Superstructure and Order-Disorder Transformation of Interstitial Oxygen in Hafnium

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Abstract

Crystal structure and phase transition in the hafnium-oxygen system containing 10–20 at% O have been studied by means of electron, neutron and X-ray diffraction and calorimetry as well. The oxygen atoms occupy the octahedral holes in h.c.p. metal lattice and two types of interstitial superstructures are found at the hypo- and hyper-stoichiometric composition $HfO_{1/6-}$ and $HfO_{1/6+}$ below 430°C. The lattice constants of the hexagonal supercells are respectively $a=\sqrt{3}a_0$, $c=3c_0$ and $a=\sqrt{3}a_0$, $c=2c_0$, where $a_0\sim3.2$Å and $c_0\sim5.1$Å are those of the metal lattice. The oxygen sublattices are described in terms of the stacking sequence of interstice layers parallel to the close-packed planes of the metal atoms, which varies continuously from A□B□C□ $\cdots$ for $HfO_{1/6-}$ to A□B□ $\cdots$ for $HfO_{1/6+}$. The concentration dependence of the ordered structures is interpreted in terms of strain ordering.

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