Measurement of over dumped phonon on protonic conductor $K_3H(SeO_4)_2$

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Protonic conductor $K_3H(SeO_4)_2$ undergoes first order phase transition at 390 K (T_C, 385 K on the cooling process), and shows high electric conductivity above T_C. We have measured the inelastic neutron scattering (INS) of the material, and observed a broad spectrum around 0 meV at zone boundary L-point above T_C. Intensity of the spectrum increases with decreasing the temperature, and the spectrum is considered to be caused by an over dumped phonon. However, quantitative nature of the spectrum was unclear because of the narrow shape of the spectrum less than the resolution. We, therefore, performed an energy scan from -0.2 meV to 0.2 meV under a possible high resolution within the scattering condition. The final momentum vector k_f was fixed at 1.39 Å^{-1}. The energy resolution was estimated as 88(3) μeV from the FWHM of incoherent scattering of hydrogen under a collimation of G-Be-20′-S-40′-Be-40′.

Figure 1 shows the temperature dependence of INS spectrum at L-point subtracted incoherent scattering which obtained at 0.7 2 0. The broad peak was observed only at L-point, therefore, the spectra are caused by an coherent scattering having the same symmetry of rotational SeO_4 tetrahedra. To analyze the data in Fig. 1, a equation formulated for neutron scattering cross section by over dumped phonon [1] was used. The equation was simplified as $AT\gamma\{(T - T_0 + B\Delta q^2)(E^2 + \gamma^2)\}^{-1}$ with the four parameters A, B, T_0 and γ. The results of fitting substituted $\Delta q = 0$ for the fitting function are illustrated as the plane in Fig 1. As shown in the figure, the data are good agreement with the calculated plane. The extrapolated Curie temperature T_0 was obtained as 368(2) K. The parameter γ was assumed as a linear function of T obtained from fitting at each temperature using a normal Lorentz function, as shown in the inset of Fig 1. The FWHM of the spectrum, 2γ, slightly depends on the temperature, and is obtained as 60(4) μeV and 70(6) μeV at 386 K and 435 K, respectively. This energy range corresponds to 14(1) GHz and 17(1) GHz, and gives the lifetime from $7.1(4) \times 10^{-11}$ s to $5.9(4) \times 10^{-11}$ s. Although it is expected that the lifetimes are little longer then this result because of the resolution, this time scale agrees with the stationary time of conduction proton, $9.0(8) \times 10^{-11}$ s at 388 K and $4.9(3) \times 10^{-11}$ s at 433 K, obtained from quasi elastic neutron scattering (QENS) [2]. It shows that proton conduction is simultaneous with the motion of rotational mode in phase I.

References

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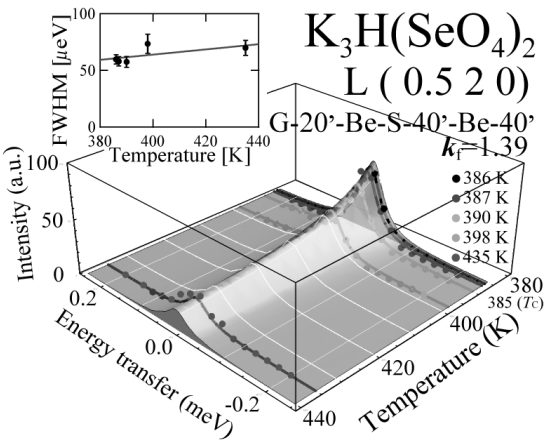

Fig. 1. Temperature dependence of INS spectra at L-point (subtracted incoherent scattering).