



EUROPEAN
SPALLATION
SOURCE



Status of texture model study

Work Package 2

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Literature review

Orientation distribution function (ODF) gives the probability of finding grains with a specific orientation in a polycrystalline material [1].

how to determine the ODF?

how to incorporate the ODF in the cross section calculation?

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Literature review

Incorporation of ODF in the cross section calculation:

Texture.comp of McStas (Laliena et al. [2]): ODF described by a series of generalised spherical harmonics and comprised in an additional term ($\Upsilon(G, k)$ or $\Upsilon(d_{hkl}, \lambda)$) in the total cross section

Sinpo1 (Dessieux et al. [3]): dedicated to neutron transmission measurements, apply ODF of single crystals (grains) to determine the transmission, then to voxel and finally to sample

March-Dollase model

March-Dollase model assumes an axially symmetric orientation distribution around the beam direction [4]:

$$P_{hkl}(\lambda, d_{hkl}) = \frac{1}{2\pi} \int_0^{2\pi} \left(R^2 B_{hkl}^2 + \frac{1 - B_{hkl}^2}{R} \right)^{-\frac{3}{2}} d\phi, \quad (1)$$

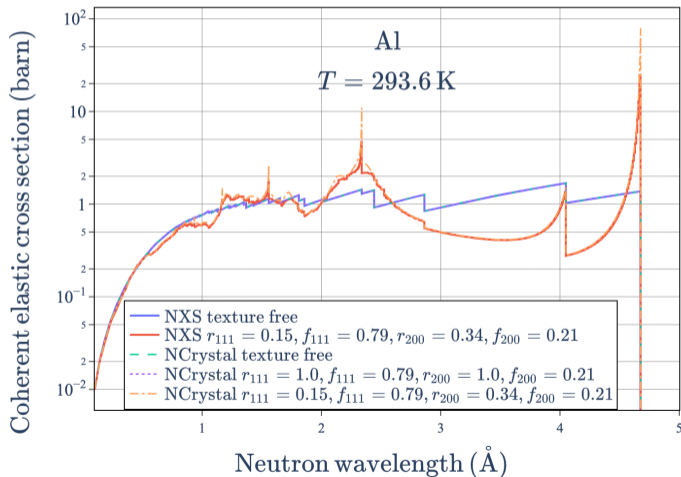
where

$$B_{hkl} = \cos(A_{hkl}) \sin(\theta_{hkl}) + \sin(A_{hkl}) \cos(\theta_{hkl}) \sin(\phi), \quad (2)$$

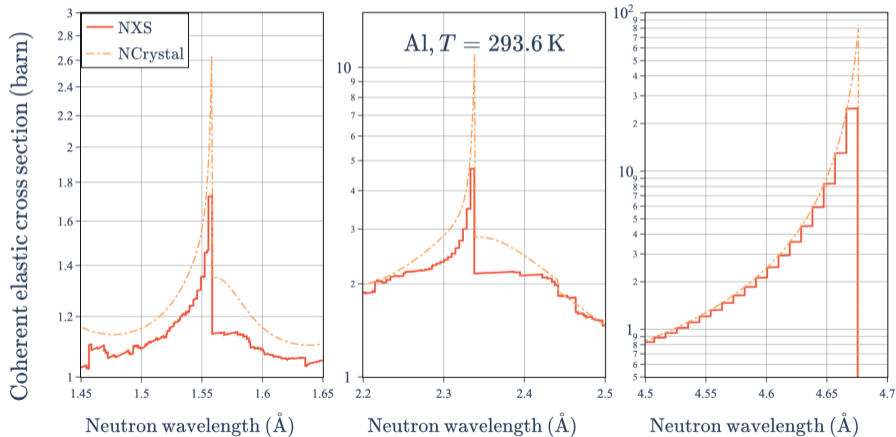
$$A_{hkl} = \arccos \left(\frac{hH + kK + lL}{\sqrt{h^2 + k^2 + l^2} \sqrt{H^2 + K^2 + L^2}} \right), \quad (3)$$

$$\theta_{hkl} = \arcsin \left(\frac{\lambda}{2d_{hkl}} \right). \quad (4)$$

Compared to NXS [5]



Compared to NXS









Thanks for your time.
Questions?

References



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-  L.L. Dessieux, A.D. Stoica, P.R. Bingham, Ke An, M.J. Frost, and H.Z. Bilheux.
Neutron transmission simulation of texture in polycrystalline materials.
Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 459:166–178, 2019.
-  Hirotaka Sato, Takashi Kamiyama, and Yoshiaki Kiyonagi.
A rietveld-type analysis code for pulsed neutron bragg-edge transmission imaging

texture: grains in poly-crystalline materials are not randomly oriented but have preferred orientations

orientation descriptions: two coordinate systems (sample coordinate and crystalline coordinate) transferred from one to another by three-dimensional rotation matrix (in $SO(3)$)

pole figure: two-dimensional graphical representation of distribution of a plan normal with respect to the sample coordinate system

inverse pole figure:

orientation distribution function (ODF): probability of finding grains with a specific orientation in a poly-crystalline material

ODF determination: from pole figures

harmonic method: ODF described by a series of generalised spherical harmonics, ODF determination problem transferred to determination of harmonic coefficients from pole figures

Backup



spherical harmonic model incorporated in cross section calculation by Laliena et al.
March-Dollase model classified as real fibre texture model