1.4.19. SPATIAL SUPER-RESOLUTION FOR LINE PARALLEL IMAGING IN ENERGY DISPERSIVE X RAY DIFFRACTION

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Abstract. We present a new approach for Energy Dispersive X Ray Diffraction (EDXRD) imaging in "line parallel" configuration. It follows an inverse problem approach using a physical model of the diffraction phenomenon. Using this approach, we show that it is possible to achieve a spatial super-resolution of poly-crystalline objects (i.e. to measure more voxels than detectors).

Introduction. EDXRD is used to provide information about crystalline structure of material. It consists in measuring photon coherently scattered by a sample at a fixed angle / the sample being illuminated by a polychromatic X-ray beam. The spectrum obtained is linked to the atomic planar spacing of the sample according to the Bragg law and then can be used for materials identification.

X-Ray Diffraction Imaging (XRDI) is a modality where measurements are made in many volume elements (voxels) of the studied object. It then provides spatially resolved maps of diffraction profiles. For practical use of this technique in security screening [2], acquisition speed is a critical requirement. As pointed in [1], each single acquisition is time consuming, and thus, designing massively parallel acquisition scheme is a necessity. One of the simplest technical solution for such scheme is the "line-parallel" XRDI defined in [1].

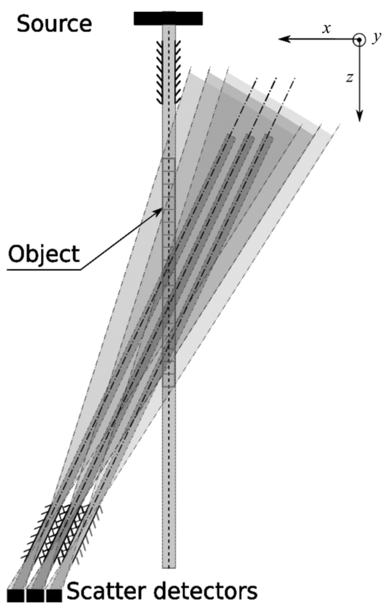

Fig. 1. Schematic Illustration of line parallel energy dispersive XRD imager

In this paper, we present a method for processing data of this line-parallel XRDI. In this framework, a line of scatter detectors provides diffraction profiles of individuals parts of the object at different depths along the illumination beam. Owing to the overlapping of areas observed by each scatter detectors, we propose an inverse problem based method which enhances spatial resolution of this line-parallel XRDI. This spatial super-resolution provides diffraction profile map with more voxels than detectors.

Inverse Problem Approach. We aim to retrieve the interference function (proportional to form factor $|F(x)|^2$ for crystalline material) in the momentum transfer space for each observed voxel. The unknowns of our problem is then a two dimensional map Z times F where Z is the depth position of the voxel and F its interference function in the momentum transfer space.

In an inverse problem approach, we estimate theses unknowns that best reproduce the measurements according to a direct model. The direct model is a physical model derived from X ray diffraction and attenuation theory, source and detector characteristics and geometrical parameters of our setup (e.g. collimators position and size, distances...). As this problem is ill-posed, we resolve it in a maximum a posteriori (MAP) framework by defining some priors about these unknowns. These prior will be injected in the problem by some regularization functions. The main issue about priors definition was the fact that pure amorphous (e.g. liquids) and pure crystalline materials present very different diffraction profiles. To bypass this problem, we defined two maps, one for crystalline, the other for amorphous materials with different priors:

– interference function of crystal is almost null everywhere except on values corresponding to inter-planar spacing distances;

– interference function of amorphous materials is smooth in the momentum transfer space;

– along the depth dimension, in an additional spatial prior, we suppose that if there a change of materials between two adjacent voxels, the interference function will change radically;

– in addition, force the estimated map to be positive.

Finally, the estimated map x is the solution which minimizes the equation:

$$x = \operatorname{argmin}[\backslash\backslash m\{x) - d \backslash f + aF_{crys} Jx) + \hat{} F_{amor} Jx) + yF_s Jx)],$$

where $m(x)$ is the model, d the measurements, $F_{amorph}\{x)$ and $F_{cry} Jx)$ the regularization functions for the amorphous map and the crystalline map respectively, $F_{cry} Jx)$ the spatial regularization function and $\boldsymbol{a}$, $\boldsymbol{p}$ an $\boldsymbol{y}$ three tuning hyper parameters. The minimization is made using a continuous optimization method (L-BFGS [3]).

Results. The direct model have been first validated using experimental measurements of known material. This method was then tested on several realistic simulated data with three or four components (crystalline and amorphous). Results show that the algorithm successfully recover the interference function in 20 voxels with only 5 five scatter detectors increasing the spatial resolution by 4. Voxels size was 2 × 2 × 2 mm and each detector “sees” about 6 voxels.

References:

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