12.6–1 LINE INTENSITY DECREASING SEMIQUANTITATIVE METHOD IN X-RAY DIFFRACTION PHASE ANALYSIS. By B. Gržeta and S. Popović, "Ruđer Bošković" Institute, 41001 Zagreb, PO Box 1016, Croatia, Yugoslavia.

The doping method in quantitative X-ray diffraction phase analysis, developed by Popović and Gržeta-Plenković (J. Appl. Cryst. (1979) 12, 205-208) and Popović, Gržeta-Plenković and Balić-Žunić (J. Appl. Cryst. (1983) 16, 505-507), requires doping of the investigated multicomponent system by known amounts of the components, the weight fractions of which are to be determined. A variation of the doping method is proposed in the present contribution. It involves the addition to the investigated system of known amounts of a crystalline substance, X, not contained in the system. One determines the added amount of X, for which the intensity of the strongest diffraction line of a particular component falls below a small detectable value. This enables the determination (estimation) of the weight fraction of that component in the original system. Also, the discussion on the applicability of the method is given.

12.7–1 RECONSTITUTION DES TRANSFORMEES DE FOURIER DES PROFILS DE RAIES DE DIFFRACTION DES RAYONS X. Par Rodolfo Vargas, Centro de Ingeniería Metalúrgica, Fundación Instituto de Ingeniería, Apartado 40200, Caracas 1040-A, Venezuela.

Dans la caractérisation de l'élargissement des profils de raies de diffraction des rayons X par l'analyse de Fourier, les transformées de ces profils, interpretées comme les "fonctions volume" des cristallites (Bertaut, Acta Cryst. (1950) 3, 14), renseignent directement sur les paramètres morphologiques du matériau. L'ajustement des profils de raies à des expressions mathématiques a été l'objet de travaux récents, des bonnes approches ont été obtenues à l'aide des fonctions de Gauss, Cauchy, Voigt, etc. Cependant il est possible de trouver une expression analytique des profils, ainsi qu'on le montre dans ce travail.

Lorsque l'élargissement des profils est dû seulement aux effets de taille et tenant compte que les cristallites ont tous la même forme alors la fonction volume relative à tout l'échantillon V est la somme des fonctions volume propres à un cristallite V, de forme et dimensions données, ponderées par la distribution de tailles G; c'est-à-dire, $V(t) = \int V(t,\ell)\ G(\ell)\ d\ell$,

où t est une variable (en Å) de l'espace directe et ℓ est la dimension moyenne apparente d'un cristallite dont la fonction volume est $V(t,\ell)$.

Une application aux raies 100, 110 et 102 d'une poudre d'oxyde de zinc, les cristallites ayant une forme cylindrique (Vargas, Thèse, Rennes (1981)), est présentée. La fonction volume pour une telle morphologie est calculée d'après Langford et Louër (J. Appl. Cryst. (1982) 15,20) et les fonctions de distributions de tailles ont été obtenus par la méthode de Le Bail et Louër (J. Appl. Cryst. (1978) 11, 50). Les resultats permettent de vérifier la validité des critères de reconstitution des transformées ainsi que des modèles considerés.

12.7–2 X-RAY LINE BROADENING DUE TO ELASTIC DEFORMATION OF POLYCRYSTALLINE SAMPLES. By C.BALASINGH and A.K.Singh, Materials Science Division, National Aeronautical Laboratory, Bangalore-560017, India.

The broadening of x-ray diffraction lines can arise from many sources, such as, plastic deformation of the specimen leading to decrease in the coherently diffracting domain size, increase in microstrains, etc (B.E. Warren, Progr Metal Phys (1959) 8, 147). The fact that elastic deformation can also lead to broadening was recognized long back (G.B.Greenough, Progr Metal Phys (1952) 3, 176). However, no detailed experimental or theoretical analysis of this aspect has been carried out. A simple consideration indicates that broadening from this source vanishes if the condition of strain continuity (W.Voigt, Lehrbuch der Kristallphysik, Teubner, 1928) across the crystallites is assumed. In this paper, expression for the variance in strain (a measure of broadening) has been derived for cubic system under the condition of stress continuity (A.Reuss, Z. angew Math U Mech (1929), 9, 49). The analysis indicates that the variance vanishes for reflections of the type (h00) and (hhh). It also vanishes for all reflections if the anisotropy factor is zero. Diffraction line profiles from annealed and deformed copper and iron specimens have been recorded and the variance due to elastic broadening calculated. A comparison has been made of the experimental results with the theory.

12.7–3 ON SUPPRESSING TEXTURE EFFECT IN QUANTITATIVE ANALYSIS BY POWDER DIFFRACTION. By M. Järvinen, Lappeenranta University of Technology, LPR, Finland and J. Zábráczky, ALUTERV-FKI, Budapest, Hungary.

The method for correcting integrated x-ray intensities for preferred orientation (Järvinen et. al. J. Appl. Cryst. (1970), 3, 313) is developed for standard use in powder examinations.

The intensities of several reflections measured by an ordinary powder diffractometer contains a lot of information about the orientation distribution of the crystallites in the specimen. This information can be extracted by representing the orientation distribution function in terms of site-symmetrized spherical harmonics and by fitting the expansion with the measured intensity data.

However, the use of a specimen spinner is necessary in order to smoothen the distribution function and to introduce cylindrical symmetry. This reduces the sufficient number of texture-parameters to 2 or 3.

As an example, the determination of Al_2O_3-concentration in an industrial alumina powder is presented. The biggest correction was 52 % the agreement between alumina and standard corundum intensities being 6 %.