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Calculation of neutron scattering libraries for liquid ortho-deuterium and hydrogen deuteride

The European Spallation Source (ESS) is an international research laboratory which is currently under construction in Lund, Sweden. Once completed, the ESS will provide the brightest pulsed neutron source in the world for neutron scattering studies. The ESS will serve a wide range of research fields using neutron scattering experiments. The neutrons are produced by accelerating protons and firing them at a tungsten target where the protons will knock out neutrons. The neutrons are then slowed down by a moderator to reach lower, more useful energies. Afterwards, they are guided to the experiment stations where they are used in various experiments. A project launched by ESS, called HighNESS, is looking to expand the array of possible neutron science experiments available at the facility. HighNESS proposes to do this by installing a second moderator, which would be able to produce a high intensity of neutrons at lower energies, compared to the first moderator. This would enable experiments in several fields of research which are currently not possible elsewhere. The choice of material which is going to be used in the proposed second moderator is currently being researched.

The performance of moderator materials at neutron sources is often characterized through Monte-Carlo simulations. An important step in this process is the accurate description of the neutron transport through the material on an atomic and molecular level. This data is collected and stored in a scattering library. The next step is to simulate the facility setup using a detailed model of the target and moderator systems, where the scattering library obtained earlier describes how the neutrons will scatter through the moderator materials. This simulation allows one to calculate how many neutrons could serve the experimental stations and what energy they will have, which is crucial to know since this relates directly to the performance of the facility.

The purpose of this thesis has been to generate scattering libraries for two materials, ortho-deuterium and hydrogen deuteride, both which could be used as a moderator at ESS. While scattering libraries exist for ortho-deuterium, these libraries use early theoretical models which could be potentially improved upon by incorporating state-of-the-art molecular dynamics techniques into the model description. The new scattering library for ortho-deuterium uses methods which account for the quantum behaviour of the moderator material, through the use of quantum molecular dynamics techniques. The work carried out for hydrogen deuteride represents the first available scattering library for this material to date. Quantum molecular dynamics techniques were also used as input to the models for hydrogen deuteride. The main difference is that the ortho-deuterium molecule has two of the same atomic nuclei, while the hydrogen deuteride molecule has two different atomic nuclei which makes it more complex in some regards. The results of the work, on several levels, were compared to experiments and simulations found in the literature. Good agreement was found where data was available.

This work builds the basis for future design work on moderator systems at the ESS. For example, a continuation of this project would be to investigate the moderator performance of hydrogen deuteride, compared to liquid deuterium and liquid hydrogen, through the use of Monte-Carlo simulation.