Equilibrium Concentration of Vacancies in Titanium Monoxide under High Pressure

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Abstract

A simple statistical thermodynamical calculation is made to estimate an equilibrium concentration of vacancies under high pressure in titanium monoxide which contains an abnormally large number of vacancies in both titanium and oxygen lattice sites. Work necessary to create a vacancy, interaction energies between vacancies and entropy of mixing are taken into account in deriving Gibbs free energy of a titanium monoxide crystal. The contribution to the free energy from thermal vibration is also considered. The result of calculation shows that the concentration of vacancies, that is 14.5% at 1 bar, decreases to 10–14% under the pressure as high as 100 kbar, the amount of decrease being dependent on the parameters chosen. Discussion is given in terms of this theoretical prediction on the results of recent high pressure experiments made on titanium monoxides.

* The **1559th** report of the Research Institute for Iron, Steel and Other Metals. Published in the Japanese Journal of Applied Physics, **10** (1971), 1149.