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## VAX adaptation of the *ROCKS* crystallographic program system.

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**Abstract**

The *ROCKS* crystallographic computing system is a general complete integrated and easy-to-use system of programs for macromolecular structure determination. However, it has heretofore been available only on IBM 360 or 370 mainframe computers. This note reports the successful adaptation of the *ROCKS* system to the DEC VAX series of superminicomputers.

The *ROCKS* system of crystallographic computer programs is described in detail by Reeke (1984). It provides a complete and unified set of programs for film scanning, initial data reduction, sorting and merging, scaling and data correlation, structure factor and least squares, and Fourier and Patterson calculations. A number of different laboratories have used it successfully.

The original version of *ROCKS* was written for the IBM 360 computer. Efficiency and ease of use were more important goals than portability, and it has not previously been possible to run the *ROCKS* programs on computers other than the IBM 360/370 series. The chief obstacle to portability was the use of large amounts of Assembler language code in certain places to avoid the inefficiency and limitations of Fortran. This code has now been converted to equivalent VAX Fortran and Assembler language, making it possible to run the *ROCKS* programs on the widely available VAX computers.

The VAX version of *ROCKS* is now a complete system, with one major exception to be mentioned below. It is used routinely in our laboratory for oscillation film processing and other tasks, and has been distributed to several other laboratories. The VAX version is highly compatible with the original version. The reference manual for the 360 version of *ROCKS* also serves for the VAX version, along with a short document listing operating system procedures and the few minor implementation differences.

Three subprograms of 360/370 *ROCKS* are written largely or entirely in Assembler language, and have not been converted at this time. These are the Fourier, contour, and structure-factor/least-squares (including isomorphous replacement) subprograms.

Alternatives to the Fourier and contour subprogram exist in the present system. A fast Fourier subprogram using Fourier transform subroutines by Ten Eyck (1973) has been added. It handles all space groups automatically by expanding the input asymmetric unit of data to a hemisphere. The program does not require that sampling intervals be powers of two; however, it does not do skew planes or orthogonal sampling as the original *ROCKS* Fourier program does. A contouring program which produces output on a plotter, rather than a line printer as in the original version, has also been added. This program was written to be portable, and will eventually be incorporated into the 360 version of *ROCKS*.

Unfortunately, there is no structure-factor/least-squares program in the current system; this is the most serious limitation of the present VAX implementation. A more portable *SFLS* program is expected to be incorporated into 360/370 *ROCKS* in the near future. When this program becomes available, it will be added to the VAX version.

The current version of *ROCKS* runs under version 3.2 or later of the VAX/VMS operating system. It is available at no charge; interested persons should send a 9-track magnetic tape to the author, specifying the density required (800, 1600, or 6250).

### References

Reeke, G. N. (1984). *J. Appl. Cryst.* **17**, 125–130.
Ten Eyck, L. F. (1973). *Acta Cryst.* A**29**, 183–191.

## Letters to the Editor

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### Comment on 'Residual Stresses in Cubic Materials with Orthorhombic or Monoclinic Specimen Symmetry: Influence of Texture on $\psi$ Splitting and Nonlinear Behaviour' by C. M. Brakman

Sir,

In determining residual stresses with X-rays, the interplanar spacing *vs* $\sin^2\psi$ is measured (where $\psi$ is the tilt of the specimen normal from the normal parafocusing position). Recently Dölle & Hauk (1977) and Dölle & Cohen (1980*a*) have shown that curvature in this plot can arise due to stress components normal to the surface, $\sigma_{33}$, $\sigma_{13}$, $\sigma_{23}$. (The latter two components cause a different shape for $\pm\psi$, which is termed $\psi$ splitting.) Brakman (1983) has suggested that an alternative explanation can be obtained without the normal stresses based on averaging the elastic constants with the symmetry associated with any preferred orientation. We wish to point out here several severe limitations in the analysis.

(1) Brakman suggests that $\sigma_{13}=\sigma_{23}=\sigma_{33}=0$ in an X-ray measurement because of the conditions of equilibrium. However, he applies these conditions at a point, whereas the X-ray beam samples a volume. A more correct application of these conditions has been presented (Noyan, 1983) and permits these stress components.

(2) Brakman's formulation is based on the Reuss limit; that is, he assumes that the stress is the same in all diffracting grains, and also neglects grain interaction stresses. It is well known that both assumptions are seldom realistic (Kröner, 1967; Hashimoto & Margolin, 1983).

(3) For his treatment to be justified, there should be no oscillations in '*d*' *vs*

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$\sin^2\psi$ for *hhh*- or *h*00-type reflections for cubic materials (Dölle & Cohen, 1980*b*). However, such oscillations have now been detected (Noyan & Cohen, 1983).

Therefore, the basic assumptions in Brakman's treatment are violated in practice. While a contribution owing to this effect may occur, it does not appear possible to use his equations to test the importance of preferred orientation.

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### References

Brakman, C. M. (1983). *J. Appl. Cryst.* **16**, 325–340.
Dölle, H. & Cohen, J. B. (1980*a*). *Metall. Trans. A*, **11**A, 159–164.
Dölle, H. & Cohen, J. B. (1980*b*). *Metall. Trans. A*, **11**A, 831–836.
Dölle, H. & Hauk, V. (1977). *Z. Metallkd.* **68**, 725–728.
Hashimoto, K. & Margolin, H. (1983). *Acta Metall.* **31**, 787–800.
Kröner, E. (1967). *J. Mech. Phys. Solids*, **15**, 319–329.
Noyan, I. C. (1983). *Met Trans. A*, **14**A, 1907–1914.
Noyan, I. C. & Cohen, J. B. (1983). *Denver X-ray Conference*, Vol. 32. In the press.

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## Reply to 'Comment on "Residual Stresses in Cubic Materials with Orthorhombic or Monoclinic Specimen Symmetry: Influence of Texture on $\psi$ Splitting and Non-linear Behaviour" by C. M. Brakman'

Sir,

Although I gave an analysis in § 9, *Conclusions*, of my paper (Brakman, 1983) of the possibilities and shortcomings of my theory it seems necessary to elaborate my points.

First of all, it is pointed out again that my treatment is concerned with (residual) macrostresses (or what is equivalent: stresses of the first kind) in textured materials with cubic crystal symmetry. Only the influence of crystallographic texture on oscillations and $\psi$ splitting is studied for the case of one-phase materials.

(1) $\sigma_{i3} = 0$; *mechanical equilibrium, X-ray diffraction sampling*

It is obvious that the conditions of mechanical equilibrium (Timoshenko & Goodier, 1970) even at a *point* leave the possibility of gradients in $\sigma_{i3}$ with respect to $z$ as far as *micro*stresses are concerned: on a *micro*scale, gradients $\partial\sigma_{ij}/\partial x$ and $\partial\sigma_{ij}/\partial y$ may be present and, as a consequence, *micro*stress gradients $\partial\sigma_{i3}/\partial z$ occur.

However, it should be clear that the macrostress gradients $\partial\sigma_{ij}/\partial x$ and $\partial\sigma_{ij}/\partial y$ *averaged* over the *sampled volume* should be equal to zero since the specimens we are discussing here cannot, physically speaking, exhibit any $x$ and/or $y$ dependency in any plane $z$ = constant.

Therefore, the *macro*stress gradients $\partial\sigma_{i3}/\partial z$ averaged over the sampled volume should be equal to zero since it can easily be shown that the conditions of mechanical equilibrium also apply for the case of averaged gradients. Since for *all* stresses (macro or micro) $\sigma_{i3}(z=0) \equiv 0$ it follows as far as *macro*stresses are concerned that: $\sigma_{i3}(z) \equiv 0$ for all depths $z$ in the sampled volume of the specimen.

Note that for the case of pseudo-macrostresses (defined as averages over the volume of a grain or a small number of grains) a different situation arises. Presumably these are the stresses Cohen & Noyan are referring to above. The averaged (over the volume of a grain) gradients $\partial\sigma_{ij}/\partial x$ and $\partial\sigma_{ij}/\partial y$ can be non-zero then. It can be shown that they, too, should obey the conditions of mechanical equilibrium (confined to the volume of averaging):

$$\left\langle \frac{\partial\sigma_{i1}}{\partial x} \right\rangle^{pm} + \left\langle \frac{\partial\sigma_{i2}}{\partial y} \right\rangle^{pm} + \left\langle \frac{\partial\sigma_{i3}}{\partial z} \right\rangle^{pm} = 0,$$

where *pm* stands for pseudo-macrostress. As a consequence, averaged gradients $\langle\partial\sigma_{i3}/\partial z\rangle^{pm}$ may be non-zero.

In most cases *these* gradients are cancelled out through the influence of other grains in the sampled volume. However, if in the case of systematic 'maltreatment' of the surface (as occurs in grinding) these gradients are 'polarized' in one direction this compensation may not occur owing to the limited penetration depth of the X-rays. Then, $\psi$ splitting may occur. However, these pseudo-macrostresses are not studied in my treatment, as their influence seems to be small in one-phase materials. In multi-phase materials the situation may be different as has been reported by Hauk, Oudelhoven & Vaessen (1981).

(2) *The Reuss model of elasticity*

It is common knowledge that the Reuss model is only approximate physically speaking. Since almost all publications in this field use the Reuss model and the setting up of the Kröner model (Kröner, 1958, 1967) for textured materials is very complicated (Kneer, 1965; Morris, 1970) it was decided to test the Reuss model first in order to find out the general tendencies. In addition to this our experiments on cold-rolled (one-phase) steel sheet specimens indicate that the Reuss model in combination with texture and the macrostresses $\sigma_{11}, \sigma_{22}, \sigma_{12}$ performs quite well in the sense that the oscillations of the graph of $\langle\varepsilon'_{zz}\rangle$ *vs* $\sin^2\psi$ are predicted very well. The grain interaction stresses mentioned by Hashimoto & Margolin (1983) can only contribute to microstress fields and X-ray diffraction line *broadening*. The elastic polarization tensors mentioned by Kröner (1967) can only give rise to pseudo-macrostresses.

(3) *The hhh and h*00 *reflections*

As was mentioned in §§ 5.1.1 and 5.1.2 (Brakman, 1983), $\psi$ splitting and oscillations would still be predicted in the case of these reflections if the stresses $\sigma_{13}$ and/or $\sigma_{23}$ were present. These can only occur as pseudo-macrostresses. For the case of grinding of carbon steel Wakabayashi, Nakayama & Nagata (1977) report a $\psi$ splitting for the 200 reflection. Obviously the same situation arises as reported by Hauk, Oudelhoven & Vaessen (1981). The non-zero pseudo-macrostresses compensate each other in both phases.

The example mentioned by Noyan & Cohen (1983) concerns a 222 reflection measured at a 90% cold-rolled α-brass. However, from the literature (Ridha & Hutchinson, 1981; Hirsch, Virnich & Lücke, 1981) it is seen that this material contains large amounts of shear bands. This fact could introduce multi-phase material behaviour and as a consequence pseudo-macrostresses. In our laboratory we measured a very strong non-linearity in the graph of $\langle\varepsilon'_{zz}\rangle$ *vs* $\sin^2\psi$ in the case of the 222 reflection measured at electrodeposited nickel. Here it seems that a few orientations (the main texture components) exhibit a stress state very different from all other crystallites. This has also been found by Naumann (1982). The phenomenon may be ascribed to a pseudo-macrostress field generated during the growth of the nickel layer.

It should be realized that all these examples are exceptions and for 'ordinary' one-phase materials (for instance our low-carbon steel sheet specimens) linear behaviour is frequently found.

### Conclusions and final remarks

(i) For one-phase materials all or most basic assumptions in my treatment are