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Analysis of Crystal Structure and Thermal Expansion Property of Li_2TiO_3 by High Temperature X-ray Diffraction using Synchrotron Radiation

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Li_2TiO_3 attracts much interest as tritium breeding materials in a thermonuclear fusion reactor. Since tritium breeder is used at high temperatures, the crystal structure at high temperatures and thermal expansion property are important information. Some of the authors performed high temperature CuKα X-ray diffraction measurements of Li_2TiO_3 and indicated possibility of existence of higher order phase transition at about 450 °C.[1)] However, measurements with higher resolution have been required to clarify the crystal structure and thermal expansion property. In this study, crystal structure at high temperature and thermal expansion property of Li_2TiO_3 have been investigated using synchrotron X-ray radiation.

Li_2TiO_3 specimen was prepared with solid state reaction method.[1)] Variation of crystal structure and lattice constants of Li_2TiO_3 on temperature has been evaluated with synchrotron X-ray diffraction employing originally designed furnace[2, 3)] at BL-4B2 in Photon Factory, KEK.

As shown in Fig. 1, Bragg angles of the diffraction peaks of Li_2TiO_3 could be measured with high resolution by using X-ray from synchrotron radiation, due to far smaller peak overlapping compared to one observed with CuKα radiation. Some diffraction peaks, for example 006 in Fig. 1, which were difficult to be observed with CuKα radiation due to low intensity, could be successfully detected with synchrotron radiation. Fig. 2 shows temperature dependence of lattice constants and molar volumes, calculated from synchrotron X-ray diffraction patterns. Discontinuous variation of thermal expansion coefficient at about 450 °C, which suggested higher order phase transition, was more clearly observed than CuKα X-ray diffraction measurements.

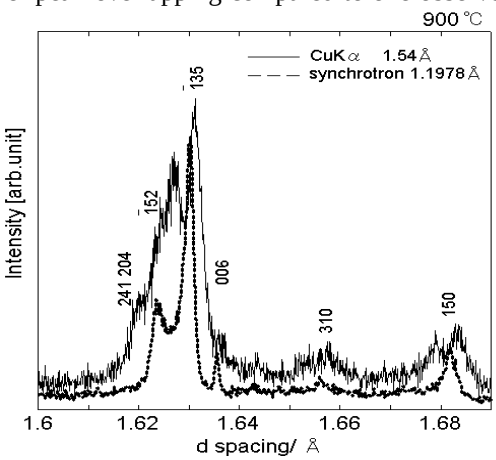

Fig. 1 X-ray diffraction patterns of Li_2TiO_3 using synchrotron and Cu*K*α radiation at 900 °C. *d* range is 1.6-1.7 Å.

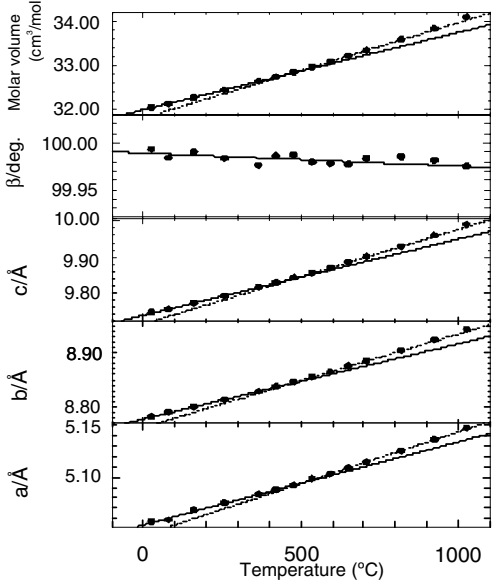

Fig. 2 Lattice constants and molar volumes of Li_2TiO_3 at various temperatures calculated from synchrotron X-ray diffraction peaks.

References

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