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【133】 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. Other fitting programs are already available and efficient, but may lack some flexibility with some of the parameters that this program allows modifying. Here the user can choose the substrate and the different materials composing an heterostructure among a long list of compounds (mainly perovskite oxides), 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 (to simulate electrodes, spacers or capping layers). 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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