phys. stat. sol. (a) 116, K141 (1989)
Subject classification: 61.10; 61.70; S5.11

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On the Transition between Dynamical and Kinematical X-Ray Diffraction in Thin Crystals with Randomly Distributed Dislocations

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One of the most important problems of X-ray diffraction consists in finding out the way of dynamical scattering transformation into the kinematical one under the condition of increasing crystal imperfection. It is possible to describe the diffraction at any level of distortions and to trace the transition between the dynamical and kinematical regimes in particular cases of the simple deformation fields /1 to 3/ or in crystals with strongly distorted surface layer /4/ only.

The problem of the X-ray dynamical diffraction in crystals with statistically distributed dislocations is very complicated and is not yet solved /5 to 10/. The integrated reflectivity R_i (in the Laue case) of a thin ($\mu t < 1$, t is the sample thickness and μ is the linear absorption coefficient) crystal with dislocations is given by /9, 10/

$$R_i = R_B + R_D = \exp(-h)\exp(-\frac{\mu_d t}{2})\Big(Be^{-L} I_o(c\varepsilon h)\exp(-\frac{\mu_d t}{2}) + + (1 - \exp(-2L)qt \,\mathrm{sh}(\mu_d t/2)/(\mu_d t/2)\Big) \quad , \tag{1}$$

where R_B and R_D are the coherent and the incoherent (diffuse parts of the reflectivity, $h = \mu t$, μ_d is the additional absorption coefficient due to diffuse scattering /11/, $B = c\,\pi\,\chi_{gr}/2 \sin 2\theta$, c is the polarization factor, χ_{gr} is the Fourier coefficient of the polarizability of the perfect crystal, L is the static Debye-Waller factor, $I_o(x)$ is the Bessel function, $\varepsilon = |\chi_{gi}/\chi_{oi}|$, $q = c^2\pi^2\chi_{gr}^2/\lambda \times \sin 2\theta$, λ is the wavelength.

In /10/ it was shown that the correlation coefficient of the expression (1) with the experimental data (observed in silicon samples with dislocation density $N_d \lessapprox 10^5$ cm^{-2} for 220, 400, 440 reflections) is rather high (95%). According to (1), the integrated reflectivity can reach the kinematical limit ($q\,te^{-h}$) if the dislocation density increases up to some boundary value N_d^* /5/. In this case the reflectivity loses its sensitivity to the degree of crystal imperfection. On the other hand, according to (1), the kinematical regime of scattering can be reached at N_d = const by increasing the value of the diffraction vector $\vec{H}$ ($|\vec{H}| \sim \sqrt{h^2 + k^2 + l^2}$). The aim of the present note is an experimental study of the peculiarities of the

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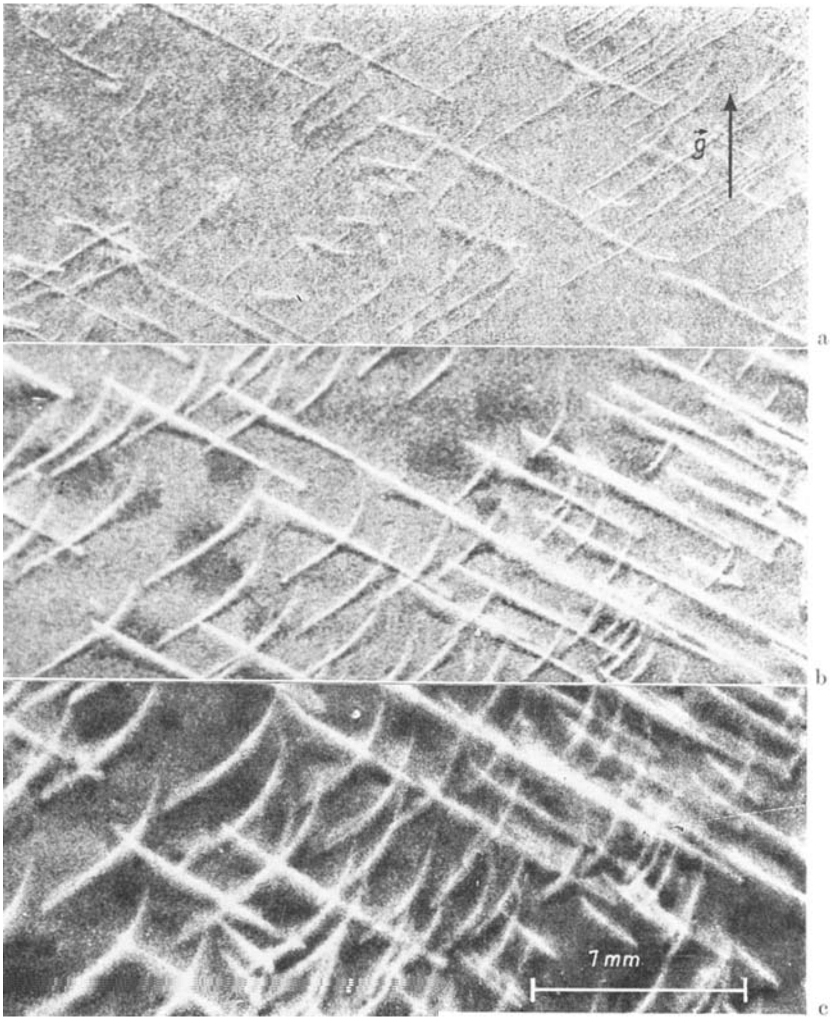

Fig. 3. X-ray transmission topograms of the dislocations in Si; MoK_{α_1} radiation. a) $\bar{2}20$, b) $\bar{4}40$, c) $\bar{6}60$

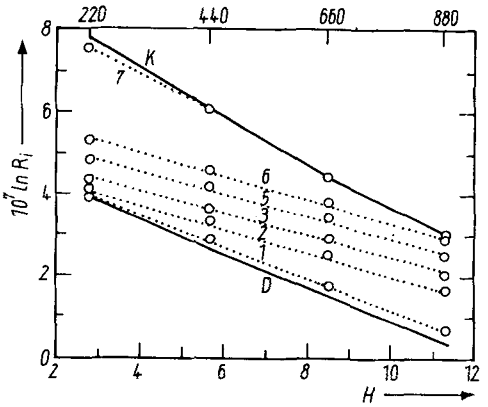

Fig. 1. Dependences of the logarithms of R_i on the modulus of the scattering vector $\vec{H}$. The solid lines D and K are the results of computation for dynamical and kinematical scattering, respectively. Dotted lines are fitted to the experimental data (O). Numeration of the dependences corresponds to the numeration of the samples in Table 1

dependences $R_i = f(N_d, H)$ for thin silicon crystals and the estimation of the values N_d^* for different types of reflections.

Silicon single-crystal plane-parallel wafers, cut parallel to {111} (t = (310 ± ± 5)μm) were measured. The wafer surfaces were etched chemically. The samples contain randomly distributed growth dislocations with density from 9×10^2 to 2.7×10^7 cm^{-2}.

Integrated intensities of 220, 440, 660, and 880 reflections were measured in MoK_{α_1} radiation with a double-crystal Bragg-Laue spectrometer. A perfect silicon crystal (220 reflection) served as monochromator. Dislocation homogeneity and density were controlled by etch pits and X-ray topography. The results are given in Table 1.

Calculated (according to expressions given in /4/) $R_i(H)$ dependences for dynamical reflections (perfect crystal) and for kinematical diffraction peaks (ideal mosaic structure) as well as experimental data are given in Fig. 1. They indicate that R_i rises with increase of the dislocation density and reaches the kinematical limit

Table 1

sample number	N_d (cm^{-2})	L^{220}	L^{880}
1	0	-	-
2	9×10^2	0.22×10^{-2}	0.11
3	1.8×10^4	0.36×10^{-2}	0.29
4	2.4×10^4	0.46×10^{-2}	0.24
5	1.35×10^5	2.07×10^{-2}	0.25
6	3.30×10^5	3.49×10^{-2}	0.98
7	2.70×10^7	0.97	-

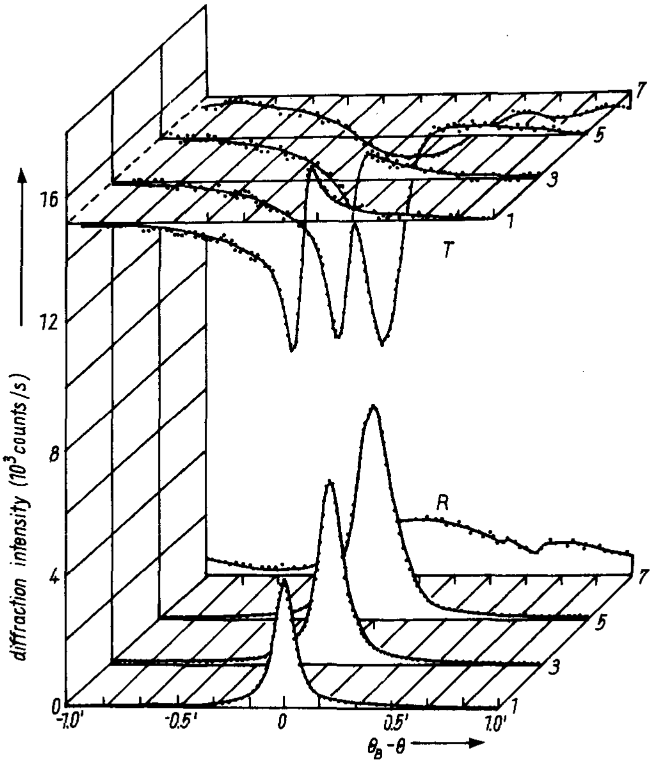

Fig. 2. The set of reflected (R) and transmitted (T) rocking curves for dislocation-free Si (1) and crystals with randomly distributed growth dislocations (3, 5, 7). Numeration of the curves corresponds to Table 1. 220, MoK_{α_1} radiation, t = (310 ± 5)μm

at a higher dislocation density (2.7×10^7 cm^{-2}) for all the reflections except 220 only (although in this case the difference is not significant - about 20%). It signifies that even for the strong (less sensitive to defects) 220 reflection the dynamical scattering in sample 7 is nearly completely suppressed.

The decrease of the peak intensity of the reflected rocking curve and the significant broadening (its halfwidth is about 36') of both reflected and transmitted curves can serve as confirmation (Fig. 2). Alongside with this the intensity maximum of the transmitted curve (which is derived from anomalous X-ray transmission /12/) is completely suppressed in the higher distorted sample 7. Therefore the value of N_d^* for 220 reflection is about 10^7 cm^{-2}.

It should be also taken into consideration that in the range of N_d = 1.4×10^4 to 3.3×10^5 cm^{-2} a linear experimental $L(N_d)$ dependence is observed (Fig. 3, see on

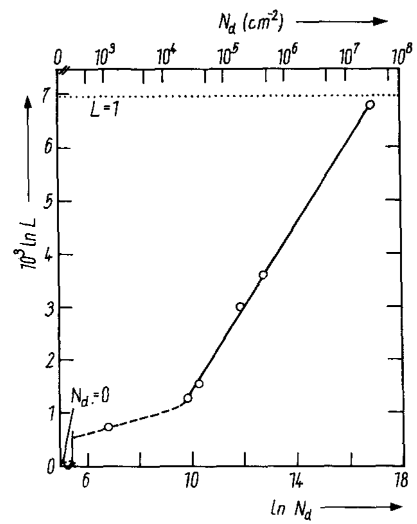

Fig. 4. Dependence of the Debye-Waller static factor L on the dislocation density in logarithmic scale. For low values of $N_d < 10^4$ cm^{-2} the dependence of ln L on ln N_d is nonlinear and indicated by the dashed line

the photo pages before the Short Notes part). These data have proved the results of the theoretical analysis /5/.

Fig. 1 also shows the possibility of reaching the kinematic limit with the increasing diffraction vector $\vec{H}$ (sample 6). Such type of transition from dynamical to kinematical X-ray diffraction is caused by the increasing higher order reflection sensibility to structure defects /13 to 15/. According to /7/ this may be explained by the strongly distorted range around the dislocation increase (in Fig. 4 dislocation image broadening with increasing order of the reflection is clearly observed) and consequently by the increase of the static Debye-Waller factor L ($e^{-L} \rightarrow 0$, $\mu_d \rightarrow 0$, $R_i \rightarrow q$ te^{-h}) /5, 9/. The experimental data presented in Table 1 and in Fig. 1 show that the N_d^* value for 880 reflection is about 10^5 cm^{-2}.

It is interesting to note that a correlation between the experimental and calculated (for a perfect crystal) values of R_i for 220 reflection exists only in dislocation-free floating zone crystal (sample 1). For other reflections the difference increases with the order of diffraction (reaching about 40% for 880 reflection). This may be explained by the presence of the growth microdefects in silicon samples /15/. We conclude that the values of the dislocation boundary density N_d^* (at which the dynamical scattering transforms into the kinematical one), decrease sharply with the increase of H. This fact may be explained by an essential increase of the static Debye-Waller factor L (characterizing the degree of crystal imperfection for a fixed reflection).

This assumption can be proved by the calculated values of L (by means of technique /16/) (Table 1).

The authors kindly acknowledge L.I. Datsenko for helpful discussions.

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(Received June 12, 1989; in revised form October 19, 1989)