

$\sin^2 \psi$ for *hhh*- or *h00*-type reflections for cubic materials (Dölle & Cohen, 1980b). 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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(Received 27 July 1983;
accepted 18 January 1984)

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Reply to 'Comment on "Residual Stresses in Cubic Materials with Orthorhombic or Monoclinic Specimen Symmetry: Influence of Texture on ψ 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 ψ splitting is studied for the case of one-phase materials.

(1) $\sigma_{13} = 0$; 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 σ_{13} with respect to z as far as *microstresses* are concerned: on a *microscale*, gradients $\partial\sigma_{ij}/\partial x$ and $\partial\sigma_{ij}/\partial y$ may be present and, as a consequence, *microstress* gradients $\partial\sigma_{13}/\partial z$ 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 $z = \text{constant}$.

Therefore, the *macrostress* gradients $\partial\sigma_{13}/\partial z$ 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) $\sigma_{13}(z=0) \equiv 0$ it follows as far as *macrostresses* are concerned that: $\sigma_{13}(z) \equiv 0$ for all depths z in the sampled volume of the specimen.

Note that for the case of pseudo-macrostress (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):

$$\left\langle \frac{\partial\sigma_{11}}{\partial x} \right\rangle^{pm} + \left\langle \frac{\partial\sigma_{12}}{\partial y} \right\rangle^{pm} + \left\langle \frac{\partial\sigma_{13}}{\partial z} \right\rangle^{pm} = 0,$$

where *pm* stands for pseudo-macrostress. As a consequence, averaged gradients $\langle \partial\sigma_{13}/\partial z \rangle^{pm}$ 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, ψ splitting may occur. However, these pseudo-macrostress 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 σ_{11} , σ_{22} , σ_{12} performs quite well in the sense that the oscillations of the graph of $\langle \epsilon'_{zz} \rangle$ 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-macrostress.

(3) The *hhh* and *h00* reflections

As was mentioned in §§ 5.1.1 and 5.1.2 (Brakman, 1983), ψ splitting and oscillations would still be predicted in the case of these reflections if the stresses σ_{13} and/or σ_{23} were present. These can only occur as pseudo-macrostress. For the case of grinding of carbon steel Wakabayashi, Nakayama & Nagata (1977) report a ψ splitting for the 200 reflection. Obviously the same situation arises as reported by Hauk, Oudelhoven & Vaessen (1981). The non-zero pseudo-macrostress 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-macrostress. In our laboratory we measured a very strong non-linearity in the graph of $\langle \epsilon'_{zz} \rangle$ 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

not violated. The theory only takes into account macrostresses. Problems associated with pseudo-macro stresses cannot be solved using my theory but neither can the methods advocated above by Noyan & Cohen as Noyan (1983) admits. Kossel techniques should be used in order to get more insight into these stresses.

The separation of macro- and pseudo-macro stresses (by definition varying from grain to grain) as suggested by Noyan (1983) seems impossible in most cases with reference to the present 'state of the art'. If the orientation dependency of the pseudo-macro stresses (Noyan, 1983) is neglected this is possible but then, strictly speaking, these stresses are treated as macro stresses.

(ii) For multi-phase materials the texture contribution to the ψ splitting and/or non-linearities can be 'subtracted' using my equations if one or more phases exhibit any significant texture.

(iii) Oscillations in experimentally obtained $\langle e_{zz}^2 \rangle$ vs $\sin^2\psi$ data need not indicate the presence of an inhomogeneous strain state but can also be a result of crystallographic texture (Noyan & Cohen, 1983).

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(Received 4 November 1983;
accepted 18 January 1984)

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Editorial comment: The authors of these two letters still do not agree on the conclusions. The technical situation is complicated, mainly due, it appears, to misunderstandings generated by imprecise terminology and incomplete mathematical models. The dialogue published here will, I hope, generate continued discussion leading to new science and better insights.

Correspondence is closed; original papers within the scope of the *Journal of Applied Crystallography* are welcomed.

M. HART

Crystallographers

J. Appl. Cryst. (1983). **16**, 217

This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Professor **Sixten Abrahamsson** died on 13 January 1984, the day before his 54th birthday. Professor P. Kierkegaard writes that Abrahamsson was born in the province of Darlecarlia in Sweden. His university education was at Uppsala, where he received his doctor's degree in chemistry in 1959. In the same year he became docent in general and inorganic chemistry. He had started his research as a student of Professor Gunnar Hägg, who at that time had widened the scope of the crystallographic research at his Institute into the field of structures of inorganic molecules of biochemical interest. This was done in close cooperation with Professor Einar Stenhagen; and Abrahamsson's thesis, which concerned long branched-chain fatty acids, was an important part of that cooperation. One year's stay with Professor Dorothy Hodgkin at Oxford was of

great importance for his development as a scientist. In 1960 Abrahamsson followed Stenhagen, who a few years earlier had moved from Uppsala to Gothenburg, and in 1966 Abrahamsson was appointed by the Medical Research Council at the Faculty of Medicine of the University of Gothenburg to a personal chair in organic molecular structure research. In that position Abrahamsson was able to develop a small but very successful research group. Their work comprised structure-function studies of molecules with biological activity, with particular emphasis during the last years on the type of lipids found in biological membranes. Abrahamsson took a great interest in instrumentation and the use of computers as aids in crystallographic research. The development of his film scanner, described in 1966, was pioneer work in fast and accurate X-ray data collection. His competence in the field of computers was also widely utilized in areas outside science, particularly for hospitals and other medical applications. As a member of the IUCr's Commission on Crystallographic Computing from 1969 until 1975 and of the Commission on Crystallographic Apparatus from 1975 (its chairman from 1978), he initiated and substantially contributed to several projects of both Commissions. Sixten Abrahamsson was personally confident, helpful and a faithful friend, and he will be mourned and remembered by many friends, colleagues and students in Sweden and abroad.

George W. Brindley, Professor Emeritus of Mineral Sciences at the Pennsylvania State University, University Park, Pennsylvania died 23 October 1983 at the age of 78. He began his X-ray studies with the Bragg school at Manchester University, England, where he received an MSc in 1928. Leeds University awarded him a PhD in 1933. Professor R. E. Newnham writes that G. W. Brindley held various posts in the physics department at Leeds, becoming Reader in X-ray Physics in 1948. His research interests, until about 1945, were mainly in the scattering of X-rays by atoms and in metal line broadening caused by mechanical deformation and thermal vibration. James and Brindley scattering factors were used by crystallographers throughout the world for more than twenty years. Shortly after World War II, he took up the study of clay minerals and achieved an international reputation for his work on the structures of kaolinite, dickite, halloysite, serpentine, and chlorite. Later, he investigated the phase transformations in clays caused by thermal and chemical treatment and, more recently, the structural aspects of