Poster

Testing *PhAI* for solving crystal structures from electron diffraction and powder X-ray diffraction data

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Recently, a new deep-learning-based method (called *PhAI*) for solving the crystallographic phase problem was developed [1]. *PhAI* is a neural network that has been trained to predict all the given reflection phase values based on their amplitudes. Initially, it has been trained to solve structures with small unit cells in $P2_1/c$ or its supergroups (for example, $C2/c$, *Pbca* and others). The initial results indicated that such a deep-learning approach can be extremely successful to solve the crystallographic phase problem. The phase values could be predicted with an outstanding accuracy from calculated and experimental single-crystal X-ray diffraction data. *PhAI* was proven to perform much better than the currently existing methods (e.g. direct methods or charge flipping), especially for low- resolution data.

Here we present examples of structures solved from electron diffraction (ED) and powder X-ray diffraction (PXRD) data. For the ED data, there are several challenges present. Firstly, the atomic scattering factors are different resulting in different input amplitudes as compared to the X-ray diffraction data based on which the *PhAI* was trained. Secondly, there are multiple scattering effects present further perturbing the data. Thirdly, the achievable data completeness is generally less than 100% due to the mechanical limit of the goniometer. Finally, the completeness and reflection intensities are also influenced by sample degradation. Despite all of that, we demonstrate some success of *PhAI* to solve structures from ED data. An example is given in Figure 1.

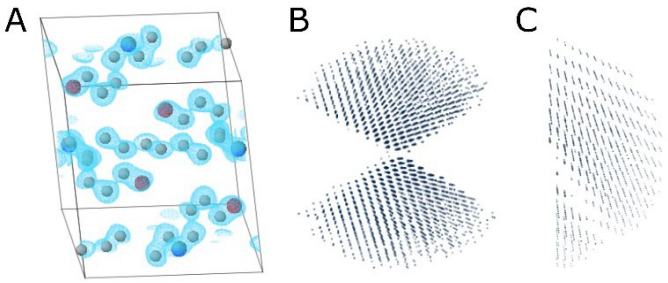

Figure 1. Structure of paracetamol solved with *PhAI*. **A:** Electrostatic potential map and structure model. **B:** Collected ED data (a 144° sweep) showing the missing wedges. **C:** The unique data according to the Laue class 2/*m*, i.e. 1/4 of the sphere showing a *stripe* of missing data that results in an 83% completeness.

In case of PXRD data, an indexing procedure followed by a Pawley fit and corrections (reflection multiplicity, Lorenz and polarisation corrections) yields intensities of the reflections. Extracting the intensities in such a way is rather ambiguous due to the strong overlap of the reflections, especially in the higher 2θ region. Nevertheless, also here we can demonstrate successful cases of *PhAI* solving the crystal structures. The results indicate that further development of such deep-learning-based methods could allow to solve the crystal structures in a general case. It is particularly important for low-completeness and/or low-resolution X-ray or ED data for which the currently available methods tend to fail.

[1] Larsen, A., Rekis, T., Madsen, A. Ø. *PhAI: A deep learning approach to solve the crystallographic phase problem*, preprint, **2023**