Phase refinement with EDEN: point defect structure in inorganic crystals.

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A crystal with point defects can be represented as consisting of two components, the host crystal and the disturbed areas around the randomly distributed defects. X-ray diffraction patterns from such crystals can be then presented as a sum of scattering amplitudes of both parts.

In that case, the defect structure can be determined using the approach proposed by A. Szöke. Analogue to the holographic principle, the intensity $I(\mathbf{h})$ measured for every scattering vector $\mathbf{h}$, is a superposition of a (known) reference wave R and an (unknown) object wave O.

$$I(\mathbf{h}) \quad |R(\mathbf{h})+O(\mathbf{h})|^2 = |R(\mathbf{h})|^2 + R(\mathbf{h})^* O(\mathbf{h}) + R(\mathbf{h})O(\mathbf{h})^* + |O(\mathbf{h})|^2$$

Using this concept, the Bragg-scattering from the “perfect” host crystal serves as a reference wave. It interferes with the wave scattered by the defects whose phase information is then conserved. In contrast to holography, the object wave can not be found by performing a direct back-transformation because of the self-interference term $|O(\mathbf{h})|^2$. The program EDEN, written by H. Szöke, uses a conjugate gradient algorithm to solve this equation and reconstruct the underlying electron density. The so determined electron density distribution can be presented as a sum of two components: the known crystalline structure and the overlaying point defects. This approach requires no preliminary models for the defect structure.

To demonstrate the feasibility of this approach, a scandium oxide (Sc_2O_3) crystal, doped with ~1% Er has been studied. Er is expected to substitute Sc atoms in the structure. The observed asymmetry of the electron density leads to a defect model with Er atoms slightly displaced from the ideal Sc positions. The result has been verified by comparison with an undoped crystal.