 MLF Experimental Report	提出日 Date of Report 30, June, 2016
課題番号 Project No. 2016A0042 実験課題名 Title of experiment Phonon density of thermoelectric bismuth chalcogenide $\text{LaOBiS}_{2-x}\text{Se}_x$ 実験責任者名 Name of principal investigator Yoshikazu Mizuguchi 所属 Affiliation Tokyo Metropolitan University	装置責任者 Name of responsible person Seiko Kawamura 装置名 Name of Instrument/(BL No.) BL14 実施日 Date of Experiment 16-22, May, 2016 6, June, 2016

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.
$\text{LaOBiS}_{2-x}\text{Se}_x$ polycrystalline samples with $x = 0, 0.2, 0.4, 0.6, 0.8,$ and $1.$

2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons.
<p>We have performed inelastic neutron scattering experiment at AMATERAS (BL14) for the polycrystalline samples of $\text{aOBiS}_{2-x}\text{Se}_x$ ($x = 0, 0.2, 0.4, 0.6, 0.8,$ and 1). The energy used in this study was $E_i = 94$ meV, and we obtained four spectra with $E_i = 5, 10, 23,$ and 94 meV for each measurements. For $x = 0$ and 1, we performed low-temperature measurements at $T = 10, 50, 100, 200,$ and 300 K using a cryostat. For all the samples, measurement at 300 K was performed, and the Se doping effect on the phonon spectrum was discussed.</p> <p>From temperature-dependent experiments for $x = 0$ and 1, we observed hardening of the low-energy phonon mode, which is corresponding to the vibration modes within the Bi-chalcogen conducting plane, with decreasing temperature. In Fig. 1, the temperature dependences of peak energy and full width half maximum (FWHM) for LaOBiSSe ($x = 1$), obtained from this study, are plotted. We observed broadening of the low-energy peak with increasing temperature, suggesting that phonon anharmonicity is induced at high temperatures in $\text{LaOBiS}_{2-x}\text{Se}_x$. To clarify the anharmonic nature of in-plane phonons, experiments at temperatures higher than room</p>

2. 実験方法及び結果(つづき) Experimental method and results (continued)

temperature are needed; hence, we submitted a proposal for this study to J-PARC (2016B period). In contrast to the low-energy modes, high-energy phonon modes, which are corresponding to the vibrations of the block-layer atoms, do not exhibit noticeable changes.

From measurements at 300 K for $x = 0-1$, we observed softening of low-energy mode with increasing Se concentration. The results can be consistent with the experimental results of thermal conductivity of $\text{LaOBiS}_{2-x}\text{Se}_x$; the suppression of thermal conductivity by Se substitution can be understood by softening of in-plane phonon mode by Se substitution

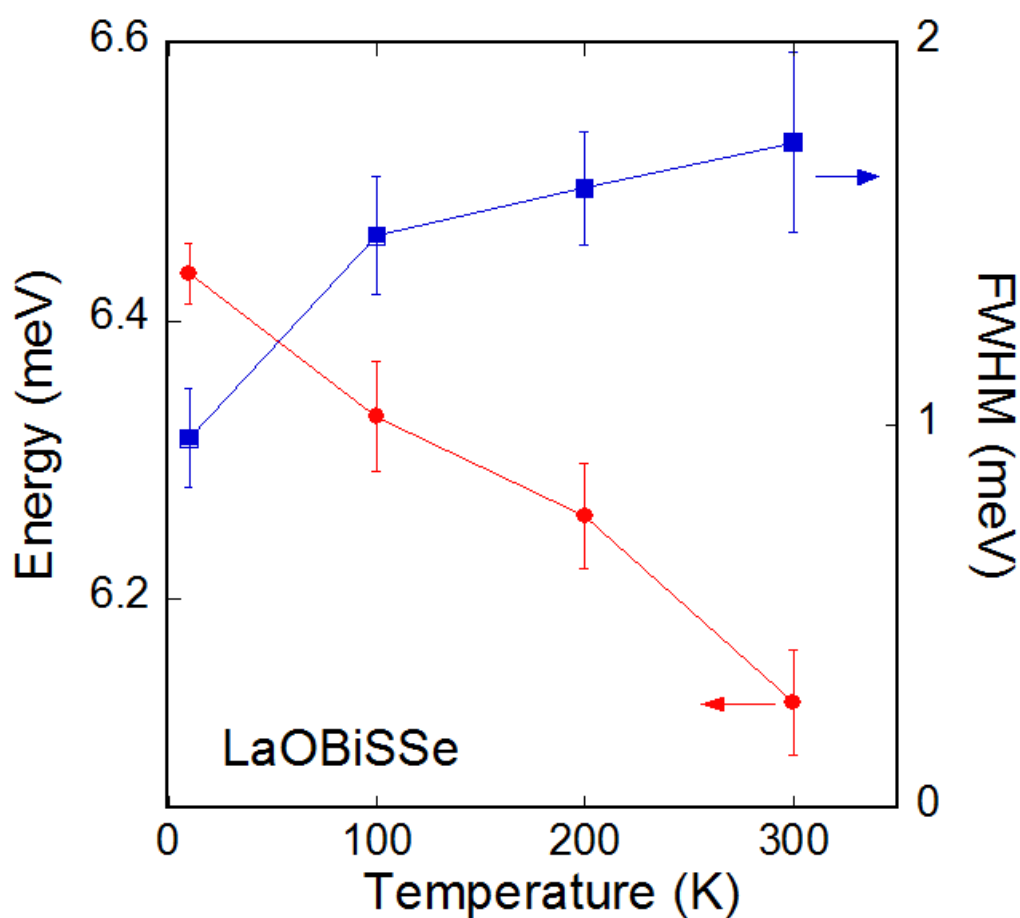


Fig. 1. Temperature dependences of peak energy and full width half maximum (FWHM) for LaOBiSSe ($x = 1$).