

11.8-3 EVANESCENT ABSORPTION IN KINEMATIC SURFACE DIFFRACTION. By H. Dosch, Cornell University, Ithaca, NY 14853, USA. Present address: Sektion Physik, Ludwig-Maximilians-Universität, München, FRG.

The Bragg scattering excited under the conditions of total reflection is discussed within a kinematic approach based on the distorted wave approximation. Due to evanescent absorption at grazing angles, the maximum of the interference function of the surface Bragg reflection is displaced into the vacuum by an amount determined by the mean electron density of the medium. X-ray scattering experiments performed on a mosaic single crystal with synchrotron radiation confirm the predictions of the kinematic theory, and indicate the potential of a controlled depth probing of near-surface atomic correlations.

11.9-1 SPIN CORRELATIONS IN  $Au_{0.85}Fe_{0.15}$ . By J. W. Cable, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U. S. A.; G. Parette, Laboratoire Léon Brillouin, Saclay, France; and Y. Tsunoda, Osaka University, Osaka, Japan.

Diffuse neutron scattering measurements were made on single crystal  $Au_{0.85}Fe_{0.15}$  to determine the spin correlations in this nearly ferromagnetic alloy. Two dimensional data were obtained in the first Brillouin zone for an [001] orientation. The results indicate free, uncorrelated spins at 295 K with the development of spin correlations below  $\sim 200$  K. The intensity distribution at 10 K is similar to that previously observed by x-rays (E. Dartyge, H. Bouchiat, and P. Monod, Phys. Rev. B 25, 6995 (1982)) with diffuse peaks at the origin and  $\{1/2\ 0\}$  along with diffuse streaks in  $\langle 210 \rangle$  directions. Intercomparison of the x-ray and neutron data suggests a tendency toward the formation of Fe platelets in  $\{420\}$  planes with some spatial correlation between the platelets. The magnetic short range order consists of ferromagnetic spin correlations in these partially correlated platelets with a magnetic correlation length larger than that of the local atomic order.

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11.8-4 CORRECTION OF X-RAY INTENSITIES FOR MULTIPLE DIFFRACTION. By B.C. Hauback and F. Mo, Institutt for røntgenteknikk, Universitetet i Trondheim-NTH, N-7034 Trondheim-NTH, Norway.

In multiple diffraction (MD) situations the intensity perturbations may become very large and are systematic in the sense that weak reflections tend to become enhanced ("Umweganregung"). Geometric conditions for N-beam diffraction are frequently satisfied, even for crystals with moderate-sized unit-cells. These facts suggest that the effect of MD should be taken into account in modern accurate structure work.

Our calculations of the magnitude of the intensity corrections are based on a first-order kinematic theory (Tanaka & Saito, Acta Cryst. (1975) A31, 841). Detailed  $\psi$ -scans over the interaction maxima have been carried out to provide parameters for the peak widths to be used in the calculations. Three crystals with unit-cell volume in the range 680-2950  $\text{\AA}^3$  have been analysed. In the data sets 5-8% of all reflections with  $\sin\theta/\lambda < 0.70 \text{\AA}^{-1}$  had  $\Delta I/I > 10\%$ . As expected, the largest effects appear in the weak intensities. Among the weakest 30% of the data, 17-20% had  $\Delta I/I > 10\%$ . Analyses and averaging of the data showed significant improvement of the weak reflection after correction. Structure parameters and details in the charge densities have been compared with and without corrections for MD included. The frequency of MD cases is proportional to  $(V/\lambda^2)$ ;  $V$ =unit-cell volume and  $\lambda$ =wavelength. The effects of path lengths of the different beams and reflecting power to the magnitude of the perturbations will be discussed.

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11.9-2 DETERMINATION OF THE CRYSTALLITE-SIZE DISTRIBUTION FUNCTION FOR ALKOXY-DERIVED OXIDE MATERIALS. By S.A. Ivanov, I.E. Obvintseva, M.I. Yanovskaya, Yu.N. Venevtsev, Karpov Institute of Physical Chemistry, Moscow, USSR.

A detailed knowledge of the morphology of crystallites in a finely divided powder is required in many fields of materials science. The purpose of this work was to determine the crystallite-size distribution function in  $Y_2Fe_5O_{12}$ ,  $Bi_2WO_6$ ,  $LiNbO_3$  powder strain-free materials prepared by the hydrolysis of alkoxides. In order to study the crystallite-size variation, X-ray diffraction experiments (DRON-3 diffractometer,  $CuK_\alpha$ ) were combined with electron microscopy and second harmonic generation methods. The Tikhonov's regularization procedure to Fourier X-ray line profile analysis was applied for calculation of domain-size distribution function. Instrumental broadening was obtained from standard specimens of the same composition. All calculations were performed by the special computer program which we have adapted to the ES-I033 computer. The effective domain size shows a tendency to increase with heating and has a maximum in the temperature range 600-700°C. Above this temperature range the crystallite size does not vary appreciably. There is a reasonable agreement between the effective domain sizes obtained from X-ray profile analysis and by other physical methods up to 1000 Å. The particles detected by electron microscopy in the 1000 Å to 1500 Å diameter range are not monocrystalline for the greater part. The values of crystallite size are computed for several crystallographic directions. The shape of crystallites is anisotropic at low temperature but the isotropy increases on heating.