Phonon dynamics of Mg_3Sb_2

K. Ono, R. Sakagami, Y. Goto, C. H. Lee

AIST, Japan

Thermoelectric materials are attracting interest because they can convert waste heat to electricity. The performance of thermoelectric materials is characterized by the dimensionless figure of merit $ZT = S^2T/(\rho^*\kappa)$ (S: Seebeck coefficient, ρ: electrical resistivity, κ: thermal conductivity). Zintl phase compounds are one of the most famous systems of thermoelectric materials. In particular, Mg_3Sb_2 is one of promising candidate exhibiting high thermoelectric performance. It shows high value of the dimensionless figure of merit ZT ~ 1.65 with quite low lattice thermal conductivity of κ_L ~ 0.7 W/mK at T = 725 K [1-3]. Although the origin of its low κ_L attracted great attention, phonon dynamics using single crystal has not been well explored.

In this experiment, we conducted inelastic neutron scattering measurements using a triple-axis spectrometer, HER installed at C1-1 beam port of JRR-3 reactor in JAEA at Tokai. The final neutron energy was fixed at Ef=6.0 meV using a pyrolytic graphite (PG) monochromator and analyzer. Solar-type horizontal collimators with 80' divergence were inserted in between sample and analyzer. Scattering plane was (hk0). A single crystal of Mg_3Sb_2 weighs 7.25g was used for the measurement.

Figure 1 shows typical spectrum of transverse acoustic phonon at a room temperature. A well-defined peak was observed, which allowed to analyze peak position and width appropriately at low energy region. Measurements were performed along Γ-M and Γ-K at room temperature. Based on the observation, phonon dispersions around Γ point were clarified. Further measurements are required to obtain information about temperature dependence to understand their anharmonic behavior.

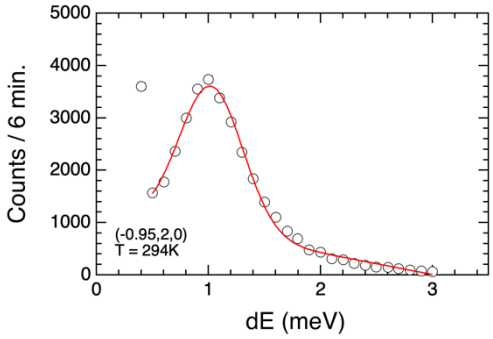

Fig. 1. Inelastic neutron scattering spectrum at ***q*** = (-0.95,2,0) at a room temperature.

[1] H. Tamaki et al., Adv. Mater. 28, 10182 (2016).
[2] J. Zhang et al., Nature Commun. 8, 13901 (2017).
[3] K. Kihou *et al*., J. Mater. Res. Technol. 10, 438 (2021).