X-ray diffraction study of intermetallic $Ba_8Ga_{16}Sn_{30}$ clathrate compound

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Intermetallic clathrate compounds have become an important research subject in condensed matter physics due to their promising technological applications that make use of thermoelectricity, that is, electricity generated in a device submitted to a temperature gradient between its extremities. Good thermoelectric materials are those that have low thermal conductivity and high electrical conductivity. These antagonistic conditions are present in the clatrates where anharmonic vibrations of the weakly bound atoms of Ba inside large cages of Ga-Sn atoms create an efficient acoustic phonon scattering mechanism reducing heat conduction without significantly altering the electrical transport. Such materials are known as "phonon glasses, electron crystals". The $Ba_8Ga_{16}Sn_{30}$ compound in the β-phase (type-I clathrate) form a structure which has two smaller dodecahedrons and six larger tetrakaidecahedrons cages with one Ba atom inside each cage[1]. In the smaller cages, the guest atoms of Ba occupy the crystallographic site 2a, but X-ray diffraction measurements done at room temperature have shown that the Ba atoms hosted in the large cages occupy the four off-center crystallographic positions (24k site) instead of the cage center (6d site) with equal probability. The acoustic phonon scattering mechanism is associated to the guest atom vibration, or rattling, inside the large tetrakaidecahedrons cages. However, it is still unknown if the atomic motion between neighboring cages is correlated or not. In this work, single crystals of $Ba_8Ga_{16}Sn_{30}$ were oriented through the Laue method and their mosaicity was found by measuring Bragg peaks with a four-circle diffractometer. X-ray diffraction measurements at low temperatures were performed to verify the existence of different occupation rates in the four crystallographic sites in order to clarify the feasibility of a time resolved X-ray diffraction measurements on these samples.

[1] Avila, M. A., Suekuni, K., Umeo, K., Fukuoka, H.,Yamanaka, S., Takabatake, T., *Appl. Phys. Lett*., **92**, 041901 (2008).

Agradecimentos: Ao suporte financeiro da Fundação de Amparo à Pesquisa do Estado de São Paulo FAPESP e ao suporte técnico do Laboratório Nacional de Luz Síncrotron LNLS.