Phase transition and internal crystal structure of spuerprotonic conductor, $Rb_{3-x}K_xH(SeO_4)_2$

R. Kiyanagi[1#], Y. Matsuo[2], T. Ohhara[1], T. Kawasaki[1], K. Oikawa[1], K. Kaneko[1], I. Tamura[1],
T. Hanashima[3], K. Munakata[3], A. Nakao[3], Y. Kawakita[1]

[1]J-PARC Center, Tokai, Ibaraki 319-1195, Japan
[2]Department of Life Science, Setsunan University, Neyagawa, Osaka 572-8508, Japan
[3]Comprehensive Research Organization for Science and Society (CROSS), Tokai, Ibaraki, 319-1106, Japan

 # a corresponding author: E-mail ryoji.kiyanagi@j-parc.jp

The materials represented as $M_3H(XO_4)_2$ (M = alkaline metal, X = Se or S) are known to exhibit high protonic conductivities at moderately high temperature. The high protonic conductivity emerges upon a structural phase transition, and the phase transition temperature varies depending on the elements of M and X. In order to clarify the roles of the elements for deciding the phase transition temperature, solid solutions of $Rb_3H(SeO_4)_2$ and $K_3H(SeO_4)_2$ ($Rb_{3-x}K_xH(SeO_4)_2$, x=0,1,2,3) were studied by means of conductivity measurements and single crystal neutron structure analyses.

The conductivities were measured in the temperature range between 300 K and 500 K with an LCR meter. The single crystal neutron diffraction experiments were conducted on SENJU, a single crystal time-of-flight neutron diffractometer at MLF/J-PARC.

The conductivity measurements revealed that the changes of the transition temperature and the conductivity were not linear to the x values (Fig. 1). The structure analyses showed that K atoms preferred to reside at one of two possible crystallographic sites (Fig. 2). In addition, the distortion of SeO_4 tetrahedron was enhanced as x increased. The variations of the phase transition temperature and the tetrahedron distortion were found to coincide with each other implying strong relation between them.

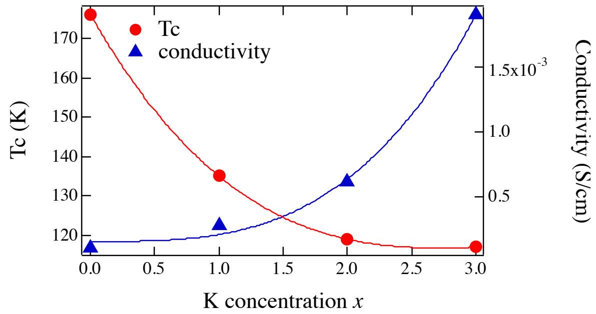

Fig. 1 Variation of Tc and the conductivities with respect to the K concentration of x. Curves are guide for eyes.

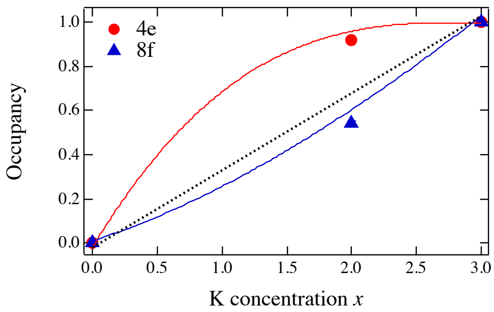

Fig. 2 Variation of the site occupancies of K atom at the 4e and 8f sites with respect to the K concentration of x.