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journal or publication title	Science reports of the Research Institutes, Tohoku University. Ser. A, Physics, chemistry and metallurgy
volume	24
page range	83-83
year	1972
URL	http://hdl.handle.net/10097/27641

Electrical and Magnetic Properties Related to Defect Structure in the Nonstoichiometric TiO and VO Phases*

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Abstract

X-ray and neutron diffractions, electrical resistivity, magnetic susceptibility, Hall coefficient, and Knight shift were measured as a function of composition or temperature for the TiO and VO phases. We considered that the large amount of randomly distributed vacancies in these phases was not produced by thermal excitation but resulted from the internal energy gain which was ascribed to the formation of a metallic band due to the extreme contraction of lattice parameters. The maximum internal energy gains were calculated as about 1 eV for both phases. In a tentative model of the energy band structure for these phases, the Fermi energy was placed at the concave part in the density of states versus the energy curve, where the overlap of the bottom of the 3d-conduction band and the top of band owing to the 3d-electrons trapped at oxygen vacancies was strongly expected.

* The **1562th** report of the Research Institute for Iron, Steel and Other Metals. Published in FERRITES: Proceedings of the International Conference, 1970, p. 568.