Hf_6Ta_2O_{17}$) structure. These constitute the reciprocal lattice basis vectors from which the orientation relationship can be extracted so as to align the $Hf_6Ta_2O_{17}$ crystal with the HfO_2 crystal.

Cubic HfO_2 (Fm3m, S.G 225) was identified as an aristotype cell for the orthorhombic $Hf_6Ta_2O_{17}$ to tetragonal HfO_2 peritectic transformation as it is the undistorted Motif (i.e. a face-centered, Z=4, cubic-cell). From the aristotype cell, symmetry decomposition was performed by means of program ISODISTORT applied to the peritectic transformation. The symmetry decomposition revealed that the mechanism of the peritectic transformation was due to polyhedral rotations and changes in cation-oxygen coordination (polyhedra) due to change in chemical composition and strain relaxation.