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SHORT COMMUNICATIONS

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Acta Cryst. (1980). **A36**, 1070–1071

The defect structure of VO_x: comparison between X-ray and electron diffraction. By M. MORINAGA, *Toyohashi University of Technology, Toyohashi, Aichi 440, Japan* and J. B. COHEN, *Department of Materials Science and Engineering, The Technological Institute, Northwestern University, Evanston, Illinois 60201, USA*

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Abstract

Discrepancies exist in the local atomic arrangements determined from diffuse X-ray and electron scattering. The possible reasons for this are examined.

In VO_x (0.8 < *x* < 1.3) there are large numbers of both anion and cation vacancies and interstitial cations. The concentrations of these vary with composition, *x*. The presence of (composition-dependent) diffuse scattering indicates that these defects are not randomly arranged. The purpose of this communication is to compare our results on the defect arrangement in VO_x (Morinaga & Cohen, 1979*a,b*) from studies of diffuse X-ray scattering with those deduced by Andersson and co-workers from their pioneering attempt to analyze quantitatively diffuse electron scattering (Andersson, Gjönnes & Taftö, 1974; Andersson, Gjönnes & Forouh, 1978; Anderson, 1979).

This comparison is presented in Table 1. While there are similarities there are also serious differences. Besides complex dynamical effects in electron diffraction, the problem in estimating background scattering makes it difficult to obtain quantitative information on local order, because a weak modulation of diffuse intensity in reciprocal space cannot be measured accurately. An advantage of the X-ray method is that this kind of problem can be treated with measurements of diffuse intensities in absolute units so that all sources of

the scattering can in principle be found. Other origins for the discrepancies that appear in Table 1 may be due to the regression method used for the analysis of diffuse electron scattering. This method is quite sensitive to the choice of fitting parameters and fitting regions in reciprocal space (Morinaga, 1978). Least-squares fitting using a limited number of parameters and restricted regions of reciprocal space sometimes yields erroneous or unstable results. Andersson and co-workers (Andersson *et al.*, 1978; Andersson, 1979) analyzed data on a few reciprocal planes with a small number of parameters. In addition, an electron microscope with an accelerating voltage of 1 MeV was employed. A wide range of reciprocal space can be measured with such an instrument, and the diffuse scattering at the highest scattering angles was used by Andersson *et al.* to detect the static and dynamic displacements of ions. But the contribution of higher-order displacements to the measured intensity is appreciable in this region. This results in problems in estimating the first- and second-order displacement coefficients in the presence of these (ignored) higher-order terms. Thus, there are several difficulties to be resolved in quantitative studies of diffuse electron scattering. On the other hand, the X-ray method averages over a much larger volume of sample than the electron method; anisotropic local structures can be lost in this averaging. Furthermore, there could be local differences in composition, and hence in the atomic arrangements, which are best examined with electron scattering. Furthermore, the X-ray method is not nearly as rapid as the electron method. But at this time it is more

Table 1. Comparison of the defect structures in VO_x determined from X-ray and electron diffuse scattering

	X-ray studies	Electron scattering
Local ionic arrangements	Composition $x > 1$. Most interstitial cations are surrounded by two–three cation vacancies. There is no correlation between interstitial cations. Composition $x < 1$. The anion and cation vacancies are arranged in rows along $\langle 110 \rangle$ directions with alternating vacancy-rich and vacancy-deficient $\{111\}$ layers.	Composition $x > 1$. Every interstitial cation is surrounded by four cation vacancies, and these form a tetrahedral cluster. There is a strong correlation between interstitial cations (or tetrahedral clusters). Composition $x < 1$. There are small $\{111\}$ sheets of anion vacancies. The arrangements of cation vacancies could not be determined.
Displacement of ions	There are displacement modulations associated with the defect arrangements. In $\text{VO}_{1.17}$, no expansion of nearest-neighbor distance. The distortion parameter ε_{110}^{xy} is negative and is the largest among the displacement parameters. (This represents the average of the product of x and y displacements at the end of interatomic vector $a/2 [110]$.)	There are no special correlations between the displacement parameters and the order parameters. In $\text{VO}_{1.23}$, the expansion of nearest-neighbor distance is large, and may occur in $\text{VO}_{0.9}$ as well. Parameter γ_{110}^x is the largest among the displacement parameters. (This represents the average x displacement at the end of interatomic vector $a/2 [110]$.)
Comparison between ordered and disordered phases	The values of short-range-order parameters for the disordered phase are much smaller than those for the ordered phase. But the change of these values with interatomic distance is similar in both phases.	There is a contradiction in order parameters between both phases. Namely, $(a/2)[211]$ is the nearest-neighbor intercluster vector in the disordered phase, but $(a/2)[221]$ in the ordered phase.

reliable for the quantitative analysis of diffuse scattering and should be employed even if some effort is required to produce a suitable crystal. Electron scattering is perhaps most suitable at the moment for a rapid estimate of the regions in reciprocal space which are of interest.

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Corrections to Sections 4.3 and 4.4 of the 1969 edition of Volume I of *International Tables for X-ray Crystallography*. By TAKESHI YAO and HIROSHI JINNO, *Department of Industrial Chemistry, Faculty of Engineering, Kyoto University, Sakyo-ku, Kyoto 606, Japan*

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Abstract

Corrections are given to §§ 4.3 and 4.4 of *International Tables for X-ray Crystallography* [Vol. I (1969), Birmingham: Kynoch Press].

(2) § 4.4, Table 4.4.3 TETRAGONAL. *Laue Class* 4/mmm on p. 350

In the first row from the top of the table (diffraction symbol 4/mmmP---), in the column of the point group 42m: Replace the space group P42m by P42m.

Errors have been found in *International Tables for X-ray Crystallography* (1969) in addition to those already pointed out (Yao & Jinno, 1979), and the corrections are given below. No other errors have been found in §§ 4.3 and 4.4.

(1) § 4.3 No. 217 on p. 326

Replace the heading I43m by I43m.

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