ing a range of cluster sizes produced by the appropriate heat treatment are currently under way.

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Quantitative Interpretation of X-ray Line Broadening of Plastically Deformed Crystals*

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Up to the present time there exists no completely satisfactory theory which explains the broadening of X-ray line profiles of plastically deformed crystals in terms of the density and the distribution of the dislocations introduced during deformation. Earlier theories {*e.g.*, Warren, B. E. [*Progr. Met. Phys.* (1959). **8**, 1473; Wilson, A. J. C. [*Proc. Phys. Soc.* (1963). **81**, 41]} explain the line broadening in terms of 'particle' size and 'mean-square strains'. However, the relationship between these parameters and those describing the dislocation distribution is fairly vague {*cf. e.g.*, Wilkens, M. [*Phys. Stat. Sol.* (1962). **2**, 692]; Wilkens, M. & Hartman, R. [*Z. Metallk.* (1963). **12**, 676]}. In particular, the term 'particle size' is badly defined in this sense, if stacking-fault broadening is negligible. In the following stacking-fault broadening will not be considered. Using an essentially different approach Krivoglaz, M. A. & Ryaboshapka, K. P. {[*Fiz. Metall. Metalloved.* (1963). **15**, 8]; [Krivoglaz, M. A. (1968). *Theory of X-ray and Thermal Neutron Scattering by Real Crystals.* New York: Plenum]} have derived a kinematical theory of line broadening in which the displacement field of dislocations is incorporated explicitly. The theory is based on the assumption of a statistically random distribution of (straight) parallel dislocations. In the final equations an 'outer cut-off radius' appears, which, in the theory, coincides with the external crystal radius. In application to practical cases the significance of this outer cut-off radius is unclear. This disadvantage is avoided in the (kinematical) theory of Wilkens, M. [*Fundamental Aspects of Dislocation Theory* (1970). Edited by J. A. Simmons, R. de Wit and R. Ballough. N. B. S. Spec. Publ. 317, Vol. I. p. 11. 95; *Phys. Stat. Sol.* (*a*) (1970): **2**, 359] which assumes a 'restrictedly' random distribution of parallel dislocations embedded in an elastically isotropic crystal. This type of distribution [Wilkens, M. (1969). *Acta Met.* **17**, 1155] is characterized by two parameters, the dislocation density ϱ and the effective outer cut-off radius R_e. The latter is defined by assuming that the elastically stored energy E of a given dislocation distribution is proportional to $\varrho\,.\,\ln(R_e/r_0)$, r_0 = inner cut-off radius. In this way, by an appropriate choice of R_e, the elastic interaction of the individual dislocations of the dislocation distribution is taken into account, for further details *cf.* Wilkens (1969). In the theory (Wilkens, 1970) instead of R_e, another parameter, $M=R_e\sqrt{\varrho}$, is used (*i.e.*, $M=R_e$, divided by the mean dislocation spacing $1/\sqrt{\varrho}$). The theory is applicable for $M\gtrsim 0{\cdot}5$ and leads to the following predictions: (i) For a given value of M the half widths of the line profiles are proportional to $g\,.\,\sqrt{\varrho}$ with g = modulus of the diffraction vector of the reflecting planes used. For a given value of ϱ the half widths increase roughly proportional to $\ln M$. (ii) The shapes of the line profiles are controlled by the value of M and lie between a

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Gaussian function (which is approached for $M \gg 1$) and a Lorentzian function (not exactly reached for the lower limit $M \simeq 0{\cdot}5$). The asymptotic tails of the line profiles as a function of ϱ were treated in detail by Wilkens, M. [*Phys. Stat. Sol.* (1963). **3**, 1718]. (A random distribution of 'infinitesimally narrow' dislocation dipoles, corresponding to $M \ll 0{\cdot}5$ in the present notation, yields exactly a Lorentzian function, *cf.* Potoskaja B. B. & Ryaboshapka K. P. [*Sb. Metallofiz. Kiew.* (1968). **24**, 97]. The validity of the theory (Wilkens, 1970) was examined by studying the X-ray line profiles (Cu $K\alpha_1$ radiation) of Cu single crystals which were deformed up to resolved shear stresses $\tau \gtrsim 3$ kg mm^{-2}. (For $\tau \gtrsim 3$ kg/mm^2 it is assumed that extinction effects are negligible.) The line profiles were measured by a monochromator technique including a photographic registration which is practically free from instrumental broadening *cf.* Wilkens, M. & Eckert, K. [*Z. Naturforsch.* (1964). **4**, 459]; Wilkens, M. & Bergenth, M. D. [*Acta Met.* (1968). **16**, 465]. Here the results of two experiments are briefly reported. (i) Herz, K., Wilkens, M. & Mughrabi, H. (To be published) have investigated the broadening of the three different {002} reflexions of a middle-oriented Cu crystal deformed in tension up to $\tau = 3{\cdot}5$ kg/mm^2. Using the theory and applying an estimated correction (reduction by $\simeq 20\%$) which accounts for the elastic anisotropy of Cu (see below) the authors obtained $\varrho_{pr} = 9{\cdot}2\,.\,10^9$ cm^{-2} and $\varrho_{sec} = 6{\cdot}2\,.\,10^9$ cm^{-2} with ϱ_{pr} and ϱ_{sec} = density of the primary and secondary dislocations respectively. The total density, $\varrho_t \simeq 1{\cdot}5.10^{10}$ cm^{-2}, and the ratio $\varrho_{pr}/\varrho_{sec} \simeq 1{\cdot}5$ compare reasonably with $\varrho_t \simeq 1{\cdot}0.10^{10}$ cm^{-2} and $\varrho_{pr}/\varrho_{sec} \simeq 1$ as estimated for $\tau = 3{\cdot}5$ kg mm^{-2} from corresponding transmission electron microscopy data of middle-oriented Cu crystals (*cf.*, *e.g.*, Essmann, U. [*Phys. Stat. Sol.* (1966). **17**, 725]. Herz *et al.* investigated further the line broadening of the {200} reflexions of Cu crystals which were fatigued with different strain amplitudes up to the saturation stress level $\tau \simeq 3$ kg mm^{-2}. For the fatigued specimens the 'shape factor' M was found to lie significantly below the lower limit 0·5 of the applicability of the theory of Wilkens (1970): the tails of the line profiles corresponded closely to the tail of a Lorentzian curve. Therefore, it was suggested, in accordance with TEM observations [Grosskreutz, J. C. & Mughrabi, H. (1974). In *Constitutive Equations in Plasticity* (1974). Edited by A. S. Argon. MIT Press], that in the fatigued crystals the dislocation distribution consists mainly of agglomerations of dislocation dipoles (multiple bundles). Application of the theory of Potoskaja & Ryaboshapka (1968) yielded values for the density of dislocation dipoles which agree reasonably with corresponding TEM data of Grosskreutz & Mughrabi (1974). (ii) Three series of Cu single crystals with the orientations ⟨111⟩, near ⟨110⟩ and near ⟨113⟩ were deformed in tension up to stresses τ between 4 kg mm^{-2} and 9 kg mm^{-2}. The deformed crystals were cut into two pieces. One piece of each crystal was used by Steffen, H., Gottstein, G. & Wallenberger, H. [*Acta Met.* (1973). **31**, 683] for a calorimetric determination of the elastically stored energy $E = E_{cal}$. The second piece of each crystal was used for X-ray line-broadening measurements [Maier, W. & Wilkens, M. (To be published)]. From the X-ray data values for ϱ and R_e were determined and subsequently used for a calculation of $E = E_x$. Since only a restricted number of {002} and {111} reflexions could be investigated, the fractional distribution of the dislocations over the 12 different slip systems could be derived from the X-ray data only with a rather large uncertainty. For symmetry reasons this uncertainty was of minor importance for the series of the ⟨111⟩ oriented crystals. In this case E_x deviated from E_{cal} by less than about 15% if mean values of E_x were taken between the values obtained from the {002} and the {111} reflexions (this average accounts for the elastic anisotropy of Cu). For the two other orientations similar agreements could be achieved. However, the results were not so conclusive since some assumptions must be made regarding the fractional distributions of the dislocations over the different slip systems. The two examples mentioned above indicate that the rather crude 'two-parameter theory' of Wilkens (1970), when applied to the complicated problem of X-ray line broadening of plastically deformed crystals, may be satisfactory in some cases but should be improved in other cases, depending on the desired accuracy. Further progress in the theory should be stimulated by a progress in the experimental technique in deriving characteristic parameters of the shapes of broadened X-ray line profiles of plastically deformed crystals.