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Local atomic ordering in nanocrystalline ZrO_2 and $\text{Zr}_x\text{Ce}_{1-x}\text{O}_2$ studied with the Atomic Pair Distribution Technique.¹ MILEN GATESHKI, VALERI PETKOV, Dept. of Physics, Central Michigan University — A number of ZrO_2 and $\text{Zr}_x\text{Ce}_{1-x}\text{O}_2$ nanocrystalline samples have been prepared using different techniques, such as ball-milling (ZrO_2) and soft chemistry (ZrO_2 and $\text{Zr}_x\text{Ce}_{1-x}\text{O}_2$). The atomic-scale structure of these samples has been studied using high-energy x-ray diffraction and the atomic pair distribution function technique. For the ball-milled materials, the studies show that the parent crystalline material, monoclinic ZrO_2 , evolves into a nanocrystalline phase that is locally similar to monoclinic zirconia but shows a cubic-type ordering at nanometer-range distances. The atomic-scale structure of the ZrO_2 samples obtained by soft chemistry techniques varies depending on the preparation method and the degree of structural coherence. The studies reveal that all samples show Zr-O distances typical for monoclinic-like local atomic ordering, while the Zr-Zr distances depend on the morphology of the samples. For the $\text{Zr}_x\text{Ce}_{1-x}\text{O}_2$ samples, interatomic distances typical for both monoclinic ZrO_2 and cubic CeO_2 are observed up to 5Å, while the longer interatomic distances are attributed solely to a cubic-type structure. The result underlines the importance of local structural disorder and the medium-range order in stabilizing the technologically important cubic zirconia at room temperature.

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