Crystal Structure of Advanced Lithium Titanate with Lithium Oxide Additives

T. Hoshino, K. Sasaki, K. Shintoku, K. Tsuchiya, K. Hayashi, A. Suzuki, T. Hashimoto and T. Terai

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Fusion Research and Development Directorate, Japan Atomic Energy Agency, 4002, Narita-cho, Oarai-machi, Higashiibaraki-gun, 311-1393 Ibaraki-ken, Japan

Department of Nuclear Engineering and Management, School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, 113-8656 Tokyo, Japan

Directors of Fusion Energy Research, JAEA, 4001 Oarai-machi, Higashi-ibaraki-gun, 311 1393 Ibaraki-ken, Japan

Graduate School of Engineering : TOKYO, University of Tokyo, Nuclear Pressional School, 22 Shirakata-Shirane, Tokai, Naka, 318-1188 Ibaraki, Japan

Department of Integrated Sciences in Physics and Biology, College of Humanities and Sciences, Nihon University, 3-8-1 Sakurajousui, Setagaya-ku, 156-8550 Tokyo, Japan

Nuclear Professional School, Graduate School of Engineering, The University of Tokyo, 2-22 Shirakata-Shirane, Tokai-mura, Naka-gun, 319-1188 Ibaraki, Japan

hoshino.tsuyoshi@jaea.go.jp

Li$_2$TiO$_3$ is one of the most promising candidates among solid breeder materials proposed for fusion reactors. Addition of H$_2$ to inert sweep gas has been proposed for enhancing the release of bred tritium from breeder material. However, the mass of Li$_2$TiO$_3$ was found to decrease with time in the hydrogen atmosphere. This mass change indicates that the oxygen content of the sample decreased, suggesting the change from Ti$^{4+}$ to Ti$^{3+}$, and also indicates that the partial pressures of Li-containing species were increased by the hydrogen atmosphere. In order to control the mass-change at the time of high temperature use, the development of Li$_2$TiO$_3$ which has Li$_2$O additive is needed. Furthermore, since Li$_2$TiO$_3$ is reduced in hydrogen atmosphere, it is important to investigate the reduction characteristic with Li$_2$O addition. In the present paper, the crystal structure and non-stoichiometry of Li$_2$TiO$_3$ added with Li$_2$O have been extensively investigated by means of X-ray diffraction (XRD), thermogravimetry, and so on.

In the case of the Li$_2$TiO$_3$ samples used by the present study, LiO-C$_2$H$_5$ or LiO-i-C$_3$H$_7$ and Ti(O-i-C$_3$H$_7$)$_4$ were mixed in the proportion corresponding to the molecular ratio Li$_2$O/TiO$_2$ of either 2.00 or 1.00. These samples are designated as L200-C$_2$H$_5$, L200-i-C$_3$H$_7$, L100-i-C$_3$H$_7$ (Li$_2$O/TiO$_2$ = 2.00), L200-i-C$_3$H$_7$ (Li$_2$O/TiO$_2$ = 2.00) and L100-i-C$_3$H$_7$ (Li$_2$O/TiO$_2$ = 1.00), respectively.

XRD measurement showed that the structure of Li$_2$TiO$_3$ which had the lithium oxide additive changed as follows. L100-i-C$_3$H$_7$, L200-i-C$_3$H$_7$ exist as double phases, and L200-C$_2$H$_5$ and L100-i-C$_3$H$_7$ exist as single phases. In thermogravimetry, the mass of L100-i-C$_3$H$_7$ was found to decrease with time by lithium defects. Further, the mass of L200-C$_2$H$_5$ increased with time by oxygen defects, where no presence of oxygen defects was indicated.

The overall results suggest that the Li$_2$O additives are able to control not only the amount of oxygen defects but also the partial pressures of Li containing species.

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