

実験報告書様式(一般利用課題・成果公開利用)

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

 MLF Experimental Report	提出日 Date of Report
課題番号 Project No. 2014A0324 実験課題名 Title of experiment Phonon dynamics in the off-center rattling system $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ 実験責任者名 Name of principal investigator Mitsutaka Nakamura 所属 Affiliation Japan Atomic Energy Agency	装置責任者 Name of responsible person Kenji Nakajima 装置名 Name of Instrument/(BL No.) AMATERAS (BL14) 実施日 Date of Experiment 2014/05/08 13:00 – 2014/05/13 13:00 2014/11/17 13:00 – 2014/11/18 13:00

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.

<p>1. 試料 Name of sample(s) and chemical formula, or compositions including physical form.</p> <p>Type-I clathrate $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ single crystal Total amount: 10.7g</p>

<p>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> <p><u>Experimental method</u></p> <ul style="list-style-type: none"> - $E_i=42.1, 15.2, 7.75$ meV (multi-E_i); Fast Disk Chopper #2 = 150Hz - Rotating crystal measurement - Temperatures: 5K, 295K (Wide angle scan) 50K, 100K, 150K, 200K, 250K (Narrow angle scan) <p><u>Experimental results</u></p> <p>The type-I clathrate compounds encapsulating guest atoms in cages are known as a candidate of "phonon-glass electron-crystal (PGEC)" materials which can be applicable to the thermoelectric devices. In this study we have investigated the phonon dynamics of single crystalline $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ where the rattling guest Ba atoms take off-center position in cages. As shown in Fig.1 and Fig.2, we succeeded to obtain the high quality data of phonon dispersion in $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ single crystal.</p>

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

In addition, we could collect temperature dependent data for several points thanks to the high-throughput performance of AMATERAS spectrometer.

We are now precisely analyzing the crossing behavior between the rattler modes and the acoustic phonon branches. The comparison of crossing behavior with on-center clathrate such as $\text{Ba}_8\text{Ga}_{16}\text{Ge}_{30}$ [1] should provide a clue to the mystery of peculiar phonon dynamics in off-center clathrates.

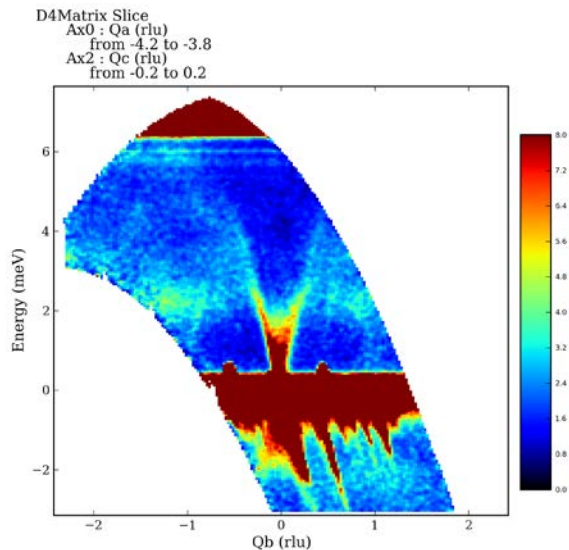


Fig.1: The neutron intensity map of single crystalline $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$. Transverse phonon along the [0LL] direction near (-400) reciprocal lattice points is shown. The INS measurements were performed at room temperature.

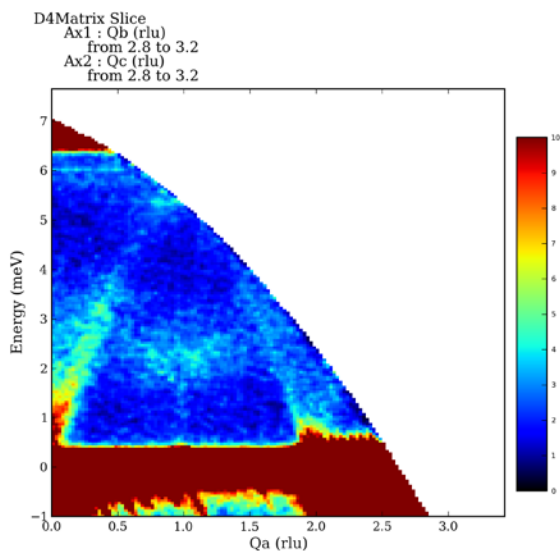


Fig.2: Same as in Fig.1, but transverse phonon along the [H00] direction near (033) reciprocal lattice points is shown.

[1] M. Christensen *et al.*, Nature Materials **7** (2008) 811.