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[219] InteractiveXRDFit: a new tool to simulate and fit X-ray diffractograms of oxide thin films and heterostructures

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InteractiveXRDFit is a Matlab program that calculates the X-ray diffracted intensity for heterostructures. The user can choose the substrate and the different materials composing an heterostructure among a long list of compounds, choose between (001) or (111) substrate orientation, and play with the different structural parameters (unit-cell size and number of layers). It is possible to build a superlattice composed of up to three different materials, and add a top and/or bottom layer. Each layer can have a different c-axis, either constant or varying as a function of depth within a layer. The simulation is quick and allows the user to compare it directly to the measurements, so as to rapidly determine the crystalline parameters of the sample.

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