c3dp: Design of a 3D printed collimator optimized for high pressure scattering

Many current neutron scattering experiments require use complex sample environments which invariably contribute significant background to the experimental data. Generally, collimators which are part of the instrument have been used to improve the sample to cell signal ratio. Particularly for high pressure, however, collimation should be customized for different pressure environments since different pressure environments produce different results. An automated workflow has been developed to design and optimize a custom collimator for a given pressure environment and manufacturing constraints. The end result of the workflow that is codded using Python in a software package called ***c3dp*** is a file ready for 3D printing used to optimize a collimator. In this workflow, first the incident beam to sample for Spallation Neutrons and Pressure Diffractometer at Oak Ridge National Laboratory is modeled using McStas. Next, the neutron interaction with the sample assembly, composed of the pressure cell and the sample, is modeled with MCViNE. In the third step, the collimator for the scattered neutrons from sample assembly is modeled using MCViNE. Next, a comparison to the optimization metrics performed. If the optimum performance is not achieved, the neutrons coming from the collimator are saved. In the fifth step, data is reduced using MANTiD to obtain the diffraction pattern. In the sixth step a differential evolution algorithm from the SciPy library was used to optimize the collimator geometry with the objective of minimizing the integrated cell peaks to integrated sample peaks ratio. Once the optimized collimator geometry is determined, it is saved to an .xml file ready for 3D printing as the last step of the workflow by using the Python script.