Texture modelling: brain dump and my inputs

Thomas Kittelmann Informal texture modelling kickoff meeting April 21, 2022

Long term goal of this collaboration!







Short term goal of this meeting!



Some things to discuss today

- What for? Both extracting texture in analysis vs. general simulation models.
- Types: Simple models (March-Dollase) vs. full ODF based. For the latter, there is a question of smooth models (expansion in spherical harmonics) versus non-smooth. In all cases, there is the issue of input data formats.
- For simulations I can see the use for both full ODF as well as simpler models.
- In particular, it would be nice to have some simple go-to models, that can be used to add simple texture to a general simulation (e.g. "rolled aluminium for entrance windows"). Does it make sense to have a bunch of standard models, like fibre / plates, rolled sheet metal, ...? With some sort of "cook book" recipes, that could be used to add some realism to a simulation (or at least gauge the importance of texture on a give figure of merit).
- For all use-cases I can see that computational speed becomes a challenge.
- Then there is the question of who / what / when. But it might be enough if we simply end today with a clear understanding of the issues, and perhaps with some ideas for next (baby) steps.
- For the rest of my slides I will go through some details of the current "texture" models in NCrystal, namely the single crystal models. They share a lot of the same issues as texture models (indeed, are a specific class of ODF), so might highlight strategies and challenges.

Experience with current "texture" models in NCrystal: Single crystals! (cf. https://doi.org/10.1016/j.cpc.2021.108082)



Single crystal with isotropic gaussian mosaicity.

Analytical formula for non-backscattering and low mosaicity, otherwise needs numerical integration. *Low chance for a given plane to contribute.* Layered crystal (a.k.a. PG, a.k.a. rotated single crystal)

x

Always needs numerical integration, High chance for a given plane to contribute.

Normal single crystal with Gaussian mosaicity uses cheap pre-check to speed up:



Single Crystals with Gaussian mosaicity

Can model monochromators, analysers, filters, samples





*: Once contributing normals Have been identified.

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NCrystal X. X. Cai & T. Kittelmann



Depending on use-case, the attention to detail in the single crystal model might be crucial.



PG : Off-axis planes are complicated and expensive to deal with. Likely similar to general texture models.



Lots of planes to consider at shorter d-spacing!



The "sccutoff" parameter: Planes with dspacing smaller than this are moved to a powder model. Default is 0.4Å.



CPU speed.



Technical check for consistency

of Single Crystals codes (must also hold for any texture model!!)

In principle an isotropically illuminated single crystal should on average give powder-like cross-sections.

In practice, a lot of edge-cases and details have to be treated correctly in the SC code before this happens!

Another check is that consistent SC codes should provide "zig-zag walk"





with this brute force validation.