Resonant Contrast and Sub-pm Resolution by means of the Parameter Space Concept

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Within the last 15 years, the Parameter Space Concept (PSC) was theoretically developed by Fischer, Kirfel and Zimmermann as an alternative approach to solve crystal structures from diffraction intensities without use of Fourier transforms \cite{1-6}. Each experimentally determined reflection restricts the 3N-\textsuperscript{dim.} parameter space of atomic coordinates for a crystal structure solution (N atoms) by a manifold of 3N-1 dimensions, equivalent to a unique isosurface, whereas the true solution vector will be the intersection of all isosurfaces. The method has already been tested on numerous, partly challenging problems of X-ray diffraction. Here, we present a study of resonant contrast to enhance the resolution of the PSC. As an example, a split position of La and Sr has been investigated in the potential high-temperature super-conductor (La\textsubscript{0.5}Sr\textsubscript{1.5})MnO\textsubscript{4}, I\textsubscript{4}/mmm. A positional shift of the cations in the order of Δ\textsubscript{z}\textapprox0.001\textapprox0.02 Å has been suggested in literature \cite{7,8}. Tuning the scattering difference of La and Sr by \f{Sr}', we now add to the discussion additional model data sets, each with (00l) reflections (l = 2,4,..20) and varied relative errors of up to 20%. A correlation of the static structural degrees of freedom within the parameter space revealed an improvement of resolution. Due to the difference in scattering power of La and Sr, a pseudosymmetric structure solution (La\textsuperscript{*}, Sr\textsuperscript{*}) exists for approximately interchanged z-positions, which we discuss in conjunction with the accurate solution (La, Sr)\cite{9,10}. There is a non-vanishing variance of the pseudosymmetric structure solution, whereas the accurate solution does not vary (Fig. 1). Depending on the relative error of the diffraction intensities, we present respective resolution limits for the split position.

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{image.png}
\caption{Model study of the real solution \textsubscript{z}_{La}=0.349, \textsubscript{z}_{Sr}=0.362 and the pseudosymmetric structure solution (\textsubscript{z}_{La:\textsuperscript{*}}, \textsubscript{z}_{Sr:\textsuperscript{*}}) as a function of scattering strength ratio \f{La}/\f{Sr}. The change in scattering power directly reflects the distortion of the respective isosurface features, whereas light weights act as elongations that increase the respective positional errors, shown for light La (left) and light Sr (right).}
\end{figure}

\begin{thebibliography}{10}
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\end{thebibliography}

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