Calculating scattering pattern from mesoscopic continuum simulation

Sassena – computes scattering pattern from Molecular Dynamics (MD) simulation

Sassena can calculate diffractions, coherent and incoherent intermediate scattering functions and elastic coherent and incoherent structure factors. This work adds a feature to subtract the unwanted scattering from the simulation box in the reciprocal space.

Calculating scattering pattern from mesoscopic continuum simulation

A continuous description of system does not provide the position of each atom. Therefore until now, complex integration had to be performed to calculate scattering patterns. This work provides an alternative approach by converting the continuous description to a discrete description.

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