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UB Matrix based on Single Crystal Orientation Program in Neutron Spectrometer

In neutron spectroscopy measurements, the orientation of single crystal samples has always been a fundamental yet still a relevant concern. Orientation refers to determining the initial orientation of a single crystal sample and calculating the sample's deviation angles, providing convenience for rotating the sample and processing data in subsequent steps. Sample positioning before conducting experiments is highly necessary because it can reduce unnecessary data processing issues, such as background subtraction and handling, while incorrect positioning could potentially lead to misleading data analysis. Furthermore, when studying certain excitations, such as phonons and magnons, their excitation directions, namely dispersion relations, must be precisely defined along specific crystallographic directions. Based on these requirements, we have referenced and developed a single crystal orientation programs using the UB matrix. By inputting lattice parameters and a predefined set of crystallographic vectors, it can assist in determining the degree of deviation of the crystal, providing information for the subsequent experimental rotations and data processing, such as with software tools like MSlice and Horace.

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