Contribution ID: **224** Type: **Oral presentation**

Dysurf: A program for simulating four-dimensional dynamical structure factor for inelastic neutron scattering measurement

Inelastic neutron scattering is a powerful technology to measure the lattice dynamics of materials, which is essential to understand the thermal transport properties and other phonon-related properties. The realization of obtaining a sufficient amount of effective data within a limited time is a major demand facing the development of the current inelastic scattering technology. Here, we develop a Fortran program that can be applied to simulate the four-dimensional dynamical structure factors (Dysurf) for inelastic neutron scattering experiments. With the underlying theoretical formalisms, the detailed implementation of the program is described. Based on the second-order force constants from the first-principles method, the Dysurf code is able to effectively calculate the four-dimensional dynamical structure factors, which can be used to design and optimize the inelastic neutron scattering measurement to save the valuable beamtime, before the measurement. It can also help the users to find the improper procedure and adjust the plan during the measurement, or analyze the neutron data to reveal the underlying physical mechanism after the measurement. Four main applications of this code with the corresponding examples will be introduced here, including the two-, there- and four-dimensional dynamical structure factors, thermal diffuse scattering and slice function at the specific point in the Brillouin zone.

Primary authors: WEI, Bing (Beijing Institute of Technology); LIN, Changpeng (École Polytechnique Fédérale de Lausanne); HONG, Jiawang (Beijing Institute of Technology); JUNYAN, Liu (Beijing Institute of Technology); REN, Qi (Beijing Institute of Technology); LI, Yongheng (Beijing Institute of Technology)

Presenter: HONG, Jiawang (Beijing Institute of Technology)

Session Classification: Software