Study of surface morphology effects on hydrogen isotope behavior in ternary lithium oxides

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In nuclear fusion reactors, understanding of tritium release process in tritium breeder materials is important for the fuel cycle. In this paper, hydrogen isotope behavior in ternary lithium oxides (LiNbO$_3$, Li$_2$TiO$_3$) with different surface morphology was studied.

In experiments, single crystals and poly crystals of LiNbO$_3$ and Li$_2$TiO$_3$ were used as samples. The samples were heated in a 100 Pa D$_2$O atmosphere for deuterium absorption. After cooling-down and evacuation, the samples were transferred to a high-vacuum TDS system. Then, in the TDS system, the samples were heated to high temperature for hydrogen isotope desorption. The desorbed gases were monitored by a mass spectrometer, and TDS spectra of mass spectrometer signals versus temperature or time were obtained. In addition, some samples were heated in a high vacuum (10$^{-5}$ Pa) or in air at high temperatures (e.g. 1233 K) in order to prepare samples of various surface morphologies.

In both LiNbO$_3$ and Li$_2$TiO$_3$, hydrogen isotopes were mainly desorbed as water species (H$_2$O, HDO, D$_2$O). Three peaks were observed in TDS spectra: (1) desorption of physically adsorbed water molecules, (2) desorption of chemically adsorbed hydroxyl groups, and (3) desorption of deuterium diffused from the bulk, respectively. The position of peak (3) moved to a lower temperature in TDS spectra as the grain size decreased. The intensity of peak (1) diminished obviously after pretreatment at 1233 K in vacuum for several hours, while that of peak (2) did not change much.

In order to check the surface morphology of each sample, SEM observation was performed. It was indicated that the surface roughness was greatly smoothened by this high-temperature pretreatment. BET was also adopted to determine the specific surface area of powder samples. The effect of surface morphology (roughness, specific surface area, reduction from atmosphere and sample holder) on hydrogen isotope behavior was discussed in comparison with results of computer simulations.