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Supporting information for article:

Determination of the cationic distribution in oxidic thin films by resonant X-ray diffraction: the magnetoelectric compound $Ga_{2-x}Fe_xO_3$

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S1. ϕ-scans

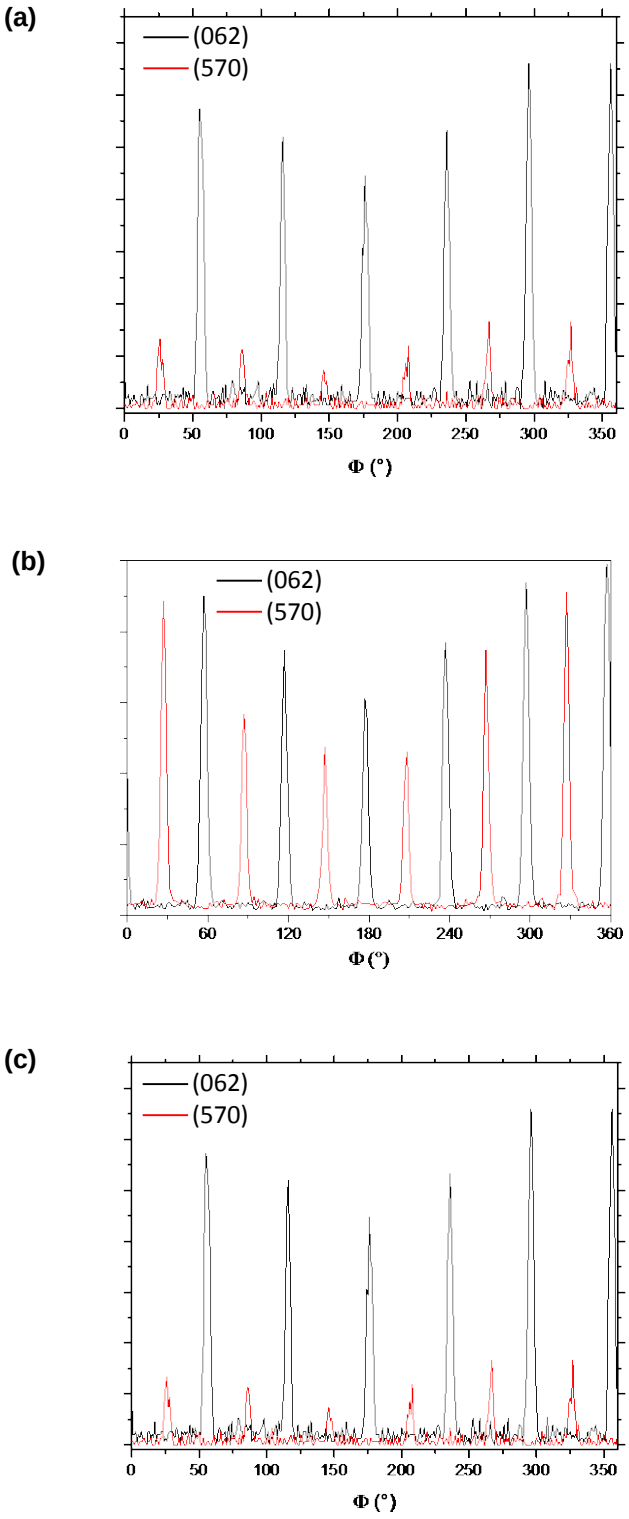

Figure S1 : Φ-scans on the 570 and 062 lattice nodes ($Pc2_1n$ space group) for the (a) GFO0.9, (b) GFO1.1 and (c) GFO1.4 thin films.

S2. Reciprocal space mapping

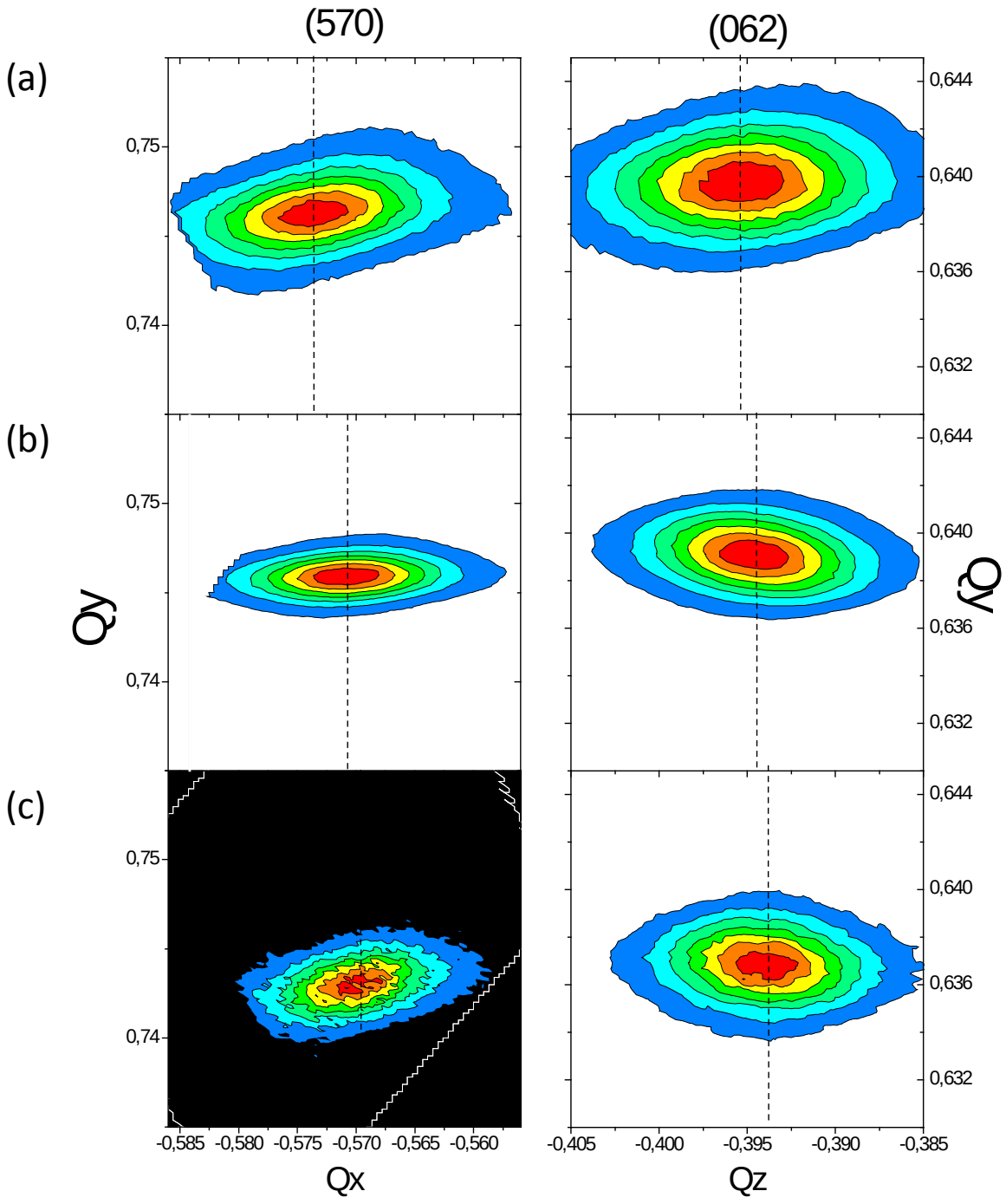

Figure S2 : Reciprocal space mapping of the 570 and 062 lattice nodes ($Pc2_1n$ space group) on the (a) GFO0.9, (b) GFO1.1 and (c) GFO1.4 thin films.

S3. Selection of the experimentally measured lattice nodes

The existence of three in-plane variants results into the superimposition of three reciprocal lattices. The issue is to avoid measuring a reciprocal lattice node which could be the locus of some node of one of the two other reciprocal lattices.

Since the growth of GFO is [0*k*0] oriented, we will consider the *k* planes of its reciprocal lattice R (within the *P*c2$_1$n space group) (Fig. S3). Within a *k* plane, if *M* is a node of R, it can be written:

$$M = \begin{pmatrix} ha^* \\ lc^* \end{pmatrix}$$

in the orthonormal basis formed by the reciprocal lattice vectors *a** and *c**, with *h* and *l* integers.
In-plane variants are described by the rotation of the direct and hence reciprocal lattice with respect the growth axis direction. If the in-plane rotation angle is α, the associated rotation matrix is:

$$R_\theta = \begin{pmatrix} cos\ \alpha & -sin\ \alpha \\ sin\ \alpha & cos\ \alpha \end{pmatrix},$$

and the coordinates of M', equivalent node to M in the rotated reciprocal lattice ($M' = R_\theta(M)$) are:

$$M' = \begin{pmatrix} ha^* cos\ \alpha - lc^* sin\ \alpha \\ ha^* sin\ \alpha + lc^* cos\ \alpha \end{pmatrix}.$$

M' overlaps with a node of the unrotated reciprocal lattice R if, and only if, *M'* belongs to *R*:

$$\exists\ (m,p)\ \in\ \mathbb{Z}^2 / \begin{matrix} ma^* = ha^* cos\alpha - lc^* sin\alpha \\ pc^* = ha^* sin\alpha + lc^* cos\alpha \end{matrix},$$

and hence if:

$$cos\ \alpha = \frac{hl+mp}{ml+hp}.$$

In our case, α=60° (three equally distributed in-plane variants). The condition for overlapping is then:

$$\frac{hl+mp}{ml+hp} = 0.5.$$

The (h,l) couples verifying this relationship are excluded from the measurements.

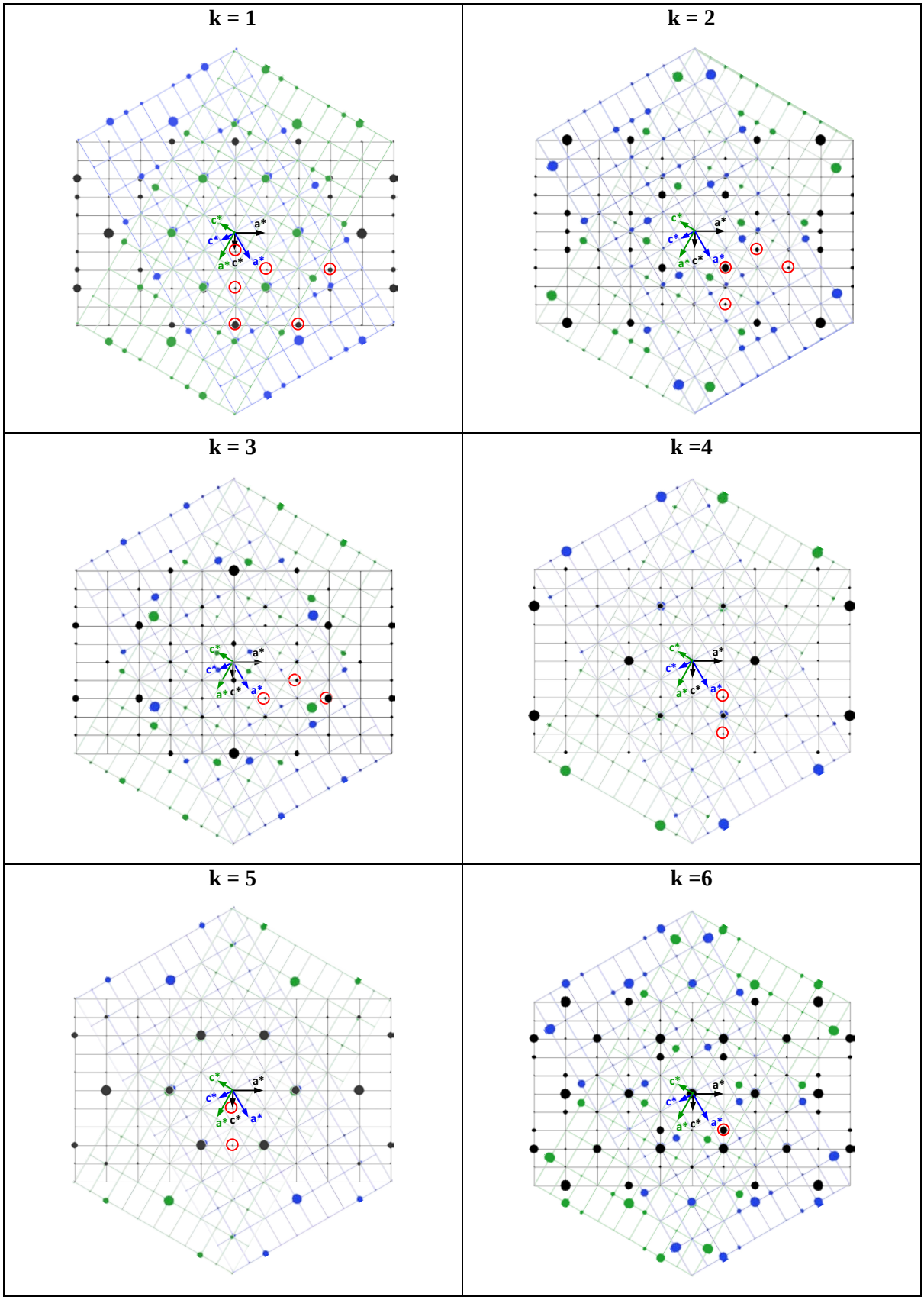

Figure S3 Reciprocal space of the $Pc2_1n$ GFO sample with 3 orientations. Red circles indicate nodes which have been recorded

S4. Influence of the direction of the growth orientation

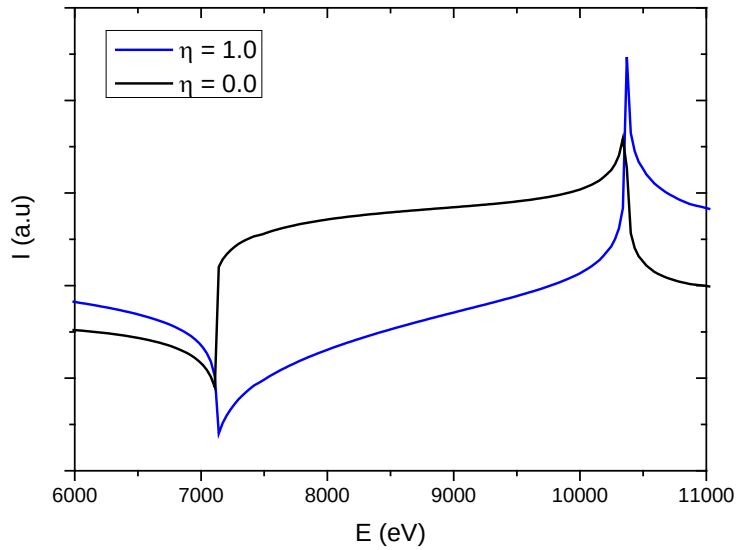

Figure S4 : Simulation of the spectra for the $GaFeO_3$ (110) peak for η = 0 and η = 1.0

S5. Experimental data and refinement of the GFO0.9 thin film using both FitREXS and FDMNES

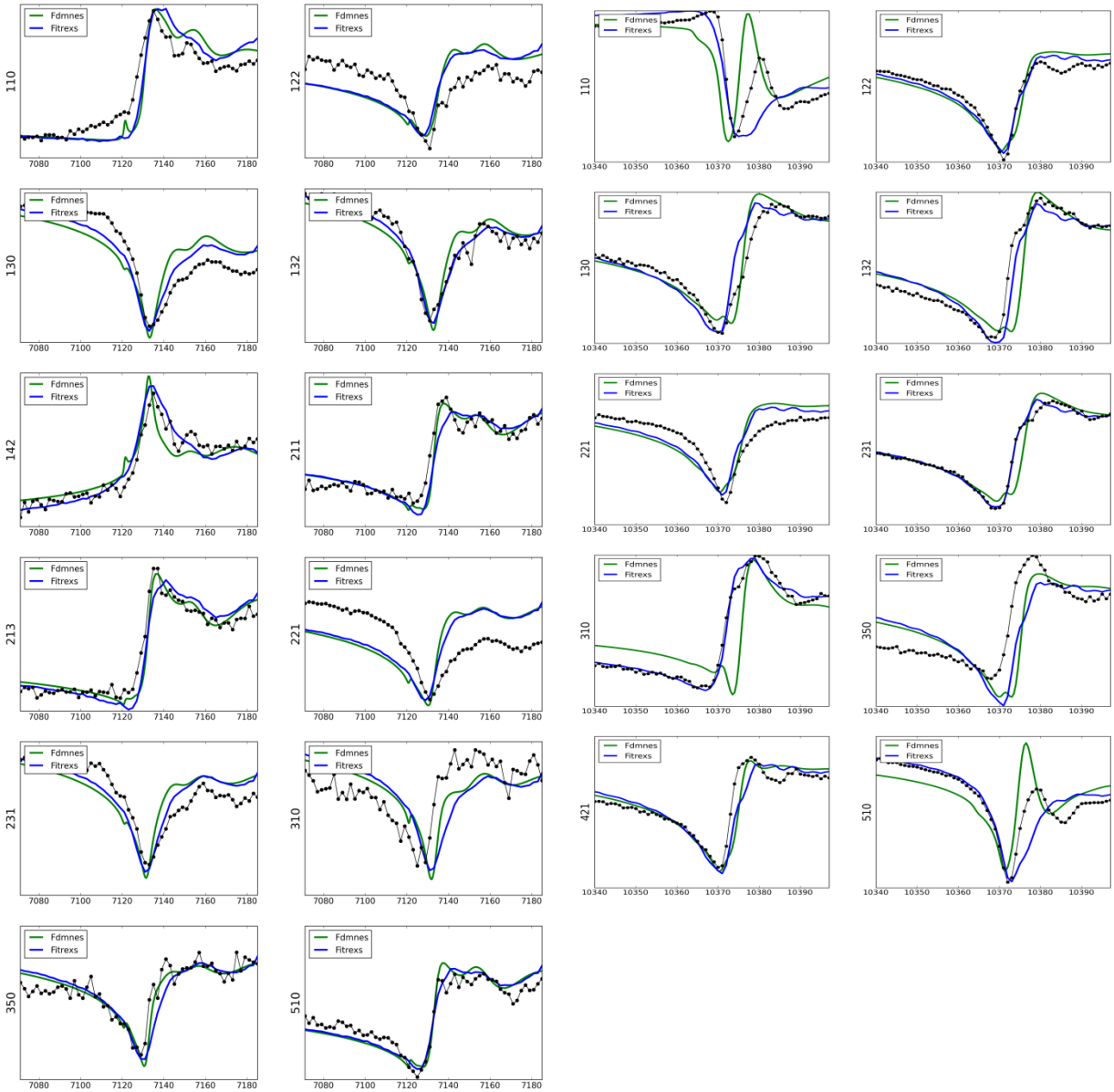

Figure S5 : Experimental data and refinement of the GFO0.9 thin film using both FitREXS (blue) and FDMNES (green).

S6. Experimental data and refinement of the GFO1.1 thin film using both FitREXS and FDMNES

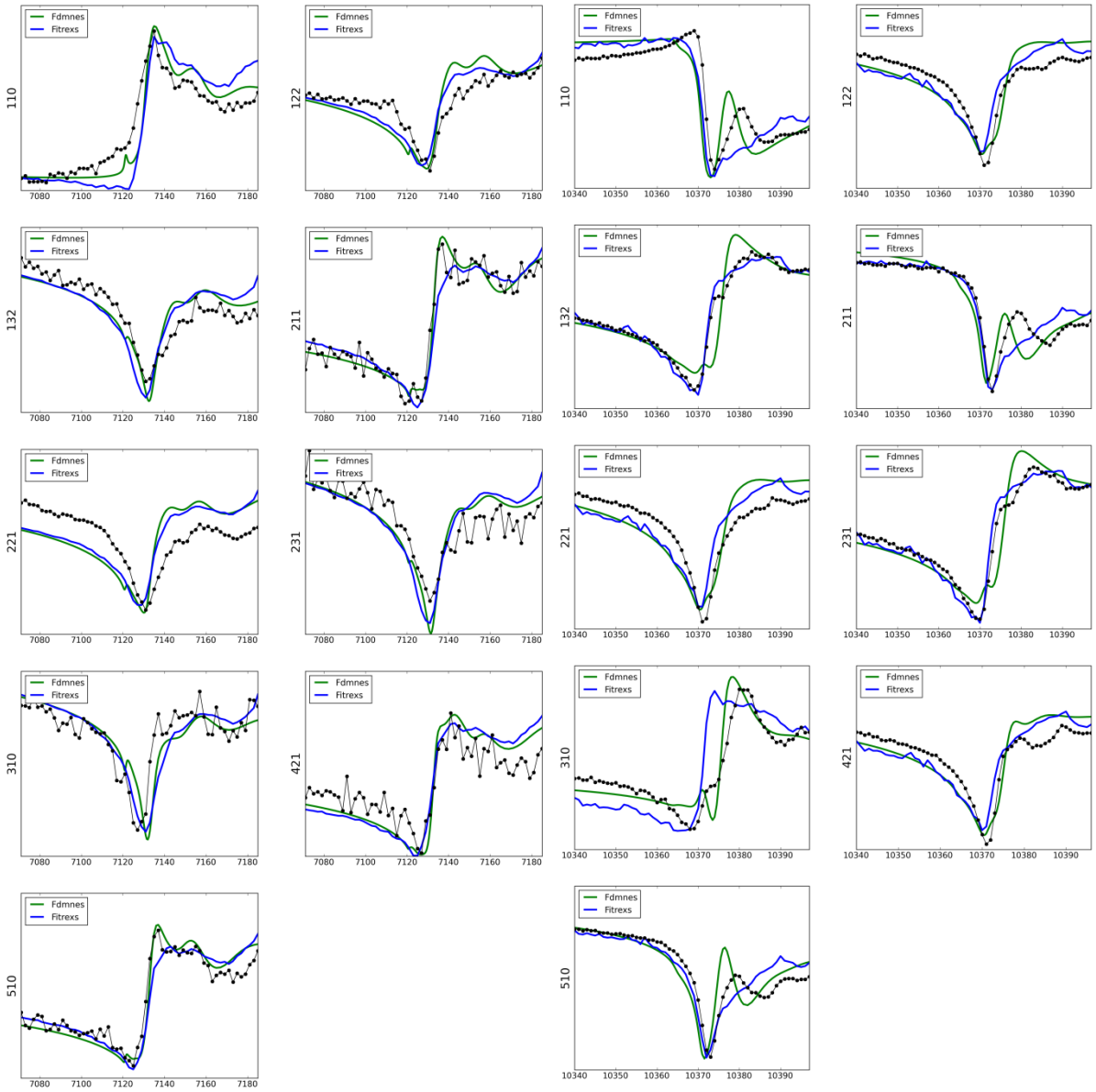

Figure S6 Experimental data and refinement of the GFO1.1 thin film using both FitREXS (blue) and FDMNES (green).

S7. Experimental data and refinement of the GFO1.4 thin film using both FitREXS and FDMNES

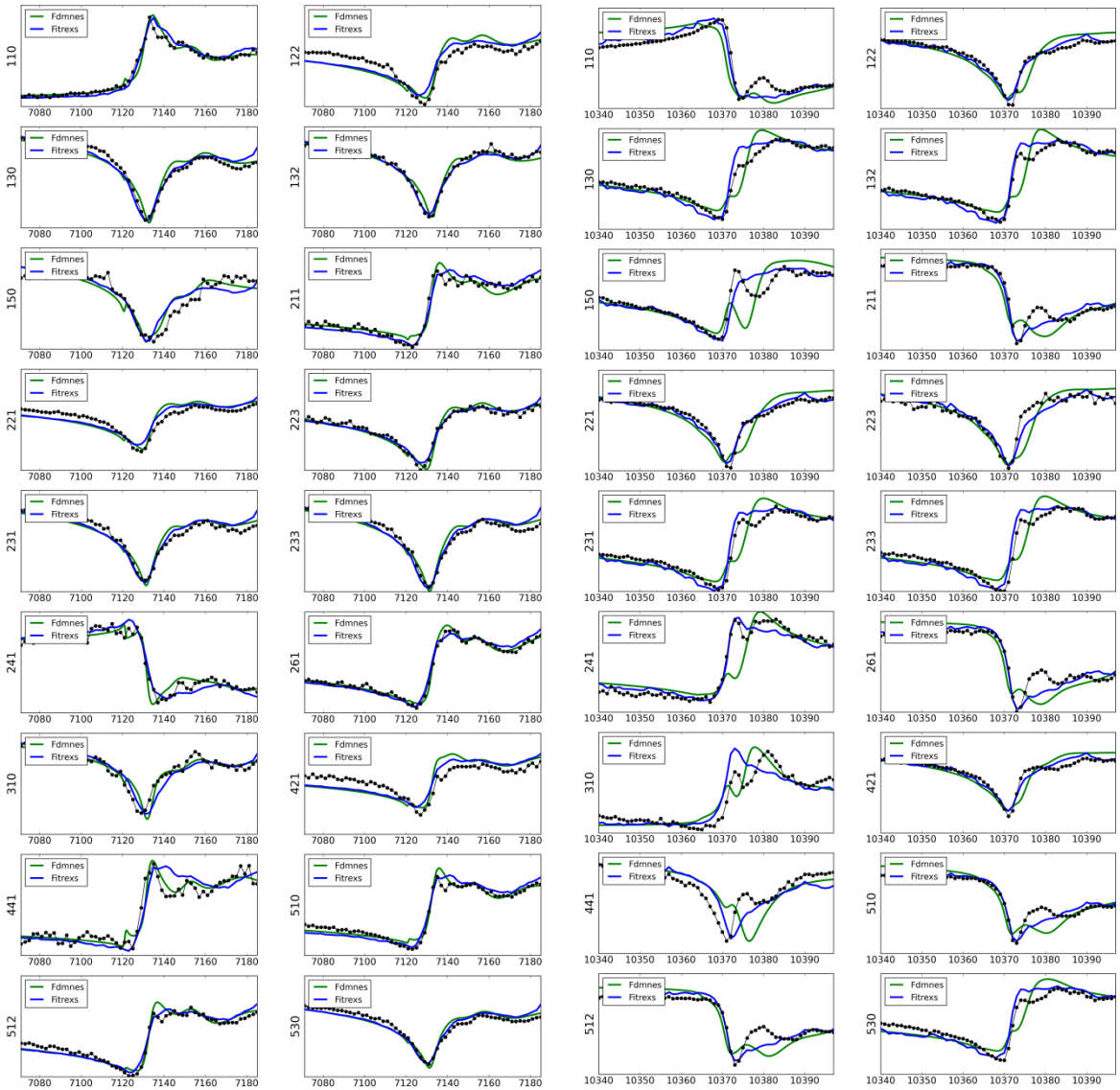

Figure S7 Experimental data and refinement of the GFO1.4 thin film using both FitREXS (blue) and FDMNES (green).