Crystal structure and the structural disorder of yttrium tantalate

T. Tsuji (A), M. Yashima (A), T. Wakita (A), Xi Qu (A), T. Ueda (A), Y. Kawaike (A) T. Komatsu (A), Y. Phat (A), R. Ali(B), Y. Matsushita(B)

(A) Department of Materials Science and Engineering, Interdisciplinary Graduate School of Science and Engineering, Tokyo Institute of Technology, (B) National Institute for Materials Science

Yttria-tantalum oxide system has various phases such as defect-fluorite, weberite phase and cubic phase. Defect-fluorite type structure has high diffusion coefficient of oxide ions. On the other hand, the weberite-type structure exhibits lower diffusion coefficient. In this study, we prepare defect-fluorite-phase Y0.79Ta0.21O1.7 and investigate the crystal structure and positional disorder of oxide ions through MEM (Maximum Entropy Method) analysis of neutron powder diffraction data measured at RT and at high temperatures

Neutron powder diffraction experiments were carried out in air in the temperature range from 298 K to 1824(3) K. Neutron powder diffraction measurements were conducted in air with a 150-detector system, HERMES, installed at the JRR-3M reactor in Japan Atomic Energy Agency, Tokai, Japan. Neutrons with wavelength 0.18207 nm were obtained by the (311) reflection of a Ge monochromator. The experimental data were analyzed by a combination technique of Rietveld analysis, the maximum-entropy method (MEM), and the MEM-based pattern fitting.

Rietveld analysis was carried out assuming the ideal fluorite-type structure where the (Y,Ta) and O atoms were put at 4a 0,0,0 and at 8c 1/4,1/4,1/4 sites of Fm-3m symmetry, respectively. The isotropic atomic displacement parameters were used for all the atoms. At higher temperatures the B(O) was larger than the B(Y,Ta), suggesting a larger diffusion coefficient of oxide ions. MEM analysis was carried out using the structure factors obtained in the Rietveld analysis. Number of structure factors derived in the analysis was 11. The spatial distribution of oxide ions is larger at higher temperatures and it seems to have disordering along <1 0 0> directions, indicating the diffusion path. (Figures (a), (b) and (c)).

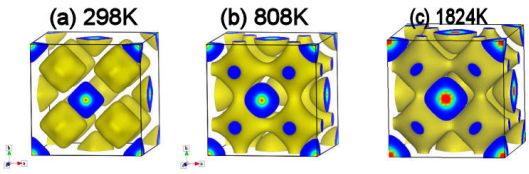

Fig. 1.