Helmholtz - OCPC - Programme 2017-2021

for the Involvement of Postdocs in Bilateral Collaboration Projects with China

PART A

Title of the project
Comparative study of lattice dynamics in thermoelectric materials

Helmholtz Centre and institute
Karlsruhe Institute of Technology (KIT), Institute for Quantum Materials and Technologies (IQMT)

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Description of the project:

Thermoelectric materials are interesting for energy applications as they can transform heat into useful electricity. The energy transformation efficiency of a thermoelectric material is determined by the figure of merit, $ZT = \sigma S^2 T/(\kappa_L + \kappa_E)$ [κ_L (κ_E): lattice (electronic) component of thermal conductivity, σ: electrical conductivity, S: Seebeck coefficient, T: absolute temperature]. As such, the electrical energy produced is in the form of a current driven by the thermoelectric voltage, which is given by $-S\Delta T$, whereas heat conduction and electrical resistance are parasitic. Thus, efficient thermoelectric materials must have a low thermal conductivity, to preserve the temperature gradient exploited to generate a voltage. Therefore, reducing κ_L is central to obtaining high-performance thermoelectrics. Inelastic neutron scattering experiments in one of the most studied thermoelectric materials PbTe [Delaire *et al.*, Nature Mat. **10**, 614 (2011)] revealed strongly anharmonic phonon scattering which was proposed to play an important role for the extremely low lattice thermal conductivity of $\kappa_L = 2\,\mathrm{Wm^{-1}K^{-1}}$ [Chen et al., Phys. Rev. Lett. **113**, 105501 (2014)].

Recently, we performed inelastic neutron scattering (INS) experiments as function of pressure (@ T = 300 K) and temperature (@ ambient pressure) on PbTe. The anharmonicity of the zone center phonon at room temperature [Fig. 1(a)] is strongly reduced under high pressure but at ambient pressure a large linewidth persists unexpectedly to low temperatures [Fig. 1(b)].

Within this project, we seek at exploring anharmonicity in the temperature-pressure parameter space not only in PbTe but also a closely related material, SnTe. Interestingly, the incipient ferroelectric-structural phase of PbTe is fully developed SnTe ($T_S \approx 40$ K). Hence, the intertwined effects of this phase transition - to which the zone center mode responds strongly - and anharmonicity can be explored by a comparative study of SnTe and PbTe.

The successful candidate will utilize inelastic neutron scattering at large-scale research facilities in order to unravel the lattice dynamical properties of (Pb,Sn)Te under variable pressure and temperatures. He/she will characterize the single crystal specimen with in-house x-ray diffraction and other methods available at IQMT. A close collaboration with the theory group of Dr. Yue Chen at HKU-SIRI is essential.

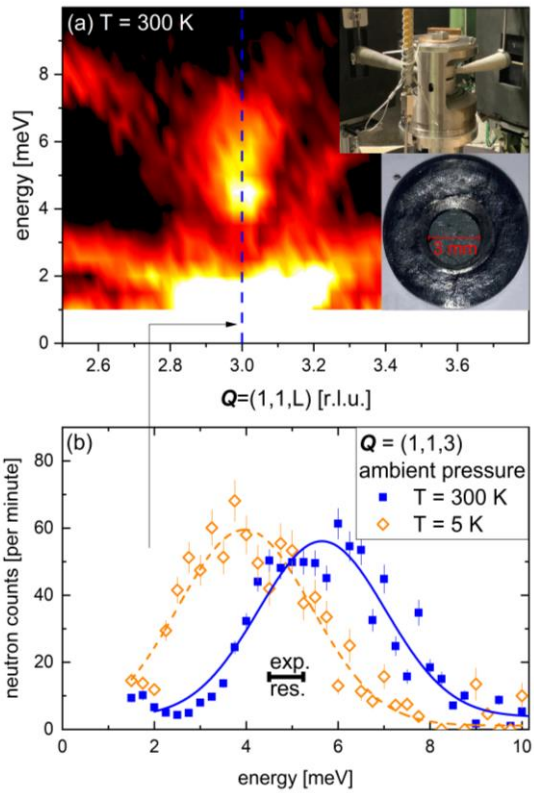

FIG. 1. Inelastic neutron scattering (INS) in PbTe. (a) Map of phonon intensities close to the zone center $\boldsymbol{\tau}$ = (1,1,3) showing the broad transverse optic mode at 5 meV and L = 3. Pictures (right) show the high-pressure setup for INS which we recently used at room temperature. (b) Energy scans at the zone center $\boldsymbol{\tau}$ = (1,1,3). Data are Bose and energy corrected.

Description of existing or sought Chinese collaboration partner institute:

The University of Hong Kong Shenzhen Institute of Research and Innovation (HKU-SIRI) established in 2011 with the support of the Shenzhen Municipal Government, is an integral part and an extension into mainland China of the research conducted by the University of Hong Kong (HKU). HKU-SIRI is a member institution of Shenzhen Virtual University Park, which has developed a postdoctoral research station registered with the Office of the China Postdoctoral Council (OCPC) to integrate postdoctoral stations of member institutions. HKU-SIRI plays an important role in transferring science and technology from HKU to mainland China.
The group of Dr. Yue Chen at HKU-SIRI specializes in the studies of materials physics for thermal and electrical transports, such as lattice dynamics and electronic structures. In particular, he has been focusing on the phonon coupling problems in thermoelectric materials using density functional theory-based first-principles methods. He is experienced in studying the intrinsic ultralow thermal conductivities of crystalline solids with strong lattice anharmonicity and the related phonon scattering mechanisms.

Required qualification of the post-doc:

- PhD in physics or related subject
- Experience with solid state physics
- Additional skills in neutron scattering and/or *ab-initio* calculations are beneficial

PART B

Documents to be provided by the post-doc, necessary for an application to OCPC via a postdoc-station in China, which is affiliated to a research institution like a university:

- Detailed description of the interest in joining the project (motivation letter)
- Curriculum vitae, copies of degrees
- List of publications
- 2 letters of recommendation
- Proof of command of English language

PART C

Additional requirements to be fulfilled by the post-doc:

- Max. age of 35 years
- PhD degree not older than 5 years
- Very good command of the English language
- Strong ability to work independently and in a team

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