GIDInd: an automated indexing software for grazing-incidence X-ray diffraction data

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Grazing-incidence X-ray diffraction (GIXD) is a widely used technique for the crystallographic characterization of thin films. The identification of a specific phase or the discovery of an unknown polymorph always requires indexing of the associated diffraction pattern. However, despite the importance of this procedure, only few approaches have been developed so far. Recently, an advanced mathematical framework for indexing of these specific diffraction patterns has been developed [1, 2].

Here, the successful implementation of this framework in the form of an automated indexing software, named *GIDInd*, is introduced [3]. *GIDInd* is based on the assumption of a triclinic unit cell with six lattice constants and a distinct contact plane parallel to the substrate surface. Two approaches are chosen: (i) using only diffraction peaks of the GIXD pattern and
(ii) combining the GIXD pattern with a specular diffraction peak (see Figure 1). In the first approach the six unknown lattice parameters have to be determined by a single fitting procedure, while in the second approach two successive fitting procedures are used with three unknown parameters each. The output unit cells are reduced cells according to approved crystallographic conventions. Unit-cell solutions are additionally numerically optimized. The computational toolkit is compiled in the form of a MATLAB executable and presented within a user-friendly graphical user interface. The program is demonstrated by application on two independent examples of thin organic films.

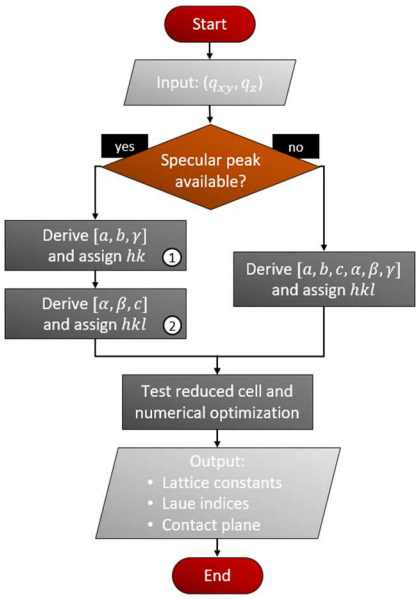

Figure 1. Process workflow of the indexing algorithm realized with *GIDInd*. The marker on the left branch indicate the split processing of the peak positions (q_{xy}, q_z) for derivation of the lattice parameters [*a, b, γ*] followed by [*α, β, c*] of the unit cell when a specular diffraction peak is available. The right branch demonstrates the single fitting procedure when working without a specular scan.

[1] Simbrunner, J., Simbrunner, C., Schrode, B., Röthel, C., Bedoya-Martinez, N., Salzmann, I. & Resel, R. (2018). *Acta Cryst.* **A74**, 373.
[2] Simbrunner, J., Hofer, S., Schrode, B., Garmshausen, Y., Hecht, S., Resel, R. & Salzmann, I. (2019). *J. Appl. Cryst.* **52**, 428.
[3] Kainz, M. P., Legenstein, L., Holzer, V., Hofer, S., Kaltenegger, M., Resel, R., Simbrunner, J. (2021). *J. Appl. Cryst.* (in press).

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