Analysing the Structure of Poly-crystalline Materials by 2-Dimensional DLS-Spectra and Neural Nets

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Abstract. A method to analyse the structure of poly-crystalline material by 2-dimensional DLS-Spectra and Backpropagation neural nets is introduced. It will be shown that DLS-Spectra “clean up” X-Ray-pictures such that the Radon-transformation of the Kikuchi-diagrams leads to better results. Further it will be shown, how these cleaned up Kikuchi-diagrams enable an automatic classification of poly-crystalline materials by neural hyper-classification systems based on the Backpropagation-algorithm.

Keywords: Kikuchi-diagrams, Radon-transformation, pattern recognition with neural nets.

1 Introduction

One of the essential features of poly-crystalline materials is that the distribution of the crystals grain-orientation (called texture of the crystal) can be detected by Kikuchi-diagrams in an automatic way. Rationale of Kikuchi-diagrams is the interaction of matter and electron beams which meet crystal probes. The interaction itself corresponds to inelastic scattering of the (wave-like) electrons by the grid system of the crystal probe, whereby the originated secondary electrons will be diffracted. This diffraction – described by Braggs law – creates a special pattern on a fluoroscopic, called Kikuchi-diagram. A Kikuchi-diagram shows straight bands – called Kikuchi-bands - and stars formed by the crosstalk of these bands. The structure of a Kikuchi-band is defined by its width which is reciprocal proportional to the shoal's distance of the of the diffracting net-planes belonging to the regarded band. The cutting angle of two bands corresponds to the angle of the according shoals of diffracting net-planes in the crystal. Thus it is depending on the orientation of the crystal which bands can be detected by Kikuchi-diagrams and how the poly-crystalline structures can be estimated. In Figure 1 a typical Kikuchi-diagram is shown; clearly the different bands and several crosstalks can be seen.

The analysis of the crystals structure is done in five steps: 1. Orientating the electron beam, 2. Recording and digitalizing the Kikuchi-diagrams, 3. Detecting the Kikuchi-bands, 4. Subscripting the detected bands 5. Computing the texture of the crystal by using the orientation of the indexed bands.
In this paper it will be shown, how an automatic detection of Kikuchi-bands (3.) can be done with the help of DLS-spectra and neural nets. Further it will be shown that the Radon-transformation can be observed as an adequate pre-processing step for such soft-computing systems, as Kikuchi-bands correspond with simple peaks in the Radon space.

2 Preprocessing Kikuchi-Diagrams

As the diffraction of the electrons results in a very poor yield of light, Kikuchi-bands normally cannot be detected directly out of a fluoroscopic's activity pattern (or its record). Only a quasi dark, lightly structured background of the activity can be observed. This background results from electrons which have been scattered in an elastic way or from electron-waves which do not fulfil Bragg's equation. To reduce or eliminate these disturbing noisy contributions of the picture we use 2-dimensional difference-autopower-spectra (2-dim DLS), as DLS-Spectra can be considered a band-pass-filter too [5]. The DLS-Operation itself consists of two calculation steps: 1. Calculating the average of a picture's background. 2. Subtracting the average from the original picture.

The first calculation step of the DLS-operation will be done by averaging a floating mask of the gray tones of the fluoroscopic's activity pattern. In detail the gray tone values of a $(m+1) \times (m+1)$ mask are added up whereby the point N denotes the epicentre of the mask. The calculated gray value is divided by the number of points added up and this value is assigned to the point N. Next the mask is displaced to the next point (pixel) of the picture and the calculation is replicated until the average has been calculated for all points of the picture. This operation can formally be regarded as convolution in the space of location for which

$$pict'_{y,x} = \sum_{i=-r}^{r} \sum_{j=-r}^{r} pict_{i,j} \cdot M_{y-i,x-j}$$