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Machine-learning tools for efficient analysis of X-ray scattering data from wood

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Wood is a heterogeneous biological material, which has a hierarchical structure extending from the molecular level to the macroscopic scale. X-ray and neutron scattering methods are particularly suited for studying wood, because they cover a large portion of the structural hierarchy and allow characterization of samples under various conditions. Wide-angle X-ray scattering (WAXS) detects the crystalline cellulose microfibrils (2-3 nm in diameter), and small-angle X-ray scattering (SAXS) their cross-sectional size and packing. Wood and other similar plants consist also of different tissue and cell types, which vary in a sample in the microscale and show differences in the scattering data measured at different locations.

State-of-the-art X-ray scattering setups especially at synchrotrons allow gathering large amounts of spatially resolved data. In samples like wood, where the structure varies in the scale of the X-ray beam diameter and above, this would ideally allow scanning-SAXS/WAXS to be measured from different cell and tissue types individually. However, often in reality the scattering contributions of different structures overlap, making them difficult to distinguish from each other. Also, when spatially resolved data from individual tissue types can be collected using a small X-ray beam, the vast amount of data makes it challenging to interpret without further reduction or classification.

Our group is addressing these challenges by implementing machine learning tools for the analysis of X-ray scattering data from woody samples. We have utilized principal component analysis (PCA) and clustering to classify fitting results from a scanning-SAXS/WAXS experiment to find representative results for earlywood and latewood tissues in Norway spruce. We also used PCA and clustering to classify spatially-resolved 2D WAXS patterns, measured by scanning radial cross-sections of wood samples from different species, into different categories according to the tissue type they represent. We also utilized X-ray microtomography to determine the ratio of different cell types in 2D WAXS patterns from bamboo, and used this information to train supervised machine learning models to estimate the same ratio from the scattering patterns directly. The results demonstrate the value of machine learning tools in helping to analyze and interpret large amounts of scattering data measured from heterogeneous biological materials.

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