Acta Cryst

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FOUNDATIONS

ADVANCES

Supporting information for article:

A real-space approach to the analysis of stacking faults in close-packed metals: *G*(*r*) modelling and *Q*-space feedback

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S1. Evaluation of Equation (9)

$$FT\left[S^b(Q)\cdot\exp\left(-\frac{\sigma^2}{2}Q^2\right)\right]=\frac{1}{2\pi}\int_{-b}^{b}dQ\exp\left(-\frac{\sigma^2}{2}Q^2\right)=$$

$$=\frac{1}{\sigma\sqrt{2\pi}}\left\{\exp\left(-\frac{r^2}{2\sigma^2}\right)\cdot\mathrm{Re}\left[\mathrm{erf}\left(\frac{\sigma b}{2}-i\frac{r}{\sigma\sqrt{2}}\right)\right]\right\}$$

(S1)

The complex error function was calculated by the CWERF routine of CERNLIB (Kölbig, 1970), implementing the algorithm of Gautschi (1970).

S2. The S=24 (=3·2^{s-1}) distinct close packed sequences of s=4 atomic layers

|						
cc	*ABCA*	*ACBA*	*BCAB*	*BACB*	*CABC*	*CBAC*
ch	*ABCB*	*ACBC*	*BCAC*	*BACA*	*CABA*	*CBAB*
hc	*ABAC*	*ACAB*	*BCBA*	*BABC*	*CACB*	*CBCA*
hh	*ABAB*	*ACAC*	*BCBC*	*BABA*	*CACA*	*CBCB*

The rows are classified according to the close packing mode: *cc* concatenation of two *ccp* sequences, *ch* for a *ccp* sequence concatenated with a *hcp* one, and so on.
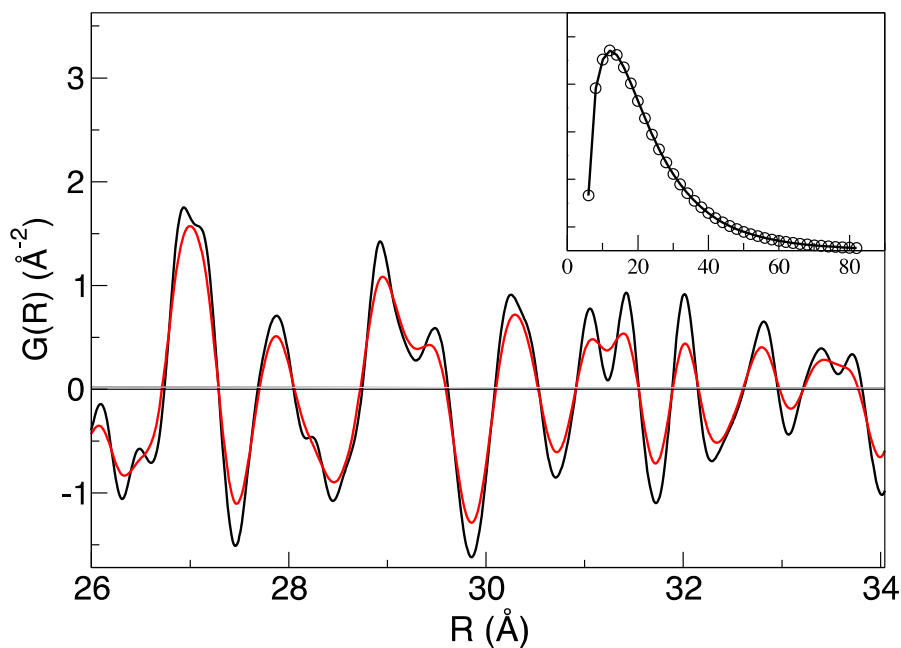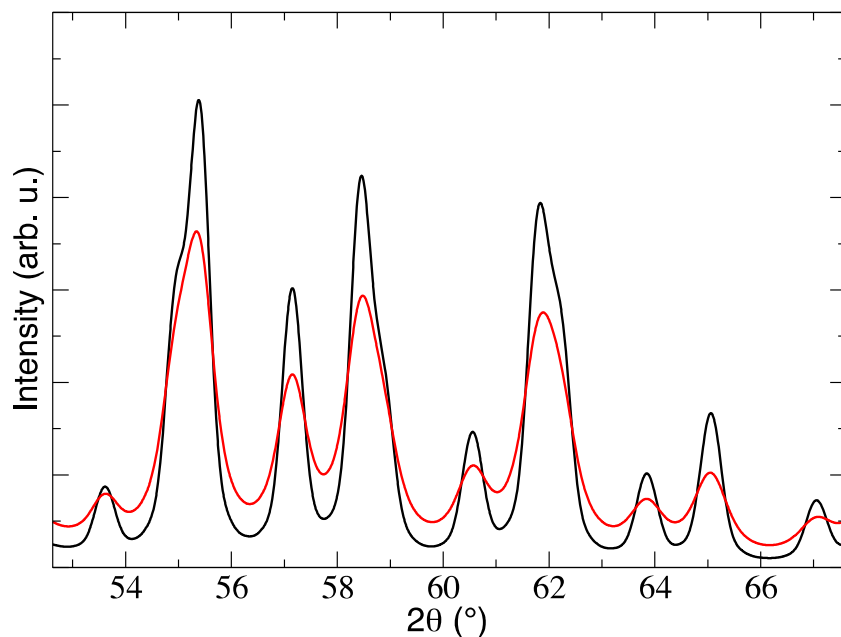
Figure S1   Effect of microstrain, as modelled by Equation (20), in direct space and reciprocal space. Upper panel: $G(R)$ relative to a *fcc* structure, particle size in the inset (black: no strain, red: strain with ζ=0.00032); lower panel: the same, in reciprocal space. At 2θ=11.2° (111 peak position) and at R=2.52 Å (nearest neighbour distance) the red and black patterns are hardly distinguishable, while at higher abscissae the width of the red peaks increases progressively, as shown in the drawings. In the inset: population distribution of diameters of spherical particles.
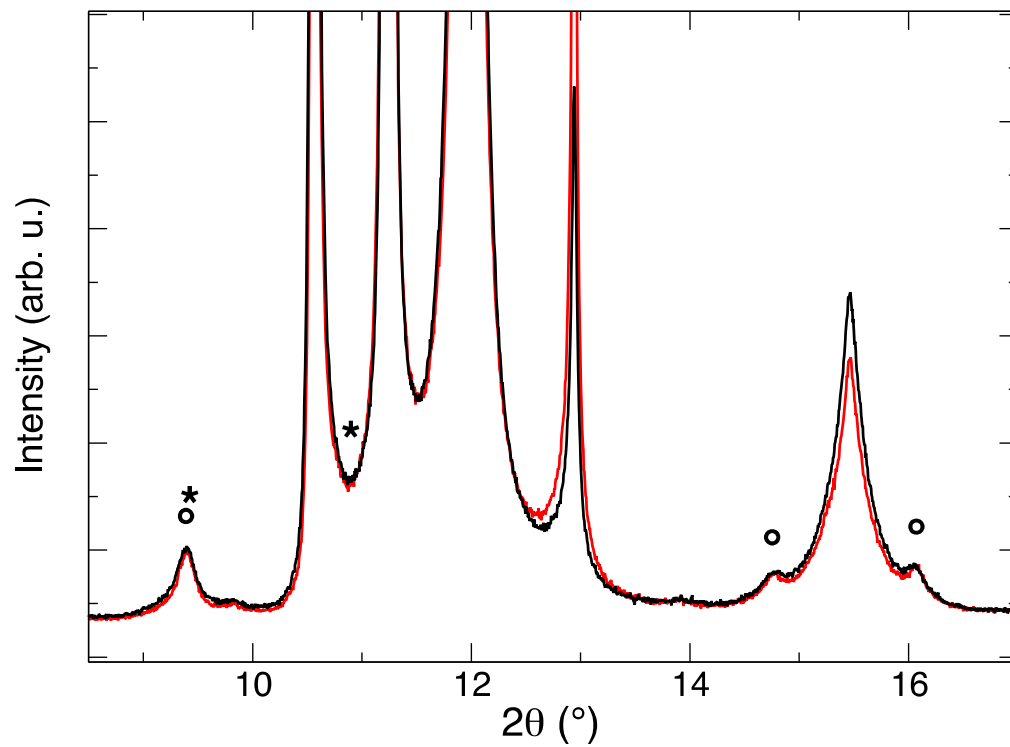
Figure S2   Q-space data of samples B1 (red) and G2 (black) zoomed in the region 8.5-17° 2θ to better show the peaks attributed to the CoO (*) and Co_3O_4 (°) phase.
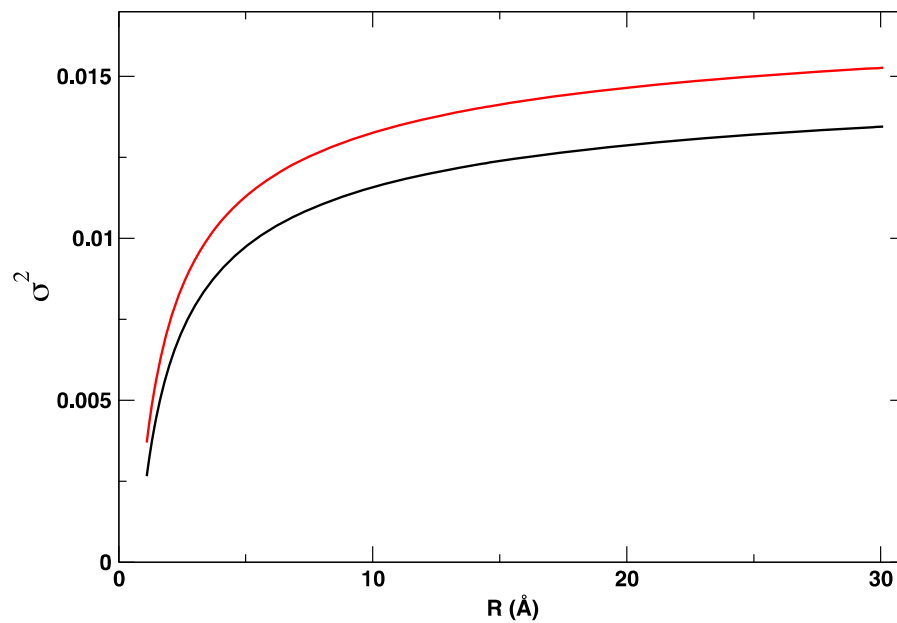
Figure S3   The σ^2 function defined in Equation (21), as a function of the distance between pairs of atoms (black:B1, red:G2)
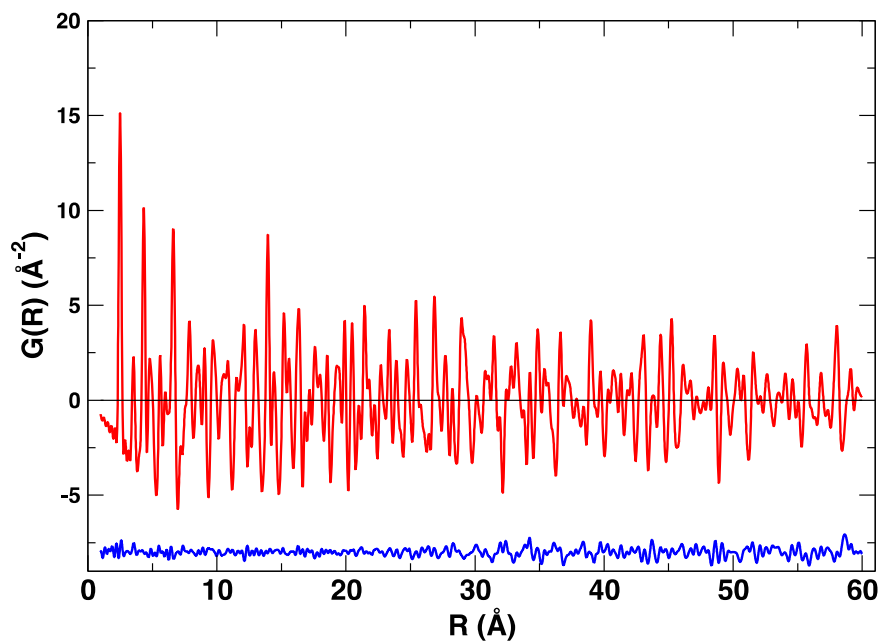
Figure S4   Simulation (red) of the G(R) pattern of sample G2. The simulation is carried out using the structural parameters determined with the fitting performed in the 1-30 Å range. The experimental data are omitted for the sake of clarity. The residual is plotted in blue.

Kölbig, K. S. (1970). Program C 335, CERN.

Gautschi, W. (1970). *SIAM J. Numer. Anal.* **7**, 187–198.