Poster Presentation

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Freeze Frames vs. Movies

C. Müller[1], S. Lidin[1]

[1]*Lund University, Centre for Analysis and Synthesis, Lund, Sweden*

Sometimes, model building in crystallography is like resolving a puzzle: All obvious symmetrical or methodological errors are excluded, you apparently understand the measured patterns in 3D, but the structure solution and/or refinement is just not working. One such nerve-stretching problem arises from metrically commensurate structures (MCS). This expression means that the observed values of the components of the modulation wave vectors are rational by chance and not because of a lock-in. Hence, it is not a superstructure - although the boundaries between the two descriptions are blurry. Using a superstructure model for a MCS decreases the degrees of freedom, and forces the atomic arrangement to an artificial state of ordering. Just imagine it as looking at a freeze frame from a movie instead of watching the whole film. The consequences in structure solution and refinement of MCS are not always as dramatically as stated in the beginning. On the contrary, treating a superstructure like a MCS might be a worthwhile idea. Converting from a superstructure model to a superspace model may lead to a substantial decrease in the number of parameters needed to model the structure. Further, it can permit for the refinement of parameters that the paucity of data does not allow in a conventional description. However, it is well known that families of superstructures can be described elegantly by the use of superspace models that collectively treat a whole range of structures, commensurate and incommensurate. Nevertheless, practical complications in the refinement are not uncommon. Instances are overlapping satellites from different orders and parameter correlations. Notably, MCS occur in intermetallic compounds that are important for the performance of next-generation electronic devices. Based on examples of their (pseudo)hexagonal 3+1D and 3+2D structures, we will discuss the detection and occurrence of MCS as well as the benefits and limitations of implementing them artificially.

Keywords: incommensurate structures, intermetallic compounds