Electronic Supplementary Material (ESI) for CrystEngComm.
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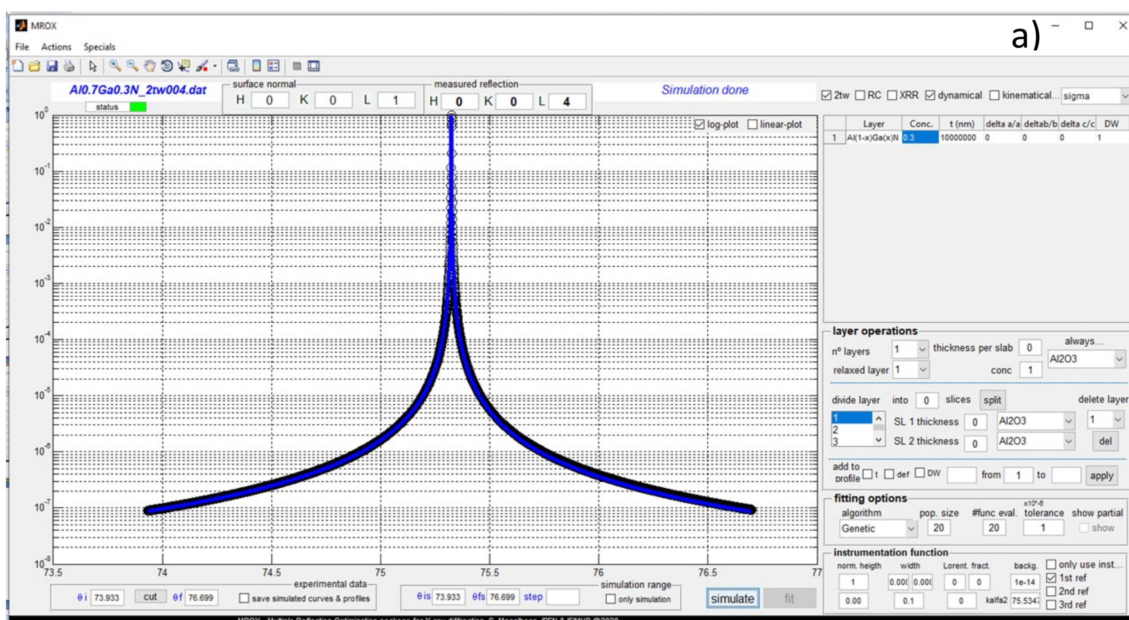
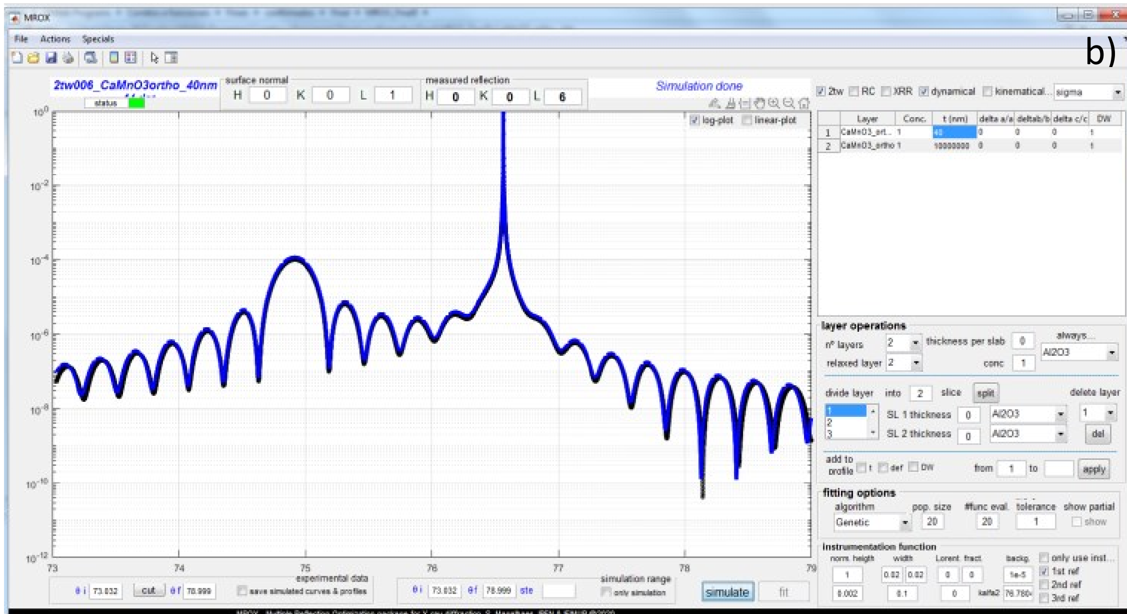
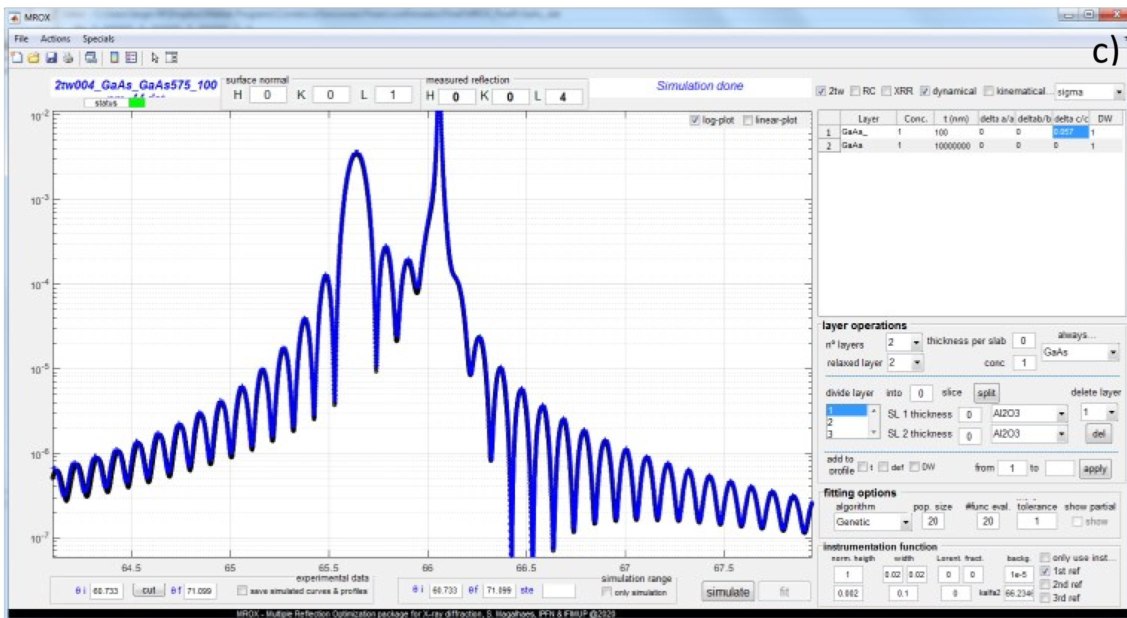
S1. Validation of MROX software

Validation of MROX is accomplished by performing several simulations using LEPTOS® commercial software, available at the Bruker D8 series AXS diffractometers. LEPTOS® implements the 2x2 and 4x4 matrix recursive methods developed by S. Stepanov *et.* al.[1] Both matrix methods are approximations to the pure dynamical theory of X-ray diffraction in order to increase the speed and versatility in the simulation and fitting algorithms. At this moment, a set of more than 160 simulations are compared and close to perfect agreement is found. The total set of figures 1 show a comparison between MROX and LEPTOS® simulations for different crystals and reflections with increasing layer complexity. In all simulations, the blue line corresponds to the simulation using the MROX code, whereas the open black circles correspond to the simulation using LEPTOS® software. Figure 1a) depicts to the case of a 0004 2θ-ω simulation of a bulk $Al_{0.7}Ga_{0.3}N$ crystal. The single layer structure of the simulated reflection is shown on the upper right side of the MROX layout (inside table). Figure 1b) reflects the comparison between both codes of a 006 2θ-ω simulation from an orthorhombic 40 nm strained $CaMnO_3$ thin film "grown" on top of relaxed-bulk $CaMnO_3$. The third comparison, shown in figure 1c) is from GaAs, a cubic crystal, where a strained layer of the same material is included at the surface. Follows in figure 1d), a strained Si 150 nm thick layer is simulated on top of a Si substrate. The comparison between figures 1b) to 1d) allows concluding that the thickness effect on the diffractogram is perfectly simulated in MROX. Moreover, the three cases refer to different crystalline structures and reflections. The fifth case is from a double Si layer of 100 and 20 nm, respectively, each layer differently strained on top of a Si substrate. The differences observed are very small and can be interpreted by the more sophisticated simulation done using the matrix recursive method developed by S. Stepanov and implemented on LEPTOS.




b)
MROX
File Actions Specials
2tw006_CaMnO3ortho_40nm
surface normal
H 0 K 0 L 1
measured reflection
H 0 K 0 L 6
Simulation done
log-plot
linear-plot
2tw RC XRR dynamical kinematical
layer operations
fitting options
instrumentation function
experimental data
simulation range
simulate
fit
MROX - Multiple Reflection Optimization package for X-ray diffraction, S. Magalhaes, IPFN & IFIMUP @2020


c)
MROX
File Actions Specials
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surface normal
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measured reflection
H 0 K 0 L 4
Simulation done
log-plot
linear-plot
2tw RC XRR dynamical kinematical
layer operations
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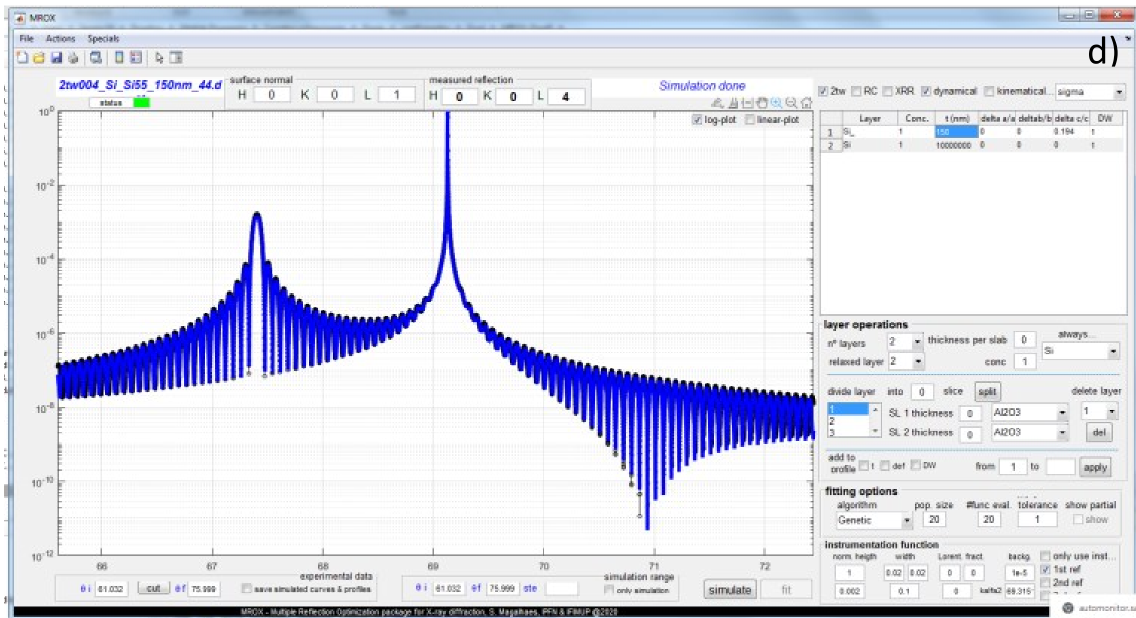

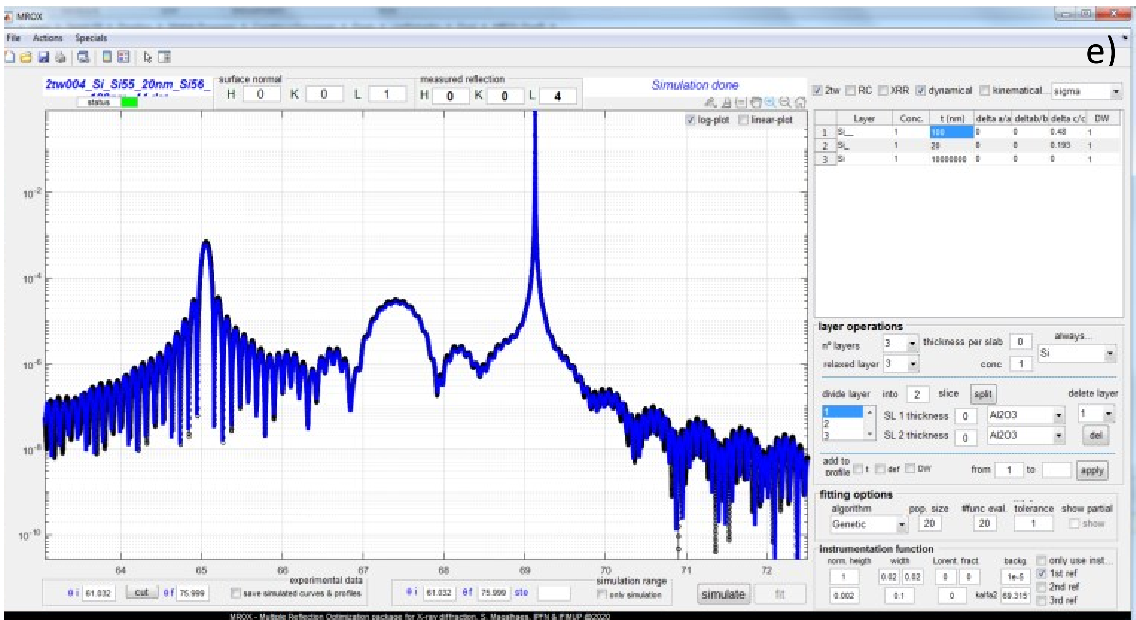

Figure 1 MROX layouts comparing the simulations of a 0004 2θ-ω scan of a bulk $Al_{0.7}Ga_{0.3}N$ alloy, a), 006 2θ-ω of an orthorhombic strained $CaMnO_3$ 40 nm thick simulated on top of the same crystal substrate, b), 004 2θ-ω of a cubic 100 nm strained GaAs simulated on top of a GaAs substrate, c), and 004 2θ-ω of a cubic Si substrate, where 1 d) and 2 layers e) of increasing strained Si and different thicknesses.

Reference

[1] S. A. Stepanov, E. A. Kondrashkina, R. Kohler, D. V. Novikov, G. Materlik and S. M. Durbin, Phys. Rev. B, 1998, 57, 4829.