Journal for Geometry and Graphics
Volume 17 (2013), No. 2, 205–211.

Application of Focal Curves for X-ray Microdiffraction Methods

Frank Henschel[1], **Jürgen Bauch**[2]

[1] *Faculty of Informatics/Mathematics, University of Applied Sciences*
D-01069 Dresden, Germany
email: henschel@informatik.htw-dresden.de

[2] *Institute for Material Science, Dresden University of Technology*
D-01062 Dresden, Germany
email: juergen.bauch@tu-dresden.de

Abstract. In order to harness the full potential of X-ray diffraction methods, in particular the Kossel and X-ray Rotation Tilt (XRT) technique, it is necessary to implement a fast and automatic detection and evaluation process for digital recordings or digitized film. A method developed by us allows, through the implementation of a largely automated processes and the application of various geometric propositions, rapid access to a diverse evaluable database of many X-ray diffraction images. Due to the registration of the reflection fine structure, the individual data can be used to, for example, for calculating the precision residual stress tensors directly. For this application it is necessary to know the complete recording geometry. In this contribution we examine the focal curves for this purpose. As all the diffraction cones have the same apex the orientation can be determined solely by the reflection lines, which result as intersection with the image plane. In this recording technique the apex of the cones is the source of X-ray radiation in the investigated sample area. In addition to the principal point, the distance from the image plane to the sample can be determined from the respective focal curves of reflection lines without the use of a scaling factor.

Key Words: conic section, focal conics, orientation, X-ray microdiffraction, Kossel technique

MSC 2010: 51N05, 51N20, 68U10

1. Introduction

Over the past several years a change from photographic paper to digital detectors has been observed for X-ray recordings. In addition, the quality of these imaging techniques has improved enormously. This development has occurred not only for the recording procedures but

ISSN 1433-8157/$ 2.50

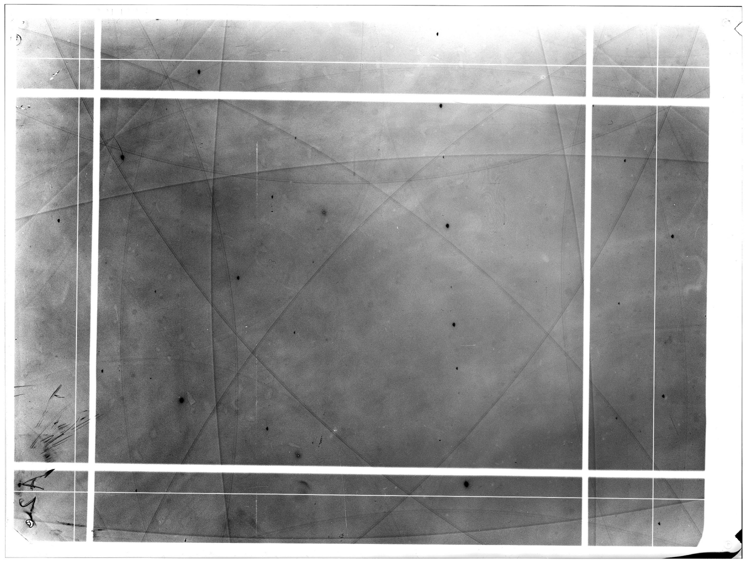

Figure 1: Synchrotron Kossel image of CuMn4 together with projection of the two level rectangular wire grid

also simultaneously for the methods of digital image processing. In our group such procedures are of great interest for the analysis of diffraction patterns. These are not generated as shadow microscopic radiographs in transmission, but by the diffraction from the crystal lattice of the sample. Only this allows any conclusions to be made about the crystallographic structure of the specimen and, subsequently a calculation of precision residual stress tensors. In order to obtain this information it is necessary to very accurately detect and evaluate the diffraction lines, which come in the form of conic sections. For this an evaluation at the digital image processing level is not enough, because the complex geometry has to be investigated as a whole.

An important aspect for the evaluation is the determination of the principal point in the recording plane and the distance to the projection centre. Previously, the calculation of the orientation has been solved with aid of extra tools: an additional construction formed from a rectangular wire grid at two different depth levels was built into the beam path (see Fig. 1). Alternatively, the distances were measured directly in the sample chamber, which is not very accurate. In this work a method is presented which implements this part of the evaluation solely on the basis of the diffraction patterns.

2. X-ray diffraction lines

The analysis chain up to the orientation evaluation is given in the following.

2.1. X-ray microdiffraction methods

The examples used in the described application are based on two microdiffraction methods: the *Kossel technique*[1] and the *XRT-technique* (X-ray-rotation-tilt) [2].

- In the first a focused electron beam or collimated X-ray beam (diameter $< 5\,\mu$m, respectively $< 100\,\mu$m) generates characteristic or fluorescence X-rays within the interaction

[1]Named after Walther Kossel (1888–1956), German physicist.

volume located in a single grain of the sample. The majority of the radiation leaves the crystal undiffracted, but a small amount of the characteristic X-rays is diffracted by the interference-capable lattice planes according to the Bragg equation[2]

$$2d \sin\theta = n\lambda \tag{1}$$

The generated interferences fall on straight circular cones with half apex angles of $90° - \theta_{hkl}$, where θ_{hkl} is the BRAGG angle for the lattice plane with index hkl. In the image plane curves of 2^{nd} order — conic sections — are generated (see Fig. 1).

- The same result is achieved using the XRT technique which is based on the same physical law; between each monochromatic X-ray beam with wavelength λ and the lattice planes there exists an angle θ_{hkl} that satisfies Bragg's Law. This diffraction generates an interference point on a detector. Moreover, for a variation over the entire angular range in the half-space above the specimen this forms a sequence of pixels: on the whole joined diffraction lines.

2.2. Detection and fine structure analysis of diffraction lines

In order to gain further information from the geometry of diffraction curves, they must first be detected on the record. This analysis is divided into two main parts: first *rough* detection followed by *fine* detection with sub-pixel accuracy. Both are described in more detail in [1].

In summary, for the first step of the object detection the image is converted into a binary image via an edge detection algorithm like the Sobel operator. The recognition of objects is based on a three-dimensional variant of the Hough transform. A reasonable first restriction is to interpret ellipses as circles (x, y, r). For each positive pixel from the obtained binary output image a circle with corresponding coordinates for this centre and also variable radius r is drawn and accumulated in the appropriate level r of the three-dimensional solution space. At the end the maxima in this space correspond to the solutions for centres and radius for the circles.

In the second step, which is based on this rough solution, sufficient transverse profiles from the diffraction lines along the previously received circular paths are measured. These profile values form the basis for the approximating function of a conic curve. An exact description of the various diffraction lines can be used in different tasks, in particular for the determination of lattice parameters, the high precision crystallographic orientation, and the strain and stress tensor for a sample. Due to the properties of the Kossel technique, the obtained data from such a recording are suitable for these computations. However, for these calculations other parameters are needed [3]: including the principal point and the distance of the detector to the sample, which form the interior orientation of the recording.

3. Application of focal curves

There are several approaches to determine the interior (and exterior) orientation of a record formed from diffraction lines obtained for instance from a Kossel recording. One way is to directly measure distances in the sample chamber. Even if the results can be compensated later, this is neither sufficiently accurate nor practicable. Another way is to install in the beam path a two depth level rectangular wire grid. Consequently, the orientation can be

[2] It was derived 1912 by Sir William Lawrence Bragg (1890–1971), an Australian-born British physicist

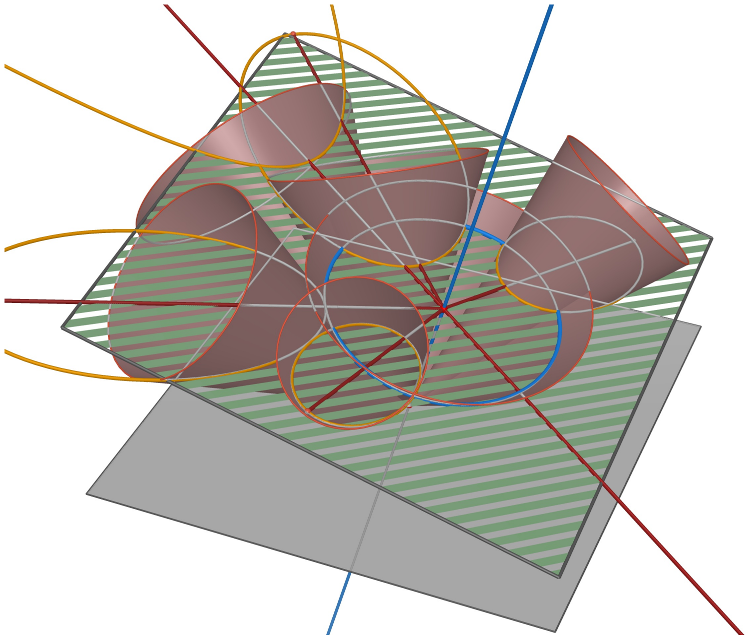

Figure 2: Intersection of all major axis from different conic sections

determined from the associated shadow projection by elementary mathematics. In practice, an exact installation and the accuracy of such two level targets cannot be guaranteed so that the solution has to be calculated over the spatial resection by adjust spatial control points to their image points. Both methods have their drawbacks, such that a solution based only on the diffraction lines is necessary. Easy to see and to explain is another way to determinate the principal point (Fig. 2).

Since there are no special cases, the diffraction lines as conic section in the image plane are hyperbolas or ellipses. All the curves are generated as intersection from all the so called

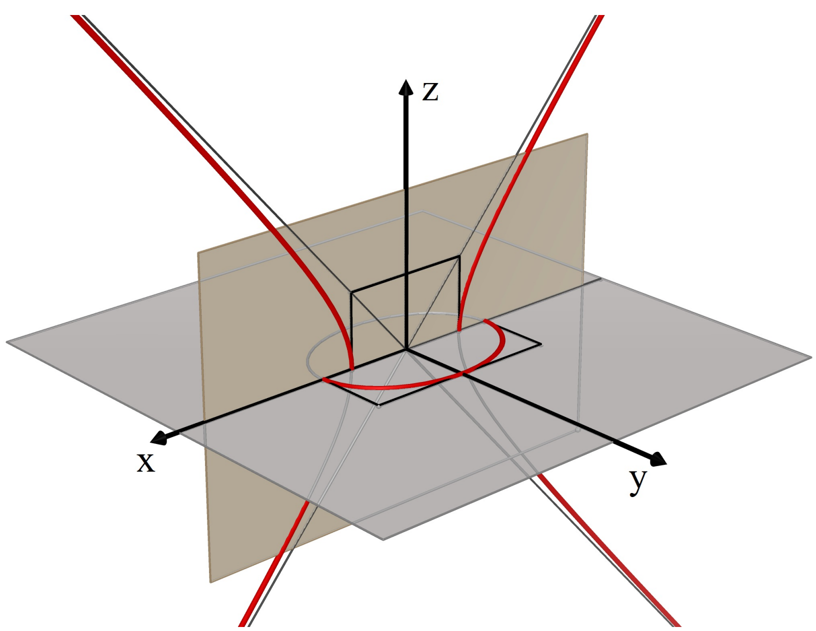

Figure 3: Example for focal ellipse and hyperbola

Kossel-cones with their different axial directions and different apertures but common apex and the image plane. Thereby the apex is the restricted sample area and the source of radiation and accordingly the projection centre. Then all major axes of the conic sections, regardless of type, intersect at a single point, which is the pedal point of the apex to the detector plane. This is the principal point.

Another possible route for the determination of the principle point is the usage of the *focal curves* of the diffraction lines: The definition of these curves can be found for instance in [4, 5, 6]: The equations of focal ellipse and focal hyperbola can be given by

$$\frac{x^2}{a^2-c^2}+\frac{y^2}{b^2-c^2}=1, \qquad z=0, \tag{2}$$

$$\frac{x^2}{a^2-b^2}-\frac{z^2}{b^2-c^2}=1, \qquad y=0, \tag{3}$$

respectively, provided $a^2 > b^2 > c^2$. Here the major and minor axes of the conics coincide with axes of the Cartesian frame. The two focal conics are located in orthogonal planes. The foci of the focal ellipse are vertices of the focal hyperbola, and vice versa (see Fig. 3).

This pair of conics has the following important property: *Each conic is projected from an arbitrary point P of the other conic by a circular cone whose axis is tangent to the latter at P (see Fig. 4). Conversely, whenever a conic $\mathcal{C}$ is projected from any point P by a cone of revolution, point P must be located on focal conic of $\mathcal{C}$.*

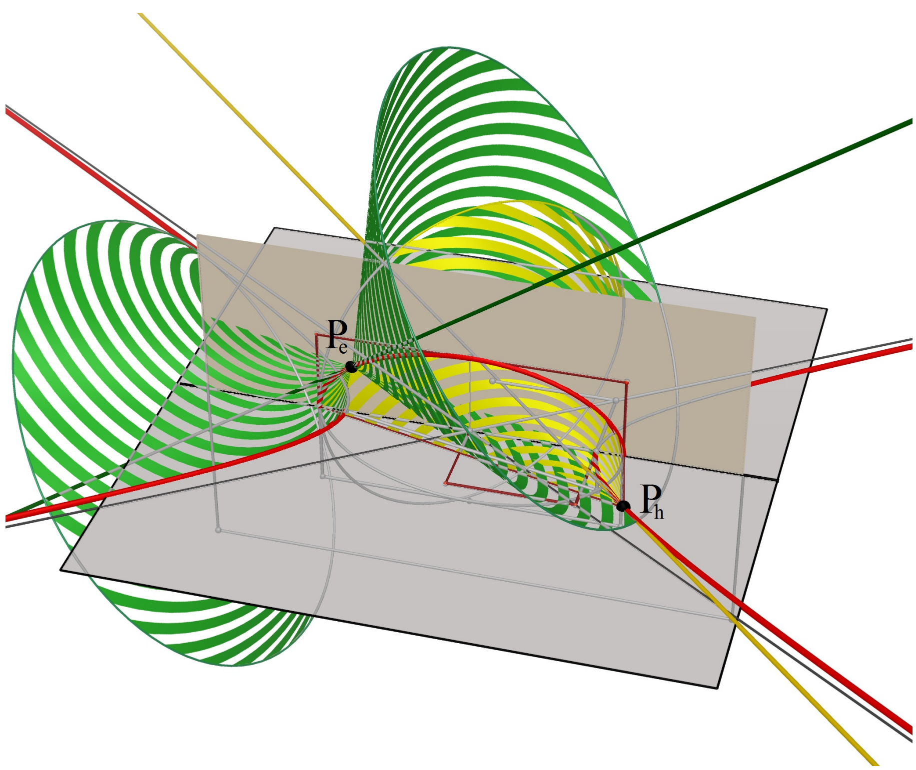

Figure 4: Focal conic sections satisfy a theorem of Ch. Dupin

This theorem is attributed to Charles Dupin (1784–1873). A proof can, e.g., be found in [5].

This property allows the determination of the complete interior and exterior orientation of the recording. Since all the cones that generate the diffraction lines on the image plane have the same apex, the different corresponding focal curves have to intersect at this point (see Fig. 5). Therefore, the principal point and the distance from the detector to the sample can be directly calculated without the use of a scaling factor. Furthermore, all the apertures of the cones are known and accordingly the diffraction angles.

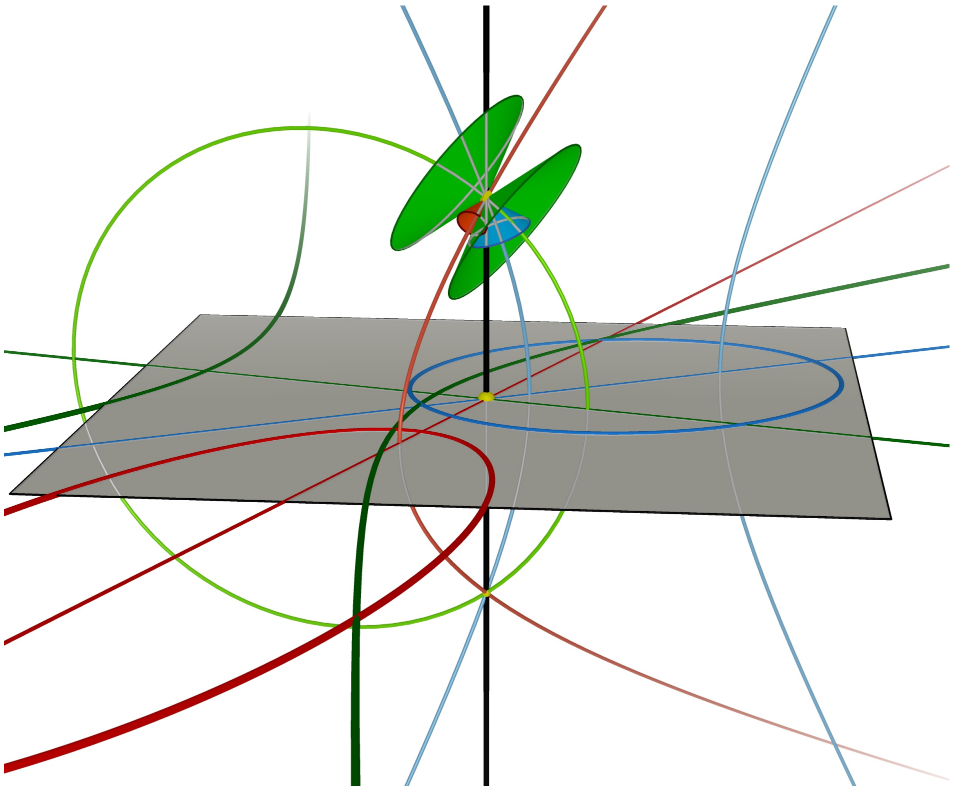

Figure 5: Diffraction curves in the detector plane with the respective focal curves which intersect at the projection centre

For the calculation, the results are averaged over a remaining inaccuracy. This is done during the whole process of determining and calculating the precise lattice parameters, which represent the real crystal.

4. Conclusions

The analysis shows that a microdiffraction record with its diffraction pattern is sufficient to determine the full imaging geometry. The characteristic of focal curves allows the determination of the orientation, which was previously complicated and imprecise. The presented method forms another link in the entire process chain of a high resolution "Residual stress microscope".

5. Acknowledgments

We are thankful for the financial support of the Deutsche Forschungsgemeinschaft, and Dr. R. Boucher and Prof. M. Hamann for their help.

References

[1] J. Bauch, F. Henschel, M. Schulze: *Automatic detection and high resolution fine structure analysis of conic X-ray diffraction lines*. Cryst. Res. Technol. **46**/5, 450–454 (2011).

[2] J. Bauch, H.-J. Ullrich, M. Böhling, D. Reiche: *A comparison of the Kossel and the X-Ray Rotation-Tilt Technique*. Cryst. Res. Technol. **38**/6, 440–449 (2003).

[3] J. Bauch, S. Wege, M. Böhling, H.-J. Ullrich: *Improved approaches to measurements of residual stresses in micro regions with the Kossel and the XRT technique*. Cryst. Res. Technol. **39**/7, 623–633 (2004).

[4] A. Clebsch, F. Lindemann: *Vorlesungen über Geometrie II*. Teubner, Leipzig 1891.

[5] K. Kommerell: *Vorlesungen über analytische Geometrie des Raumes*. Stuttgart 1950.

[6] O. Staude: *Die Focaleigenschaften der Flächen zweiter Ordnung / ein neues Capitel zu den Lehrbüchern der analytischen Geometrie des Raumes*. Teubner, Leipzig 1896.

Received August 2, 2012; final form November 27, 2013