

REPORT OF THE EXPERIMENT HS 4821

PDF investigation on short range correlations between Fe and Ru in $\text{La}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}$ compounds

Aim and execution of the experiment

The aim of this experiment was to investigate the local structure and possible short range correlations between Fe and Ru taking place at the transition metal plane in $\text{La}(\text{Fe}_{1-x}\text{Ru}_x)\text{AsO}$ compounds. Specimens with $x = 0.00, 0.10, 0.30, 0.40, 0.50$ and 0.80 , were analyzed ID31 beam-line, collecting data at 290 K. Reduction of the total scattering data to obtain $G(r)$, the PDF function, was done by the PDFgetX3 software, using $Q_{\text{max}} = 30.0 \text{ \AA}^{-1}$. Full-profile fitting of the $G(r)$ function was carried out using the PDFgui software, using the average structures obtained from the Rietveld refinements as models

Results

Figure 1 shows the PDF of LaFeAsO (upper panel) and $\text{La}(\text{Fe}_{0.70}\text{Ru}_{0.30})\text{AsO}$ (lower panel) after fitting. The change of the agreement factor R_w as a function of the Q range used for fitting $G(r)$, revealing significant local deviations from the average structure. Below $\sim 8 \text{ \AA}$ the fit is significantly worsened, indicating that the real short-range structure is not adequately described by the average structural model within this r range. Conversely, the average structure of LaFeAsO fairly fits $G(r)$ above $\sim 15 \text{ \AA}$ ($R_w \sim 7\%$), indicating that beyond this distance the local distortions are no longer correlated.

A similar behaviour is observed in the Ru substituted sample (Figure 2, on the right), indicating that Ru substitution does not determine a notable variation in the length scale of the local distortion.

The analysis of $G(r)$ in the region of the (Fe,Ru)-(Fe,Ru) pair ($r \sim 2.85 \text{ \AA}$) gives useful insights about the distribution of these atomic species. A single peak is observed in this region, smoothly varying in distance and intensity as a function of Ru content, indicating that the sample is single phase and no phase separation or clustering takes place.

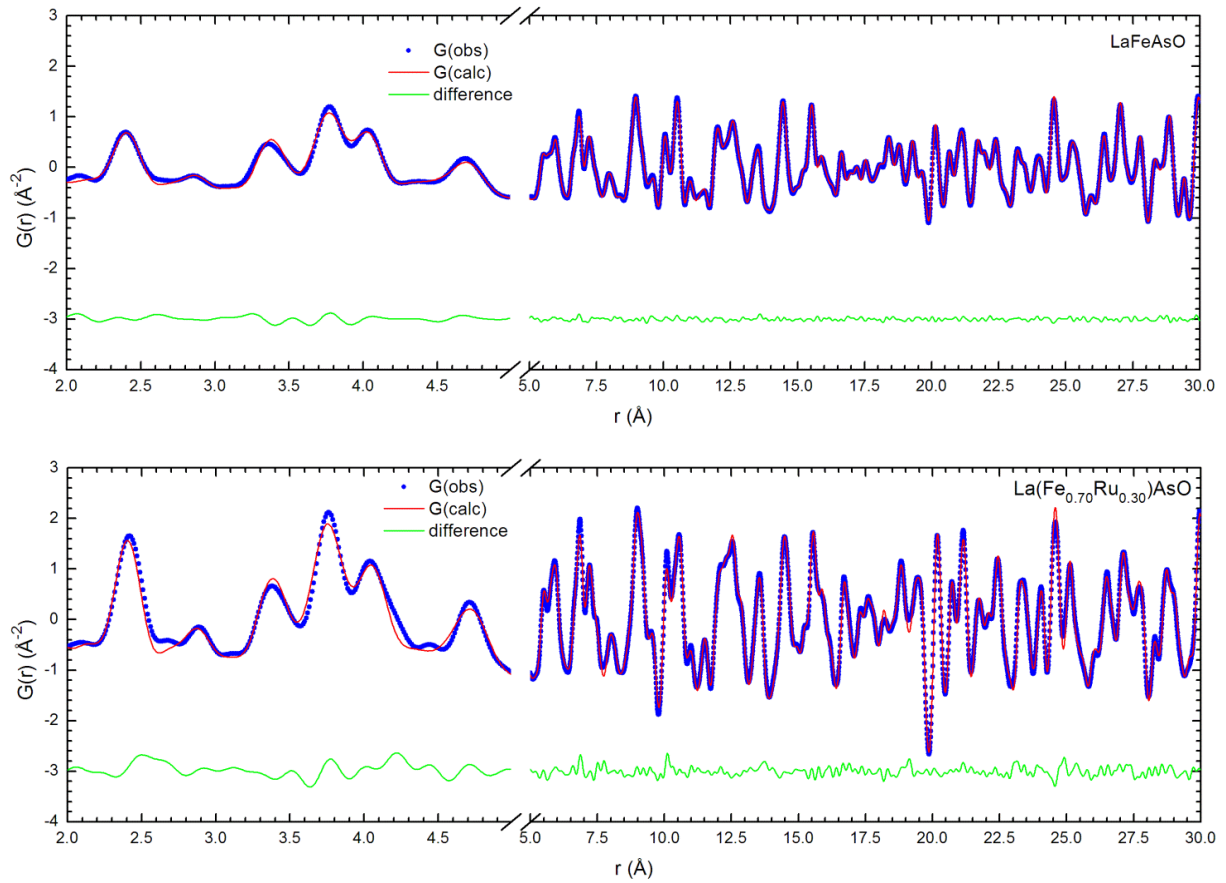


Figure 1: PDF data of LaFeAsO (upper panel) and $\text{La}(\text{Fe}_{0.70}\text{Ru}_{0.30})\text{AsO}$ (lower panel) fitted with the $P4/nmm$ structural model; the difference between observed data and calculated PDF is shown in the lower field.

Unfortunately the different types of short range correlation do not produce significant changes in the PDF. As a consequence it is not possible to determine by PDF nor if short range ordering between Fe and Ru takes place, nor even less distinguish between different types of the possible correlations.