

Do Q!

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Why bother with reciprocal space, if my instrument measures just the diffraction angle? What is behind the synonyms of Reciprocal Space, Q -space, K -space, G -space, Momentum Space and why is it important? X-ray and neutron powder diffraction patterns can be displayed as a function of many independent quantities, such as scattering angle 2θ , lattice spacing d , neutron time of flight τ , energy E , wavelength λ , wave vector k , radius R on a 2-dimensional diffraction image and so on. In most of the cases, experimentalists plot data just against the independent quantity in which their instrument operates without thinking further. This has been escalated with the tradition of X-ray measurements on Cu-K_α tubes to the extreme, that whole evaluation programs work in 2θ only and powder diffraction databases even store patterns in 2θ of Cu-K_α , the profile matching programs re-calculating patterns measured at different wavelengths to this scale. Beamlines at the world's brightest synchrotron sources have been built on Cu-K_α energies for this reason and only slowly, after ten years of the operation of such facilities, the community realizes that other wavelengths may be of advantage. At the end of the chain peer referees and journal editors have become reluctant to authors presenting on this arbitrary scale.

So why bother ? - Because:

- reciprocal space is the NATURAL space diffraction takes place;
- reciprocal space is LINEAR and symmetries can be identified by eye;
- the representation directly reflects crystal SYMMETRY;
- the representation is INDEPENDENT of the instrument geometry and type of radiation (electrons, neutrons, X-rays, light, atoms...)
- the representation is INDEPENDENT of the wavelength used;
- presentations and publications would become directly COMPARABLE;
- reciprocal space is WIDELY USED outside the powder diffraction community;
- modern instruments with 2D detectors DO NOT WORK in 2θ space;

The contribution will point out these issues and animate for a lively discussion.

Keywords: Powder Diffraction; Single Crystal Diffraction; Standardization;