Decomposition methods for analysis of specific radiation damage

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Radiation damage is driven by charged states generated by ionization reactions. These states can migrate even in cryo-cooled samples and can trigger chemical reactions and physical (collective) processes. Methods of analysis should assume that these processes, while occurring in parallel, can occur at various rates and in particular for physical processes, can have complex time/dose dependence. One of the challenges is due to the accumulation of random displacements in the sample, which cause the decay of the diffraction signals so later stages have limited signal quality. We would like to learn the rules of how these processes depend on sample composition, its structure, and experimental conditions.

We developed an approach based on matrix decomposition that allows us to accurately quantify radiation damage and separate components of specific radiation damage from each other. The non-decay components resulting from decomposition can be imaged in real space as difference electron density maps and interpreted appropriately. We applied this approach to the analysis of multiple datasets acquired at different time scales of data collection, and in the presence of different additives from the standard crystallization conditions. We observed an unexpected richness of specific radiation-induced effects, with independent components originating from: (1) specific chemistries induced by radiation, (2) time-dose effects, (3) modulations due to subtle changes in crystallization conditions. Additionally, the robustness of the matrix decomposition showed that we can separate radiation-caused components from other data variability, in particular that which comes from the uncorrected part of crystal absorption.

The method applies well to problems which have a complex dependence on experimental conditions that were introduced either intentionally or accidentally. We will present these results and discuss possible applications.