

Iterative phasing of 2D crystal XFEL data

Yun Zhao¹ and John Spence¹

¹Dept. of Physics, Arizona State University, Tempe, AZ 85287-1504.

Abstract

The phase problem for Bragg diffraction from two-dimensional(2D) crystalline monolayer in transmission is marginally unique with a compact support which sets the density to zero outside of the monolayer. In practice, the reconstruction can hardly be achieved from intensities alone as this one-dimensional support function fails to link the reciprocal space rods correctly unless some prior information is available. The charge flipping algorithm can be used to solve structures from intensities, however it requires atomic resolution data. Here we explore the different type of prior information required for successful three-dimensional(3D) structure retrieval from a 2D crystal diffraction dataset. This method provides us with an alternative way to phase 2D crystal datasets, which is less dependent on the existence of a high quality model or high resolution data.

Supported by NSF BioXFEL STC award. 1231306