Powder diffraction on graphics processing units

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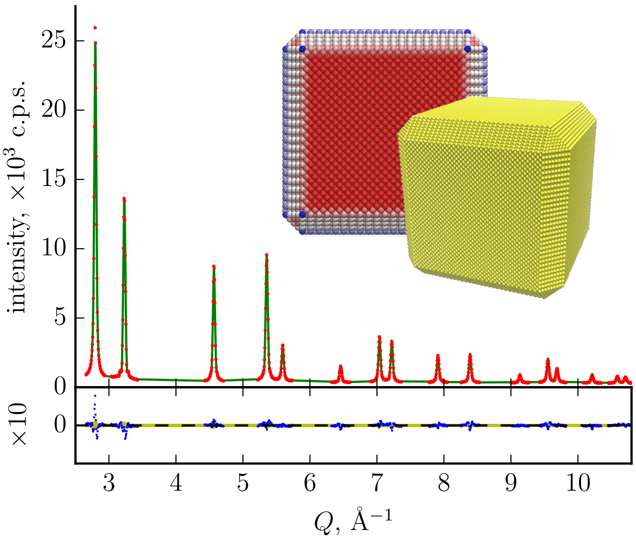
Paradigms for the interpretation of intensity scattered by finite bodies are tremendously evolving, providing enhanced resolution at the price of increased computational demand. Particularly, the signal emanated by small aggregates can be described employing an atomistic approach, *i.e.* considering each atom in an aggregate. The Debye scattering equation [1] provides an elegant solution in this framework for the case of powder diffraction, a technique frequently employed to investigate structural and vibrational properties of nano-structured particles. Although one century has passed since the formulation, the major limitation to its widespread use has been the time complexity, proportional to the squared number of atoms in a scattering domain. While clever solutions implying different levels of approximations have been proposed to alleviate the computational cost [2–5], an approximation-free implementation of the above-mentioned equation might be needed to describe fascinating features decorating diffraction patterns induced directly or indirectly by the finiteness of bodies.

Graphics processing units have been exploited to perform a brute-force calculation of the Debye scattering equation, dramatically lowering computational time [6, 7].

Implementation details and selected case studies illustrating the potentiality of this approach in unveiling insights into nano-structured particles will be discussed.



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