

s8.m27.p16 **New-Discovered Principles of Substructure Inhomogeneity in Metal Materials with Developed Crystallographic Texture.** Yu. Perlovich, M. Isaenkova and V. Fesenko, *Moscow Engineering Physics Institute (State University), Moscow, Russia.* E-mail: perlovich@hotmail.com

**Keywords: Substructure inhomogeneity; Crystallographic texture; Lattice condition**

A number of formerly unknown principles, controlling the substructure development in metal materials under plastic deformation, were established by use of advanced X-ray diffractometric methods. Elaboration of a new approach to X-ray measurements was connected with necessity to widen the usual description of real metal materials, having always very inhomogeneous substructures. The standard geometry of X-ray line profile measurement allows to obtain information only on the grains with reflecting planes, parallel to the surface, whereas in the general case these grains constitute the minor portion of the sample. Therefore the ways were found to measure or to reconstruct profiles of the same X-ray reflection from grains of all orientations, presented in the texture, and thus to compare their conditions. Obtained data are plotted as Generalized Pole Figures depending on the orientation of reflecting planes and as diagrams of the correlation between diffraction or substructure parameters. This became possible only by use of automated X-ray measurements and computer data treatment. The transition to the new level of experimental technique results in the fundamental change of characterization of metal materials - the description of their substructure conditions now proves to be many-dimensional, much more systematic and includes statistically confirmed regularities.

As applied to metal materials, subjected to the plastic deformation by their technological treatment, the following new regularities were established:

(1) A spectrum of coexistent substructure conditions is very wide, simultaneously including regions with extreme fragmentation of crystallites and highest lattice distortion as well as regions with a relatively perfect structure.

(2) The development of substructure inhomogeneity under plastic deformation accompanies the process of texture formation and is caused by action of the same mechanisms.

(3) The most effective criterion for systematization of substructure inhomogeneities in textured metal materials is the crystallographic orientation of regions with different substructures and, in particular, their orientation relative to texture maxima and minima.

(4) When passing from texture maxima to texture minima, the substructure condition changes gradually, so that both fragmentation of coherent domains and distortion of the crystalline lattice are intensifying.

(5) Equilibrium of residual microstresses within deformed metal materials realizes in such a way, that each structure element with some particular orientation of axis  $\langle hkl \rangle$ , along which the crystalline lattice is elastically compressed, has in the orientation space its mirror pair, where along axis  $\langle hkl \rangle$  with the same orientation the lattice is extended by the same absolute value.

(6) The distribution of residual elastic microstrains in rolled materials shows in the orientational space a distinct system, consisting in the mutual alternation of quadrants with predominant extension and predominant compression; in some cases texture maxima divide into halves with opposite signs of elastic strain.

s8.m27.p17 **The focusing mirror: a new optical setup for measuring samples in glass capillaries.** Stjepan Prugovecki and Martijn Fransen, *PANalytical B.V., The Netherlands.* E-mail: Stjepan.Prugovecki@panalytical.com

**Keywords: Focusing mirror; Capillary transmission; Pharmaceutical formulations**

The capillary transmission geometry is generally accepted as the best way for minimizing preferred orientation effects in powder X-ray diffraction experiments. Normally, incident beam focusing monochromators are used to enhance resolution, or graded multilayer parabolic mirrors to enhance intensity. Focusing incident beam monochromators are significantly reducing intensities. Multilayer graded parabolic mirrors are converting divergent beam to parallel beam, therefore instrument resolution is defined by capillary diameter. In order to combine both, high resolution of focusing beam, and high intensity of graded multilayer optics, graded multilayer elliptical mirror has been developed. The graded multilayer elliptical mirror is a special kind of beam conditioner, which is able to convert the divergent beam from a line focus X-ray tube to an intense monochromatic (K-Alpha) beam that is focused onto the goniometer circle. This is possible because of the combination of the elliptical shape of the mirror and the changing of the multilayer period over the length of the mirror. In this presentation, a novel geometry setup for the X'Pert PRO diffractometer will be shown, employing graded multilayer elliptical mirror as incident beam conditioner and X'Celerator as detection system. Resolution of such setup is almost independent of capillary diameter, and intensities are comparable with standard parabolic multilayer mirrors. This will be demonstrated by measurements using capillaries of different diameters. Application of graded multilayer elliptical mirror on transmission measurements of pharmaceutical formulations (tablets) will be shown, demonstrating detection limits of an active ingredient far below 0.5%.