Combined-technique structure refinements in RMCProfile

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The RMCProfile software package has been extended to enable simultaneous fitting of real and reciprocal space representations of neutron and X-ray total scattering data combined with multiple EXAFS datasets and 2D and 3D single-crystal diffuse scattering. The ability to include different types of radiation and EXAFS provides chemical resolution, which is critical for the analysis of complex multielement materials, while diffuse scattering emphasizes interatomic correlations with directional resolution. New types of implemented structural restraints stabilize fitted atomic configurations. The total number of data sets and structural restraints may be a couple of tens.

Introducing new algorithms combined with parallel and GPU computing, noticeably reduced the computational times. Now, models that contain up to 500,000 atoms and interrogate distances up to ten nanometers can be refined within one week. Thus, structural solutions that were deemed impractical are now routine.

The speed-optimized RMC software also incorporates algorithms that correct the calculated X-ray and neutron total scattering signals for instrument resolution in both reciprocal and real spaces, as required for fitting these data over larger length scales. The convergence of multi-signal RMC refinements has been facilitated by introducing a procedure for automated assignment of weights to individual datasets during fits. The new capabilities of RMCProfile will be illustrated using structure refinements in several representative material systems.