s4.m13.p1 **Comparison of intensities from glass photo plates and Imaging Plates.** M.S. Nickolsky,[a] P.N. Oleynikov[b] and A.P. Zhukhlistov[a], [a]*Institute of Ore Deposits, Petrography, Mineralogy and Geochemistry (IGEM) RAS, 109017, Moscow, Staromonetny, 35, Russia, and* [b]*Stockholm University, Structural Chemistry, SE-10691 Stockholm, Sweden. E-mail: sir_Maxus@mail.ru*

Keywords: Electron diffraction; Texture patterns; Quantification of intensities

A series of multiply exposure of oblique texture electron diffraction pattern of brucite mineral $Mg(OH)_2$, recorded on glass photo plates, were processed by means of TexPat software [1]. Intensities were estimated as profile areas across arc reflections passing through their centers. The background being subtracted, the approximation of the profile shape was made using the Gaussian-Lorentzian Sum (Area) providing the best agreement between experimental and calculated profiles. In the case of partial overlapping, the reflections could be separated. The structure amplitudes were calculated from intensities according to their local values $|Fhkl| = \sqrt{Iobs/dhkldhk0p}$, where indices hkl and hk0 are related to the one and the same ellipsis, and p is the multiplicity factor [2]. The intensities of reflections coinciding in texture patterns were subdivided proportional to corresponding $|Fhkl|^2$ values. The relative F-values were normalized and reduced to the same scale as obtained with Imaging Plates [3]. The correspondence of both sets of values is displayed in the scheme (Fig.1). The small deviation of the real points from the direct line for the ideal coincidence of values provided by the two techniques indicates that there is a good agreement between them. This work is supported with RFBR project # 02-05-64952 and the Royal Swedish Academy of Sciences.

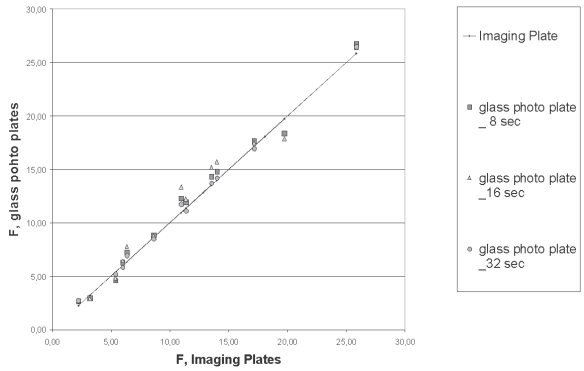

Fig. 1. Comparison of intensities from glass photo plates and Imaging Plates.

[1] Oleynikov P.N., Hovmöller S., Zou X.D., Zhukhlistov A.P., Nickolsky M.S., Zvyagin B.B., *Z. Krist*, **219**, 2004, 12-19.
[2] Vainshtein, B.K.: Structure analysis by electron diffraction. Pergamon Press, 1964.
[3] Nickolsky M. S., Zhukhlistov A. P., Zvyagin B. B.: Combination of electron diffractometry, Imaging Plates (IP) and electron diffraction structure analysis (EDSA): *Abstracts of XIX Congress of the International Union of Crystallography, Geneva*, 2002.

s4.m13.p2 **Two-dimensional pattern decomposition for quantitative analysis of texture patterns.** P.N. Oleynikov, S. Hovmöller and X.D. Zou, *Stockholm University, Structural Chemistry, SE-10691 Stockholm, Sweden. E-mail: oleyniko@struc.su.se*

Keywords: Electron diffraction; Texture patterns; Pattern decomposition

The electron diffraction from textured samples makes this powerful method especially useful for structure analysis [1]. The main problems arising during the quantification of texture patterns are overlapping reflections especially for low symmetries (see figure for example) and complications with intensities extraction. In order to solve these problems a two-dimensional pattern decomposition method was developed and implemented in the program TexPat [2]. It allows refining of different parameters simultaneously. Among them are: a tilt angle of the texture specimen, a centre, a main axes tilt, unit cell parameters, a misorientation angle of micro-crystallites within a sample, peak shape of reflections and amplitudes of selected reflections. Before the refinement a pattern is converted into polar coordinates since this significantly simplifies calculations. The Pawley method was used for pattern decomposition, where single reflections substituted the groups of almost or exactly overlapping ones. After the refinement the equipartition was applied for those highly overlapping reflections. TexPat was used to process the texture patterns of several minerals, such as brucite, lizardite 1T, muscovites 1M and $2M_1$ and kaolinite. The calculated unit cell parameters were in good agreement with published data [3, 4]. The R-factors for extracted intensities were below 15.0%.

Fig. Texture pattern of the triclinic mineral kaolinite.

[1] Zvyagin B.B., Plenum Press, New York, 1967, 124-181.
[2] Oleynikov P.N., Hovmöller S., Zou X.D., Zhukhlistov A.P., Nickolsky M.S., Zvyagin B.B., *Z. Krist*, **219**, 2004, 12-19.
[3] Zhukhlistov, A.P., Zvyagin, B.B., *Kristallografiya (Rus)* **43**, 6 (1998) 1009-1014.
[4] Zhukhlistov, A.P., Avilov, A.S., Ferraris, D., Zvyagin, B.B., Plotnikov, V.P. *Crystallography Reports*, 42 (1997) 774-777.