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The Measurement of Defect Parameters in Imperfect Crystals using X-ray Diffraction

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Abstract

Correlation lengths and defect-strength parameters, related to the separations and magnitudes of discontinuities in imperfect crystals, are obtained from X-ray rocking curves using a stochastic model of crystal defects. The model describes the diffraction of X-rays from an imperfect crystal containing surfaces of defects, such as stacking faults, and misoriented crystal grains. The two defect parameters provide a measure of crystal quality. A method of extracting the parameters from rocking curves is described in the limit of kinematic X-ray diffraction. The method is applied to X-ray diffraction data obtained from thin films of CdTe and $Hg_{1-x}Cd_xTe$ grown on GaAs substrates. The ability of the model to fit the X-ray data is a test of the stochastic model.

Introduction

X-ray diffraction is used extensively to measure the quality of thin crystalline films grown by techniques such as molecular-beam epitaxy and metalorganic chemical vapour deposition. A single parameter, the full width at half-maximum of the Bragg reflection, is the usual measure of the crystal quality. However, many theories of X-ray diffraction from imperfect crystals involve two parameters related to the nature of the imperfections (Zachariasen, 1967; Kato, 1980; Becker & Al Haddad, 1990; Davis, 1992). Therefore, it should be possible to obtain a better measure of the crystal quality by extracting two parameters from the X-ray data.

The stochastic model of X-ray diffraction developed by Davis (1992) describes the mean reflectivity from an imperfect extended-face crystal containing surfaces of defects and misoriented crystal grains. These defects produce discontinuities in the strain and strain gradients in the crystal. The model contains two parameters: a defect-'strength' parameter, σ, and a correlation length, l. The correlation length is defined by a correlation function and is the distance over which the correlation between the phases of the diffracted X-rays falls by $1/e$. If the width of the Bragg reflection, related to $\nu^2 = \sigma^2/2l$, is chosen as one independent measure of the crystal quality, then a possible choice for the second independent parameter is the correlation length.

The aim of this paper is to verify that the stochastic model can fit X-ray data from a number of thin films and to demonstrate the method by which the two defect parameters may be obtained. The model is applied in a kinematic limit to X-ray data sets obtained from thin films of CdTe and $Hg_{1-x}Cd_xTe$ grown on GaAs substrates. In the following sections, the stochastic model is briefly reviewed, the method for fitting the model to the data is described and the experiments and their results are discussed.

Theory

The stochastic defect model for X-ray diffraction from imperfect crystals is based on a form of the Takagi–Taupin equations (Takagi, 1962, 1969; Taupin, 1964). The main aspects of this model are summarized below. For a complete description of the model the reader is referred to Davis (1992).

For thin films in which the change in the amplitude of the transmitted wave is small, a *kinematic* solution for the complex reflectance $R(t)$ at depth t is

$$R(t) = \exp[-i2\alpha \int_0^t \beta(t')\,dt'] \int_0^t i\alpha\chi_h(t') \times \exp[i2\alpha \int_0^{t'} \beta(t'')\,dt'']\,dt', \quad (1)$$

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where t is measured from the lower boundary of the film (*e.g.* the epilayer–substrate boundary) and $R(0) = 0$ at this boundary, *i.e.* there is no interference between substrate and epilayer reflections. This situation arises when there are significant lattice-parameter differences between the substrate and the film, such as occur with CdTe grown on GaAs.

The symbols are defined as follows: $\alpha = -\pi k/\gamma_h$; $1/k = \lambda$ is the X-ray wavelength; γ_h is the direction cosine of the diffracted wave with respect to the coordinate axis; $\chi_h = C\chi'_h$, where C is a polarization factor and χ'_h is the Fourier component of the dielectric susceptibility associated with the reciprocal-lattice vector $\mathbf{h}$. χ'_h is a complex quantity and includes the anomalous scattering factors. The resonance parameter, β, is given by

$$\beta = n^2[(k_h^2 - k^2)/2k^2] - n[\hat{\mathbf{k}}_h \cdot \nabla(\mathbf{h}\cdot\mathbf{u})/k], \qquad (2)$$

where $n = (1 + \chi'_o)^{1/2}$ is the refractive index for the X-rays; $\mathbf{k}$ and $\mathbf{k}_h$ are the wave vectors of the transmitted and diffracted waves, respectively, in the crystal interior; $\hat{\mathbf{k}}_h$ is the unit vector in the direction of $\mathbf{k}_h$; and $\mathbf{u}$ is the displacement of a point in the lattice from its relaxed position resulting from strains in the crystal.

Bragg's law, $h = 2k\sin\theta_B$, and the relation $\mathbf{k}_h = \mathbf{k} + \mathbf{h}$ allow the first term in (2) to be written as

$$n^2[(k_h^2 - k^2)/2k^2] \simeq -\sin 2\theta_B(\theta - \theta_B) - (\chi'_o/2)(1 + b), \qquad (3)$$

where θ is the angle of incidence of the X-ray beam, $|\theta - \theta_B| \ll 1$ and b is the asymmetry parameter defined by

$$b = \sin(\theta_B - \theta_s)/\sin(\theta_B + \theta_s), \qquad (4)$$

where θ_s is the angle in the diffraction plane between the crystal-surface normal and the reciprocal-lattice vector for the Bragg reflection. It is defined here to be positive if the peak of the Bragg reflection occurs when the angle between the incident beam and the plane of the crystal surface is greater than the Bragg angle, θ_B. The second term in (3) is a refraction term resulting from the boundary conditions at the crystal surface [see, for example, Zachariasen (1945)]. The effects of absorption are contained in the imaginary component of χ'_o.

The strain at a point in the crystal is assumed to arise from two sources: (i) smoothly varying strains, such as arise from lattice mismatches or from stresses at the crystal boundaries; (ii) strains arising from the defects in the crystal, such as stacking faults and misoriented crystal grains. The second source of strains can be separated into a smoothly varying component, which is the average of the strains over a surface at depth t, and a rapidly fluctuating component, which is the difference between the true strain at t and the smoothly varying average. The smoothly varying strain components in the second term in (2) and the angle-dependent and refraction terms in (3) are written as $\langle\beta\rangle$, and the fluctuating strain components are written as β_ξ, so that

$$\beta(t) = \langle\beta(t)\rangle + \beta_\xi(t), \qquad (5)$$

where the average $\langle\beta_\xi\rangle = 0$. Strictly, the average here is an ensemble average over an idealized imperfect crystal. However, in practical terms, this is taken as an average over that area at depth t in the crystal that is diffracting the X-ray beam. For this purpose, the X-ray beam must be sufficiently broad to be influenced by (or averaged over) a statistically significant number of defects.

In an experiment using X-rays, it is the average reflectivity $\langle R^*R\rangle$ that is measured. If the fluctuating part of the resonance parameter is Gaussian distributed with variance ν^2, then the average reflectivity is a function F of the two-point correlation, $\langle\beta_\xi(t_1)\beta_\xi(t_2)\rangle$:

$$\langle R^*R\rangle = F(\exp[-2\alpha^2 \int_{t''}^{t'}\int_{t''}^{t'} \langle\beta_\xi(t_1)\beta_\xi(t_2)\rangle \mathrm{d}t_1\,\mathrm{d}t_2]). \qquad (6)$$

The stochastic defect model describes stacking faults and misoriented crystal grains in terms of discontinuities in the strain and the strain gradients in the crystal, leading to a correlation given by

$$\langle\beta_\xi(t)\beta_\xi(t+\tau)\rangle = \nu^2\exp(-|\tau|/l), \qquad (7)$$

where the variance $\nu^2 = \sigma^2/2l$. Although (7) has been derived from a consideration of stacking faults and crystal grains, it is applicable to any system in which the resonance parameter, β, and its gradients are discontinuous and are delta-function correlated with position. From (6) and (7), the mean reflectivity depends on

$$\begin{aligned}\exp[-2\alpha^2 \int_{t''}^{t'}\int_{t''}^{t'} \langle\beta_\xi(t_1)\beta_\xi(t_2)\rangle \mathrm{d}t_1\,\mathrm{d}t_2] \\ = \exp\{-4\alpha^2\nu^2 l^2[(|\tau|/l) + \exp(-|\tau|/l) - 1]\} \\ \equiv (1/2\pi)\int_{-\infty}^{\infty} \gamma(\kappa)\exp(-i\kappa\tau)\mathrm{d}\kappa, \qquad (8)\end{aligned}$$

where $\tau = t' - t''$ and (8) defines the Fourier transform of the function $\gamma(\kappa)$. It can be shown that

$$\langle R^*R\rangle = \int_{-\infty}^{\infty} [\gamma(\kappa)/2\pi]|R(2\alpha\langle\beta\rangle - \kappa)|^2\mathrm{d}\kappa, \qquad (9)$$

where $2\alpha\langle\beta\rangle$ is a function of the angle of incidence of the X-ray beam, as shown in (3). The term

$|R(2\alpha\langle\beta\rangle)|^2$ in (9) is the reflectivity of the crystal in the absence of the *discontinuities*, or random perturbations, resulting from the defects and can be calculated from (1). In this sense, it represents a continuous crystal and it contains all the smoothly varying strain terms, including the average of the strains resulting from the imperfections, as discussed above. This term is called the *continuous-crystal reflectivity*. The effects of the random fluctuating strains are obtained by convolving the continuous-crystal reflectivity with the function $\gamma(\kappa)$.

With the mean reflectivity $\langle R^*R\rangle$ of a crystal obtained from a diffraction experiment with a broad incident beam, the aim is to deduce $\gamma(\kappa)$ from (9) and then to extract the defect parameters ν^2 and l using (8). This is conveniently done by taking the Fourier transforms of both sides of (9) and using the fact that the Fourier transform of the convolution of two functions is equal to the product of the Fourier transforms of the functions. The Fourier transform of $\gamma(\kappa)$ is simply the correlation factor given in (8). Then,

$$\left[\int_{-\infty}^{\infty}\langle|R(\kappa_\beta)|^2\rangle\exp(-i\kappa_\beta\tau)\mathrm{d}\kappa_\beta\right] \times\left[\int_{-\infty}^{\infty}|R(\kappa_\beta)|^2\exp(-i\kappa_\beta\tau)\mathrm{d}\kappa_\beta\right]^{-1} = \exp\{-4\alpha^2\nu^2l^2[(|\tau|/l)+\exp(-|\tau|/l)-1]\}, \quad (10)$$

where κ_β is the real part of $2\alpha\langle\beta\rangle$ averaged throughout the volume of the crystal. That is, if the crystal thickness is t_c, then

$$\kappa_\beta = (1/t_c)\mathrm{Re}\left(\int_0^{t_c}2\alpha\langle\beta(t')\rangle\mathrm{d}t'\right). \quad (11)$$

In practical terms, κ_β is linearly related to the mean deviation of the angle of incidence from the angle at maximum reflectivity [see (3)].

The actual count $D(\kappa_\beta)$ measured by the detection system in an experiment will be related to the crystal reflectivity by a scale factor A:

$$D(\kappa_\beta) = A\langle|R(\kappa_\beta)|^2\rangle, \quad (12)$$

which depends on the incident X-ray-beam intensity, losses by absorption and scattering between the sample and the detector, detector efficiency *etc.* Then the left side of (10) represents the correlation factor in a sample obtained from a diffraction experiment and the right side is the predicted correlation factor based on the stochastic model.

The aim of this present work is to demonstrate that the predicted correlation factor has a functional form suitable for fitting X-ray data from crystalline films of varying degrees of perfection. To do this, the continuous-crystal reflectivity must be known, as required by the left side of (10). If the smoothly varying strain in the crystal is known as a function of t then $\langle\beta(t)\rangle$ can be determined and the reflectivity can be calculated from (1). This is particularly simple if there is no strain or if the strain is constant. Furthermore, if the crystal film is thick enough for the continuous-crystal reflectivity to approximate a delta function at the Bragg angle, then the Fourier transform of the continuous-crystal reflectivity is approximately constant and can be neglected altogether in (10). A strain that varies with t usually gives rise to an asymmetry in the reflectivity about the Bragg angle. If the t dependence of such a strain is not known, then the mean reflectivity can be obtained from a triple-crystal or high-resolution experiment, which will resolve regions of constant strain in the crystal. This is discussed below.

The imaginary part of the ratio of the Fourier transforms in (10) should be small (ideally zero) because the correlation factor is real. A significant imaginary component may arise if the imperfect- and perfect-crystal rocking curves are not centred about the same angle. This is a trivial 'phase' effect, which is removed by taking the absolute value of the ratio. An imaginary component can also occur if the imperfect-crystal rocking curve has a significant asymmetry that cannot be accounted for in the calculation of the continuous-crystal rocking curve. In this case, the stochastic model cannot provide a realistic description of the defects in the sample.

Experiment

X-ray data were collected using the configuration in Fig. 1. A dispersive arrangement of channel-cut silicon monochromators provides a parallel and monochromatic X-ray beam in the plane of diffraction using a succession of reflections from silicon (111) planes. The analyser is a two-reflection channel-cut silicon (111) monochromator that can be mounted onto the 2θ arm of the diffractometer when a high-resolution experiment is required. This is a slitless system that projects an image of the source onto the sample. The slits shown in the figure merely limit the

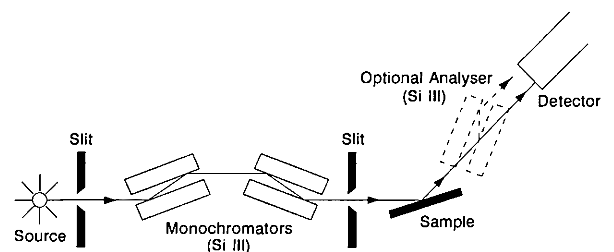


Fig. 1. Diffractometer configuration. The analyser monochromator is only used for high-resolution diffractometry.

Table 1. *Data for each thin-film sample*

No.	Material	Orientation	Thickness (μm)	θ_s (°)	θ_B (°)
1	CdTe	400	0.90	0.0	28.38
2	CdTe	400	0.84	0.0	28.38
3	CdTe	422	1.63	0.0	35.61
4	$Hg_{0.75}Cd_{0.25}Te$	311	1.5	4.3	23.27
5	$Hg_{0.78}Cd_{0.22}Te$	400	1.0	0.0	28.46

amount of diffusely scattered radiation reaching the sample and define the size and divergence of the beam out of the plane of diffraction. The beam properties in the diffraction plane are determined by the monochromators. The beam properties at the sample were: (i) a divergence in the diffraction plane of 12.8″ and a width of 0.8 mm; (ii) a divergence out of the diffraction plane of 36″ and a height of 4 mm. The X-ray wavelength was 0.154 nm, obtained using the Cu $K\alpha_1$ characteristic radiation from a sealed-tube source. The advantage of this system is that it produces an incident beam that closely approximates the assumption in the stochastic model of a monochromatic plane wave incident on the sample. It also produces a broad X-ray beam that averages over a large volume of the sample.

X-ray rocking curves (Figs. 2*a*, *b*, *c* and *d*) were collected from five samples of thin films of CdTe and $Hg_{1-x}Cd_xTe$, each about 1 μm thick, grown on GaAs substrates (see Table 1). The data from sample 4 (Fig. 2*d*) and sample 5 (not shown) had significant asymmetries on the high-angle sides of the Bragg peaks, consistent with nonconstant compressive strains in the films. Because the dependences of these strains on depth in each film are not known, alternative data sets were collected using the analyser in a fixed orientation in front of the detector. In this configuration, only those X-rays diffracting from regions with the same lattice parameter (constant strain) are detected. The data from these high-resolution experiments are shown in Figs. 2(*e*) and (*f*).

Analysis

The continuous-crystal reflectivities were calculated from (1) using the data for each sample given in Table 1. The scattering factors required in the calculation of χ_h were obtained from Doyle & Turner (1968) and Cromer & Liberman (1970). The scattering factors for the $Hg_{1-x}Cd_xTe$ alloys were calculated from weighted averages of the scattering factors for HgTe and CdTe according to the fractions of mercury and cadmium. Linear trends between the first and last counts in each experimental data set were subtracted to remove the background. Each data set was padded with zeros to extend its length to a power of two, as required by the fast Fourier transform (FFT) algorithm (Press, Flannery, Teukolsky & Vetterling, 1987). Both the experimental and the calculated data sets were Fourier transformed and the ratios of the transformed data were taken in accordance with equations (10) and (12). In principle, these ratios should be real and positive. However, the noise in the X-ray data introduces an imaginary component and causes this and the real component to fluctuate about zero for large τ. To allow the logarithms of these data to be taken for both fitting and plotting, the absolute values of the ratios were taken. The scale factor A is assumed to be constant and is chosen for each experiment so that the ratio in (10) is unity at $\tau = 0$. This procedure yields the experimental correlation factors as functions of τ (Fig. 3).

For large τ, the noise from the X-ray data dominates the correlation factor. Fluctuations in the data will arise from the shot noise associated with photon counting, which is governed by Poisson statistics. The standard deviation of these fluctuations can be estimated from the zeroth-order Fourier coefficient of the transformed data, as discussed in the Appendix, giving a measure of the expected level of noise. The shot-noise levels for the data sets are shown as dashed lines in Fig. 3.

The argument of the exponent on the right side of (10) was fitted to the logarithm of the ratios using a Levenberg–Marquardt nonlinear least-squares algorithm (Press *et al.*, 1987). The algorithm optimized the parameters ν^2 and l to obtain the best fits through the data, shown as the solid lines in Fig. 3. The defect parameters were used in (8) and (9) to calculate the imperfect-crystal rocking curves from the continuous-crystal reflectivities. Each curve was scaled to match its peak with the peak value of the data and the average background count was added. The curves appear as the solid lines through the data points in Fig. 2.

While the fits to the data in Fig. 3 appear reasonable, objective measures of the quality of each fit are required. For this purpose, we define

$$\Gamma(\tau) \equiv -4\alpha^2\nu^2 l^2[(\tau/l) + \exp(-\tau/l) - 1] \quad (13)$$

and let $\Delta\Gamma(\tau)$ be the difference between the logarithm of the ratio of the data and the calculated value, $\Gamma(\tau)$, at τ. Then the change Δl in the correlation length required to produce a change $\Delta\Gamma(\tau)$ in the fit at τ is

$$\Delta l = \Delta\Gamma(\tau)/(\mathrm{d}\Gamma/\mathrm{d}l) \quad (14)$$

and similarly for ν^2. Note that $\nu^2 = \sigma^2/2l$ is a function of l that must be included in the derivative $\mathrm{d}\Gamma/\mathrm{d}l$. If there are N data points, each at a particular τ_n, then the mean-square deviations of the defect

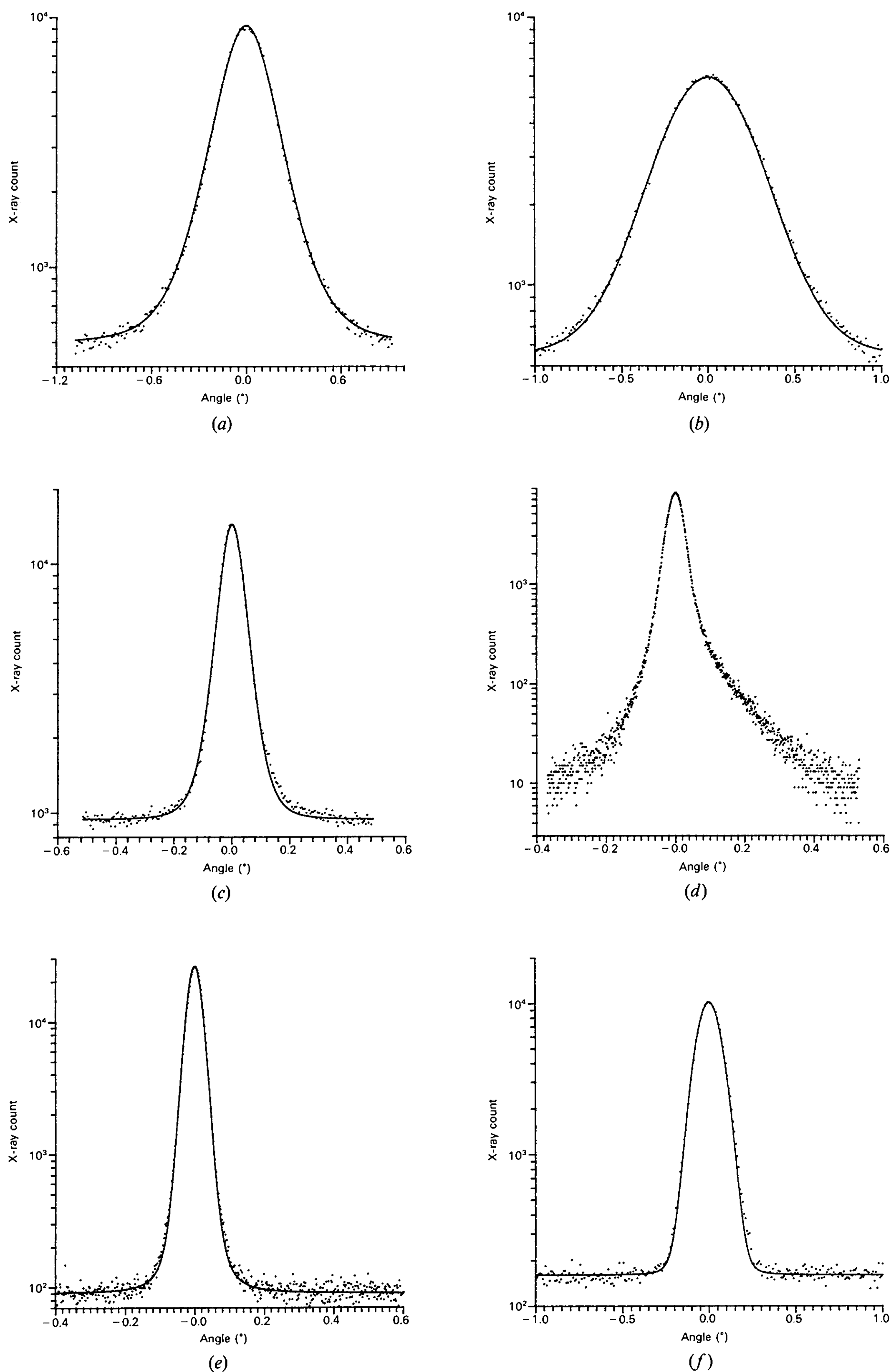
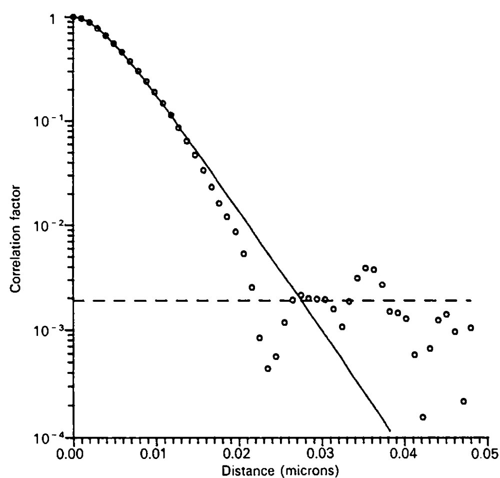
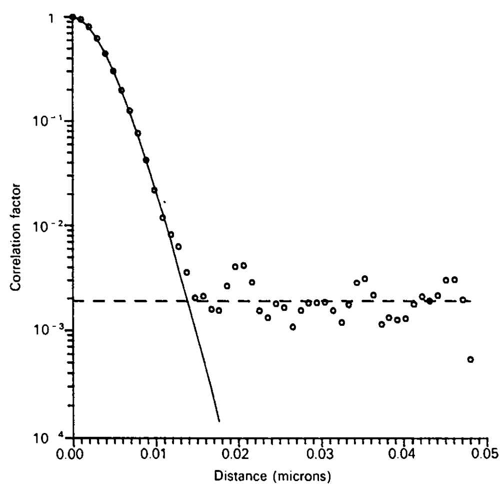


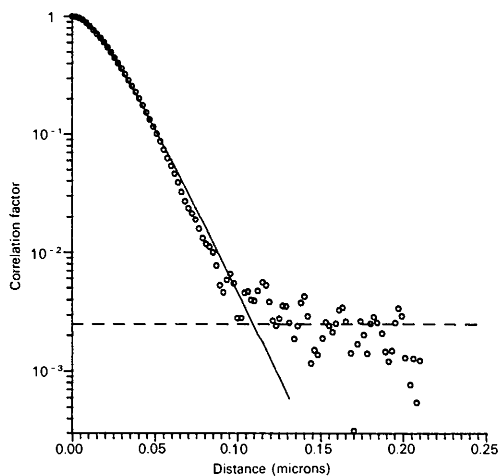
Fig. 2. X-ray rocking curves from (*a*) sample 1, (*b*) sample 2 and (*c*) sample 3; (*d*) rocking curve from sample 4 showing marked asymmetry. High-resolution data from (*e*) sample 4, (*f*) sample 5.



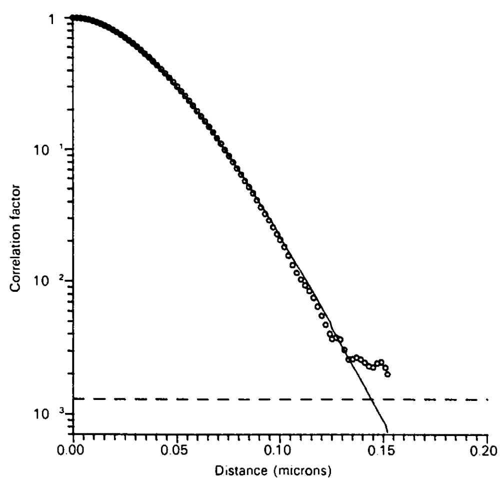
(a)



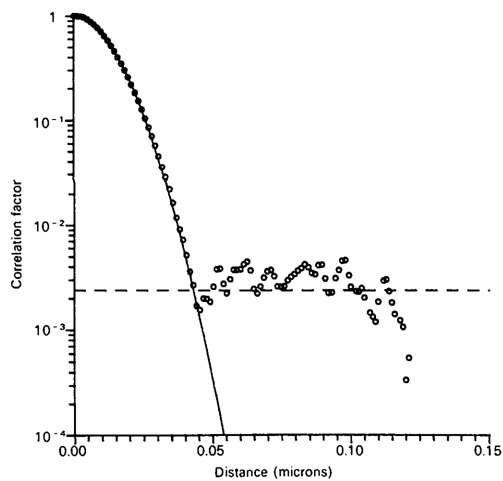
(b)



(c)



(d)



(e)

Fig. 3. Experimental correlation factors (points) and curves of best fit (solid lines) for (a) sample 1, (b) sample 2, (c) sample 3, (d) sample 4 and (e) sample 5. The dashed line in each figure is the estimate of the shot noise in the data.

Table 2. *Results from fitting the model to X-ray data*

No.	N	ν^2	l (μm)	$\Delta\theta$ (°)	Shot noise $\times 10^{-3}$	$\langle(\Delta\mathrm{fit})^2\rangle^{1/2}$ $\times 10^{-3}$
1	29	$9.90\,(160)\times 10^{-6}$	$3.59\,(314)\times 10^{-3}$	0.216	1.93	5.08
2	15	$1.76\,(7)\times 10^{-5}$	$5.53\,(44)\times 10^{-3}$	0.287	1.98	2.95
3	52	$7.94\,(52)\times 10^{-7}$	$1.66\,(35)\times 10^{-2}$	0.0539	2.49	5.15
4	75	$7.92\,(57)\times 10^{-8}$	$5.95\,(48)\times 10^{-2}$	0.0222	1.29	1.49
5	36	$1.01\,(23)\times 10^{-6}$	0.110 (26)	0.0687	2.39	5.75

parameters and the fit to the data can be written as

$$\langle(\Delta l)^2\rangle = (1/N)\sum_{n=1}^{N}\{\Delta\Gamma(\tau_n)/[\mathrm{d}\Gamma(\tau_n)/\mathrm{d}l]\}^2,$$

$$\langle(\Delta\nu^2)^2\rangle = (1/N)\sum_{n=1}^{N}\{\Delta\Gamma(\tau_n)/[\mathrm{d}\Gamma(\tau_n)/\mathrm{d}\nu^2]\}^2,$$

$$\langle(\Delta\mathrm{fit})^2\rangle = (1/N)\sum_{n=1}^{N}\{\exp[\Gamma(\tau_n)+\Delta\Gamma(\tau_n)] - \exp[\Gamma(\tau_n)]\}^2. \quad (15)$$

The r.m.s. deviations for each data set were calculated from (15) and are given in Table 2. The r.m.s. deviations for ν^2 and l are shown as errors in these parameters. The value of N was determined by that part of the fit that lies above the shot-noise level. The half-width of each rocking curve, $\Delta\theta$, defined by that value of $\theta-\theta_B$ for which $\beta(\theta)^2 = \nu^2$, is also given in the table.

Discussion

A comparison between the last two columns of Table 2 shows that the r.m.s. deviation of each fit from the data is within a factor of three of the shot-noise level, which indicates that the stochastic model provides the correct functional form for the defect correlations in all samples, to a level of accuracy approaching the noise level in the data.

There are significant numbers of fluctuations in the noisy regions of the data (Fig 3), which exceed the shot-noise levels by factors close to the r.m.s. deviations of the fits. Fluctuations of this magnitude were observed in the imaginary components of the ratio in (10). This suggests that there are additional noise sources and long-range small-magnitude correlations that have not been accounted for in the analysis. The origins of these fluctuations may be nonuniformities, or biases, in the distributions of the defects, which introduce asymmetries in the X-ray data, leading to fluctuations of this type in the correlation factor. Spurious Fourier components may also be introduced when each data set is padded with zeros as required by the FFT algorithm.

In some instances, notably for samples 1 and 3 (Figs. 3*a* and *c*), the experimental correlation factors show progressive deviations from the fit, well before the noise levels are reached. Such deviations indicate that the assumptions in the stochastic model of Gaussian-distributed strain and strain-gradient fluctuations, and the correlation assumptions leading to (7), are beginning to fail. The extent of the failure of the model is ultimately gauged by the resultant errors in the defect parameters.

A comparison of correlation lengths between samples shows that the defects in samples 1 and 2 are point-like, these samples having correlation lengths equivalent to about six unit-cell widths; *i.e.* there are strain fluctuations in these samples that, on average, are only coherent over short distances, suggesting the existence of a large number of closely spaced defects. The other samples have longer correlation lengths and the defects have more the character of mosaic blocks; *i.e.* the strain fluctuations are coherent over longer distances, which is suggestive of crystal subgrains. The differences between the samples arise from the different growth conditions of the films and also from the different crystallographic orientations of the substrate surfaces. Note that, although the rocking-curve widths of samples 3 and 5 are similar, both the correlation lengths l and the defect strengths σ^2 differ by an order of magnitude. This implies that the distributions of defects and their structures, measured from these two samples, are quite different. The usual measure of crystal quality, based solely on the rocking-curve width, would not distinguish between these samples.

The method presented above for measuring the defect parameters is based on a kinematic description of X-ray diffraction. Although the stochastic model has been incorporated in a dynamical formulation by Davis (1991), the resulting equation is difficult to solve analytically and numerical solutions are likely to require intensive computations. For crystals in which dynamical extinction effects are important, the kinematic method is only applicable to data collected well away from the Bragg peak where the scattering becomes kinematic.

Summary

A model for the diffraction of X-rays from imperfect crystals has been used to obtain two parameters that characterize the statistical properties of the crystal

defects. A method of extracting these parameters from X-ray data in the kinematic regime has been discussed. In its simplest form, where the rocking-curve width from the imperfect sample is very much greater than that from the continuous crystal, the method only requires the Fourier transform of the data and the fit to this of an analytical expression involving the unknown defect parameters. On a modest personal computer, this process takes a few minutes at most. For other crystals, the continuous-crystal reflectivity must be calculated, which either requires knowledge of the strain profile in the crystal, or requires the data to be collected in a high-resolution triple-crystal experiment.

It was shown that the correlation factor predicted by the defect model has the correct functional form to fit experimental data obtained from five samples of CdTe and $Hd_{1-x}Cd_xTe$ films grown on GaAs. If this form is sufficiently general to fit the data from a large class of imperfect extended-face crystals then, through the two defect parameters in the model, it will provide an objective measure of the crystal quality and a means of characterizing the statistical nature of defects.

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APPENDIX

Let $f(x) = \langle f(x)\rangle + \xi(x)$ represent the X-ray count from a diffraction experiment, dependent on some parameter x (for example, the angle of incidence of the X-ray beam on the sample), which can be written in terms of an ideal or average value $\langle f(x)\rangle$ and a noise term $\xi(x)$, where $\langle \xi(x)\rangle = 0$. The noise term represents fluctuations in the count owing to random effects and is assumed to obey a Poisson distribution. The Fourier transform of this is

$$\begin{aligned} F(k) &= \int_{-\infty}^{\infty} [\langle f(x)\rangle + \xi(x)] \exp(-ikx)\,\mathrm{d}x \\ &= \langle F(k)\rangle + \Xi(k), \end{aligned} \qquad (A1)$$

which defines the transforms of the average and noisy parts of the data. The variance in Fourier space is

$$\sigma^2(k) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \langle \xi(x)\xi^*(x')\rangle \exp[-ik(x-x')]\,\mathrm{d}x\,\mathrm{d}x'. \qquad (A2)$$

This depends on the two-point correlation function $\langle \xi(x)\xi^*(x')\rangle$, which, for uncorrelated fluctuations, is given by

$$\langle \xi(x)\xi^*(x')\rangle = \sigma_\xi^2(x)\delta(x-x'), \qquad (A3)$$

where $\sigma_\xi^2(x)$ is the variance of the X-ray count. Substitution of ($A3$) in ($A2$) yields

$$\sigma^2(k) = \int_{-\infty}^{\infty} \sigma_\xi^2(x)\,\mathrm{d}x, \qquad (A4)$$

which is independent of k. This is the standard result demonstrating that uncorrelated noise has a constant spectral density. If Poisson statistics are assumed, then the variance of the measurement is equal to the mean. Therefore,

$$\begin{aligned} \sigma^2(k) &= \int_{-\infty}^{\infty} \langle f(x)\rangle\,\mathrm{d}x = \langle F(0)\rangle, \\ \sigma(k) &= \langle F(0)\rangle^{1/2}, \end{aligned} \qquad (A5)$$

where ($A1$) has been used to relate the integral of $\langle f(x)\rangle$ to $\langle F(k)\rangle$ at $k = 0$. Thus, the standard deviation $\sigma(k)$ of the Fourier transform of data obtained from a counting experiment (*i.e.* one governed by Poisson statistics) is constant and equals the square root of the value of the Fourier transform at $k = 0$. Note that it is $F(k)$ that is determined from the data and not $\langle F(k)\rangle$. However, an estimate of the likely error can be obtained by using $F(0)$ instead of $\langle F(0)\rangle$ in ($A5$). Furthermore, note that $F(0)$ used in ($A5$) should be calculated from the complete data set, including the background count.

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