Mandatory XRR parameters required to run Measurement and Analysis (All about XRR)

For XRR measurements and analysis, please provide the essential parameters for both the substrate and each layer of the thin film. Fill the following details of the substrate material and Film.

Substrate Material _____

Expected Average Density of Film (layers), (g cm^{-3}) _____

Please complete the table below by specifying whether each substrate and each layer of the film is crystalline or non-crystalline.

For Structured Material of Substrate/Film (fill detail for each layer separately if film is multilayer)

Custom name/ Material	
Layer(s) No. / Substrate	
Estimated layer Thickness	
Space group name	
a, nm	
b, nm	
c, nm	
α, °	
β, °	
γ, °	
Volume, nm³	

Atoms

Atom	Wyckoff	Occupancy	X	Y	z

For Structureless Material of Substrate/Film (fill detail for each layer separately if film is multilayer).

Custom name/ Material	
Layer(s) No. / Substrate	
Estimated layer Thickness	
Density, g/cm3	0.000

Atoms

Atom	Concentration

To perform XRR analysis for a new crystalline material in the Rigaku SmartLab SE software, you need to input accurate crystallographic parameters. Here's how you can source the correct values:

1. **Lattice Constants (a, b, c, α, β, γ):** Lattice constants refer to the set of six parameters that define the geometry of a unit cell in a crystal lattice
2. **Space Group:** It specifies the symmetry group of the crystal lattice, which defines how the unit cell repeats in space.
3. **Wyckoff Positions:** It represents the symmetry-equivalent positions of atoms in the unit cell based on the space group.
4. **Atom Types and Coordinates (x, y, z):** Atomic coordinates are usually expressed in terms of fractional coordinates, (x, y, z). This coordinate system coincides with the cell axes (a, b, c) and relates to the position of the atom in terms of the fraction along each axis.
5. **Volume:** The calculated volume of the unit cell based on the lattice parameters and angles

Recommended Approach:

1. **Search in Databases:** Use crystallographic databases like ICSD (Inorganic Crystal Structure Database), COD (Crystallography Open Database) or Pearson's Crystal Data to search for your material or closely related ones.
2. **Experimental Methods:** If your material is new or unavailable in databases, perform XRD or similar characterization techniques to gather the necessary lattice parameters and atomic coordinates.
3. **Literature Review:** You can source this data from specialized literature or material property databases such as Materials Project or MatWeb. If the material is not in the database, starting with a closely related material for initial analysis and refining the parameters experimentally would be a good approach.