MS26 Quantum mechanical models for dynamics and diffuse scattering

MS26-01
Thermal diffuse scattering and ab initio phonons in LaPdSb
M. Gutmann [1], D. Adroja [1], B. Rainford [2], K. Refson [1], M. Von Zimmermann [3]
[1]Rutherford Appleton Laboratory - Chilton Didcot (United Kingdom), [2]University of Southampton - Southampton (United Kingdom), [3]DESY - Hamburg (Germany)

Abstract
LaPdSb has been found experimentally to be a potential high temperature thermoelectric material[1]. The compound crystallises in a hexagonal structure with layers of La alternating with layers containing Pd and Sb [2]. Here, we present results combining ab-initio phonons computed using the CASTEP code along. These show a number of low-energy phonon modes supporting the thermoelectric properties. The ab-initio phonons are used to compute thermal diffuse scattering. Neutron diffuse scattering patterns were collected using the SXD beamline at the ISIS spallation neutron source and complementary high-energy X-ray diffuse patterns were obtained using beamline BW5 at DESY. These patterns are compared with the theoretical thermal diffuse scattering patterns. Alternatively, the thermal diffuse scattering can also be modelled using a simple balls-and-springs model. This gives complementary information on the bonding-strength between the various metal ions.

References
[1] T. Sekimoto et al., Appl. Phys. Lett _89_, 092108 (2006).
[2] The crystals for our experiments were grown by Drs. K. Kathoh (National Defense Academy, Yokosuka, Japan) and H. Aoki (Dept. of Physics, Tohoku University, Sendai, Japan).