Contribution ID: **36** Type: **Invited**

Correcting Non-isomorphism

Thursday, 15 October 2020 17:10 (20 minutes)

The problem of non-isomorphism has plagued macromolecular crystallography since the beginning [1, 2, 3], and it is essentially unavoidable in radiation damage studies. The unit cell changes with dose and that means the molecules in the cell must be adjusting somehow to the new cell. This will change the structure factors, but what if the molecular distortions could be corrected? Rigid-body motions cannot be the whole story because these lead to steric clashes. The true underlying distortion of the molecule must be both smooth across space, and also obey crystallographic symmetry. Here I present how periodic rubber-like distortions may be modelled using a collection of sine waves in space. This spatial distortion field (SDF) is similar in mathematical form to the Fourier synthesis of electron density from structure factors. The main differences are that the SDF is not a scalar field but a vector field describing changes in atomic position at every point in the unit cell. The number of orders needed to describe typical non-isomorphism is small, usually only 3-5 orders. SDFs may also be applied to electron density, allowing multi-crystal averaging across non-isomorphous crystal forms. Structural flexibility inherent to function may also be excited by these rubber-like distortions, making SDFs a potentially useful tool for elucidating subtle changes by eliminating the "noise"of rubber-like non-isomorphous distortion.

References

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Session Classification: Session 3 - Damage at New Sources - XFEL and 4th generation synchrotrons