Structure relations in the family of the solid solution $Hf_xZr_{1-x}O_2$

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Hafnium Zirconium Oxide $Hf_xZr_{1-x}O_2$ is a potentially ferroelectric material with great perspectives in semiconductor applications, due to its compatibility with silicon technologies and its low toxicity. Despite its chemical simplicity, the solid solution $Hf_xZr_{1-x}O_2$ comprises a large variety of different phases. We compiled a complete list of experimentally and theoretically reported $Hf_xZr_{1-x}O_2$ structures. All of them are symmetrically related to the common aristotype with Fluorite type structure. The summetry relationships between those structures have been determined and are presented in a Bärnighausen-like tree [1]. Interestingly, not all symmetry reductions follow the conventional group-subgroup relations and involve severe atomic shifts. Further, the structures were compared to each other in detail regarding the dimensionality of atomic shifts and the accompanied lattice distortions. In total, nine of the 23 structure types have a polar space group allowing for ferroelectricity; six of them still lack for experimental evidence. Finally, the information provided by the Bärnighausen-like tree was used to transform the indices of a reflection before and after a phase transition. This conversion allows the study of (dis)appearing reflections during phase transitions.

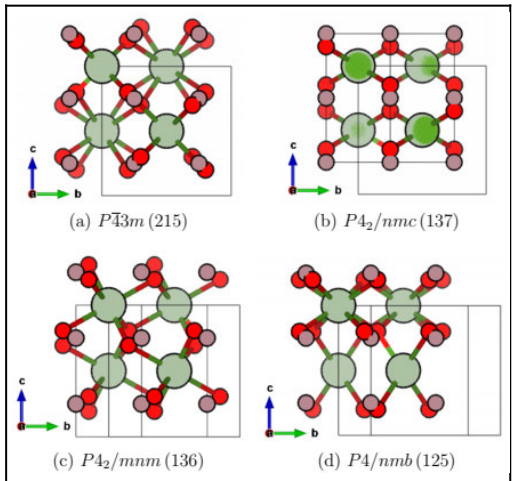

Fig. 1: Structure types of the solid solution $Hf_xZr_{1-x}O_2$ with only slightly distorted lattices compared to the aristotype.

[1] H Bärnighausen Group-subgroup relations between space groups: a useful tool in crystal chemistry" MATCH, 9, 139 (1980)

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