著者 | 山口 智
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ABSTRACTS OF PAPERS
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Interstitial Order–Disorder Transformation in the Ti–O Solid Solution. I. Ordered Arrangement of Oxygen*

Sadae Yamaguchi
The Research Institute for Iron, Steel and Other Metals

Abstract

The crystal structure of the interstitial solid solution of alpha titanium-oxygen system has been investigated by a combined method of electron, neutron and X-ray diffraction as functions of composition and annealing temperature. The existence of two-types of interstitial superstructure has been established over nearly the whole composition range below the critical temperature. One of them designated as $\alpha'$ has a layer-ordered structure of the anti-Cd(OH)$_2$ type (space group $P\overline{3}m1$) involving out-of-steps with regard to oxygen distribution. The other is a low-temperature form $\alpha''$ which has a trigonal symmetry (space group $P\overline{3}1c$) with the cell dimension of $a=\sqrt{3}a_0$ and $c=2c_0$ ($a_0$ and $c_0$ are the lattice constants of the original h.c.p. cell). The oxygen distribution in this phase is generally specified in terms of composition dependent parameters of occupation probabilities for the three octahedral interstitial sites 2(a), 2(c) and 2(d). The structure of $\alpha''$ at a special composition of TiO$_{0.33}$ coincides with the model proposed by Holmberg.