isotropic error'. The 'maximum deviation' is the largest value of $|\sigma_x - \sigma_n|/\sigma_n$, or the analogous fraction for the y or z coordinate, of any atom.

Estimates of $\sigma(R)$ from equation (1) were typically within the round-off error; the poorest agreement noted between calculated and reported values is given in Table 1. The same can be said for the estimates of $\sigma(\varphi)$, from equation (4*b*); the poorest agreement found is included in the table. The corresponding value of $\sigma(\varphi)$ calculated from equation (2) is also given for these cases; it is not markedly superior to the approximate value from equation (4*b*).

The assumption of isotropic uncorrelated errors appears to be satisfactory for typical crystal structure determinations, and the error estimates provided by equations (1) and (4*b*) are surprisingly good.

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Extinction in single crystals of UO_2.

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Abstract

The measurements of nuclear neutron diffraction intensities for a single crystal of UO_2 by Faber & Lander [*Phys. Rev. B* (1976), **14**, 1151–1164] have been re-analysed using both the Cooper–Rouse and Becker–Coppens extinction formalisms. The results indicate that this crystal is type I in nature, not type II as was suggested by Faber & Lander, and this conclusion is essentially the same as that obtained for a different single crystal of UO_2 used in our earlier study of the wavelength dependence of extinction in this material [Sakata, Cooper, Rouse & Willis (1978). *Acta Cryst.* A**34**, 336–341]. The analysis of the Faber & Lander data gave a value for the scattering-length ratio $b_U/b_O = 1{\cdot}448$ (2).

Introduction

In a recent study of the magnetic structure of UO_2 Faber & Lander (1976) carried out a series of accurate neutron diffraction measurements on a single crystal of UO_2 at three different temperatures, *viz* 300, 80 and 4·2 K. In analysing their data they assumed the model for extinction given by Zachariasen (1967) and found this adequate to describe the extinction results for the purpose of their study. However, they concluded that the high value they obtained for the mosaic-spread parameter g, *i.e.* about 1000, suggested a type II extinction, as defined by Zachariasen (1967).

Recently we have carried out an independent neutron diffraction study of the wavelength dependence of extinction in UO_2 (Sakata, Cooper, Rouse & Willis, 1978), analysing our results on the basis of the improvements to the Zachariasen extinction model derived by Cooper & Rouse (1970) and Becker & Coppens (1974). This study led to the conclusion that these formalisms gave similar results for the crystal studied and indicated a type I extinction in this case. Since almost every recent study of extinction has indicated type I extinction or a tendency to type I extinction we have therefore carried out an analysis of the Faber & Lander data to determine whether the extinction type in their crystal was any different from that in the one we studied.

Results of the new analysis

Detailed experimental results for the nuclear scattering in the Faber & Lander (1976) experiment were kindly supplied by these authors and were re-analysed using the Harwell *TAILS* computer program (see Sakata, Cooper, Rouse & Willis, 1978). In order to determine the most suitable model for the extinction in this crystal the data were analysed using the following models:

(1) Cooper–Rouse
(2) Becker–Coppens type I Gaussian (secondary)
(3) Becker–Coppens type I Lorentzian (secondary)
(4) Becker–Coppens type II (secondary)
(5) Becker–Coppens mixed-type Gaussian (secondary)
(6) Becker–Coppens mixed-type Lorentzian (secondary)
(7) Becker–Coppens general (mixed-type Lorentzian plus primary).

The Cooper–Rouse model gave reasonable agreement, with values of the effective domain radius which do not differ significantly for the three temperatures. The Becker–Coppens type II model gave a fit which is significantly worse than that for the type I models, particularly for the most severely extinguished reflections. Of the type I models, that using a Lorentzian mosaic-spread function gave slightly better overall agreement than that using a Gaussian mosaic-

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spread function, although the latter gave slightly better agreement for the 300 K data.

The Becker–Coppens mixed-type models gave no significant overall improvement over the type I models and, although the extinction parameters were less well determined, gave values for which $r \gg \lambda g$ indicating again the preference for a type I model. Inclusion of primary extinction in the mixed-type model also gave no significant overall improvement. It is concluded, therefore, that the most appropriate model for these results in the Becker–Coppens formalism is a type I model with a Lorentzian mosaic-spread function. This model gives slightly better agreement than the Cooper–Rouse model, but significance tests on the weighted discrepancy index (Hamilton, 1965) indicated that this difference is only significant at the 25% level.

In order to compare our results with those obtained by Faber & Lander (1976) we tabulate in Table 1 values for the parameters derived for the Becker–Coppens type I Lorentzian model (BCL) together with those derived by Faber & Lander (FL). There is clearly no significant difference between the parameters derived from these two analyses indicating that, at the level of extinction involved ($y_{min} \simeq 0{\cdot}6$), the unmodified Zachariasen model is also adequate, as would be expected for a type I crystal.

Table 1. *Parameter values derived for the Becker–Coppens type* I *Lorentzian model (BCL) and those derived by Faber & Lander (FL)*

		$T = 300$ K, $\lambda = 1{\cdot}05$ Å	$T = 80$ K, $\lambda = 0{\cdot}992$ Å	$T = 4{\cdot}2$ K, $\lambda = 0{\cdot}992$ Å
g	BCL	909 (70)	1076 (44)	1087 (41)
	FL	936 (73)	1110 (46)	1155 (43)
B_U (Å^2)	BCL	0·27 (3)	0·11 (1)	0·07 (1)
	FL	0·25 (2)	0·10 (1)	0·07 (1)
B_O (Å^2)	BCL	0·42 (3)	0·25 (1)	0·21 (1)
	FL	0·41 (2)	0·24 (1)	0·22 (1)

Table 2. *Results obtained from the final analysis*

	$T = 300$ K, $\lambda = 1{\cdot}05$ Å	$T = 80$ K, $\lambda = 0{\cdot}992$ Å	$T = 4{\cdot}2$ K, $\lambda = 0{\cdot}992$ Å
b_U/b_O	1·443 (3)	1·448 (7)	1·450 (2)
g	806 (38)	1022 (17)	1072 (18)
B_U (Å^2)	0·24 (2)	0·09 (1)	0·06 (1)
B_O (Å^2)	0·44 (1)	0·27 (1)	0·25 (1)
R (%)	1·49	0·64	0·42

Re-analysis of earlier measurements on a single crystal of UO_2 (Rouse, Willis & Pryor, 1968) gave a value of $b_U/b_O = 1{\cdot}43$, rather than 1·47, which was used by Faber & Lander (1976), and this lower value was used in the wavelength-dependence study (Sakata, Cooper, Rouse & Willis, 1978), together with a fixed value of $B_U = 0{\cdot}28$ Å^2. Analysis of the Faber & Lander 300 K data with these values of b_U/b_O and B_U gave $B_O = 0{\cdot}52$ (1) Å^2, in good agreement with the earlier value of $B_O = 0{\cdot}55$ (2) Å^2, but with a worse overall fit to the data. A further analysis was therefore carried out with the Becker–Coppens type I Lorentzian model and b_U/b_O refined, the results of which are given in Table 2. These give a weighted mean value of $b_U/b_O = 1{\cdot}448$ (2). Correlation between the other parameters was considerably less in this analysis than in that with $b_U/b_O = 1{\cdot}47$ and the parameters were therefore determined more accurately. The weighted discrepancy factors are also significantly less and it is concluded therefore that this represents the best model for these data.

Further details of this analysis are available elsewhere (Cooper & Sakata, 1978).

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