Poster Presentation

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Debye function and Reverse Monte Carlo refinement of nano-sized FeOOH

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Debye scattering equation is known since 1915 [1]. Altought this formula can, in principle, describe scattering from any multiple particle systems, its application is normally limited to small domains as clusters or low-sized nanoparticles. This is mostly due to the very high computational effort needed. Indeed, computing time strongly depends on the number of atoms. In recent years, the availability of highly performant graphics processing units (GPU) allowed their use for general purposes including strongly demanding scientific applications. This feature was exploited in the Debye Function Analysis to study more complex systems with several thousand of atoms [2]. Here, we present a refinement code using both the Debye scattering equation implemented on a commercial GPU and the Reverse Monte Carlo algorithm [3] to study the structure of two disordered nano-sized iron oxy-hydroxides, feroxyhite and ferrihydrite. The determination of their structure appears rather complex. Different interpretations of the X-ray diffraction pattern have been put forward and debates remain about the exact nature of their crystalline structure. The proposed models show some structural features that are not in accordance with the known structures of other iron oxy-hydroxides: goethite, akaganeite and lepidocrocite. To evaluate their validity, these models are used as starting atom sets in the refinement procedure. To reach a quantitative agreement between the experimental diffraction pattern and the calculated one, the atom positions are randomly modified. X-ray diffraction pattern is calculed using Debye scattering equation; to speed up calculation time, a parallelized version of the equation is optimized to run on Nvidia GeForce 690 GPU.

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