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Comment on *A universal treatment of X-ray and neutron diffraction in crystals. I. Theory* by Hu (1997)

A. McL. Mathieson *at Chemistry Department, La Trobe University, Bundoora, Victoria 3083, Australia, and CSIRO Manufacturing, Science and Technology, Private Bag 33, Clayton South MDC, Victoria 3169, Australia. E-mail: gauit@lure.latrobe.edu.au*

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Abstract

The re-interpretation by Hu [*Acta Cryst.* (1997), A**53**, 484–492] of the data of Mathieson [*Acta Cryst.* (1975), A**31**, 769–774] is shown to be fallacious by reference to the subsequent experimental measurements on the same LiF boule by Mathieson [*Acta Cryst.* (1977), A**33**, 610–617]. It is pointed out that a match of theoretical values with a set of experimental values does not, of itself, establish the physical reality of the assumptions underlying the theoretical model.

In the mid 1970's, I carried out measurements of the intensity of Bragg reflections from the surface of an LiF crystal over a wide range of asymmetry. There were two sets of measurements, both with the same LiF boule, one set with the surface abraded (Mathieson, 1975) (= M1) and, subsequently, the other with the surface polished flat to within one optical fringe (Mathieson, 1977) (= M2). The two sets were dramatically different. For the first, the plot of normalized intensity *versus* asymmetry was concave downwards (see Fig. 6 in M1), *i.e.* the normalized intensity decreased progressively with increase in asymmetry. This trend was interpreted in terms of the absorptive surface layer. For the second, the corresponding plot was concave upwards (see Fig. 4 in M2), *i.e.* the normalized intensity increased progressively with increase in asymmetry. This trend was interpreted as due to the progressive reduction of the effect of extinction on intensity.

Recently, Hu (1997) has used the experimental data in M1 and, ignoring the existence of the surface layer, has analysed the LiF situation as a single-component system. Within this context, she has succeeded, with appropriate selection of parameters, in curve-fitting my data (see her Fig. 8) virtually as well as I did on the basis of the surface layer (see Fig. 5 in M1). According to her theoretical analysis, the deviation of the experimental points from curve (*a*) (the kimematical limit curve) in her Fig. 8 is due to '*multiple reflections and not to a surface layer*'. Under her interpretation, the effect of multiple reflection, *i.e.* extinction, is to reduce the diffracted intensity and this effect *increases* with increasing asymmetry.

This interpretation by Hu is completely at odds with my experimental results in M2 where there was no abraded surface layer. Fig. 4 in M2 shows the increase in normalized intensity with increasing asymmetry, which results from the 'decoupling of multiple diffraction, leading to *reduction* of extinction' (see M2, p. 616). This latter conclusion is in accord with the earlier theoretical treatment of Hirsch & Ramachandran (1950) and with the normalized presentation of their curves that I gave in M2.

It is evident that if one forces a model to fit a preconceived notion (in this case that there is no surface layer), then theory may provide parameters so that calculated values closely fit experimental values but the physical situation implied by the parameters is not compatible with reality.

References

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Response to Mathieson's (1998) comment on *A universal treatment of X-ray and neutron diffraction in crystals. I. Theory*

Hua-Chen Hu *at China Institute of Atomic Energy, PO Box 275(18), Beijing 102413, People's Republic of China. E-mail: ciaednp@sun.ihep.ac.cn*

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Abstract

There is an obvious difference between the behaviour of the dependence of the integrated reflection power ratio on the asymmetric parameter for plane crystals predicted by the H–D equations on mosaic crystals and that predicted by the theory of Hirsch & Ramachandran on perfect crystals. It is most important to get rid of the surface layer effect of the crystal sample as much as possible for the verification of such a difference by experiment. This paper is in response to the comment by Mathieson [*Acta Cryst.* (1998), A**54**, 251].

I did not include Mathieson's second experiment (Mathieson, 1977) (= M2) in my work (Hu, 1997) because he did not mention in any of his published articles that the sample with different cutting angle used in M2 was taken from the same