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Letter to the Editor

J. Appl. Cryst. (1986). **19**, 491

Errors in a recent critique of the Borie–Sparks method in diffuse scattering

Sir,

In a recent paper, Bubeck & Gerold (1986) have purported to report on the limitations of modern methods of analysis of diffuse scattering (Borie & Sparks, 1971; Georgopoulos & Cohen, 1977). In particular, they attempt to show that it is essential that a region close to the origin of reciprocal space be included if the effects due to chemical order and atomic displacements are to be properly separated. However, they have apparently misunderstood the analysis procedures.

They attempt to show this by synthesizing diffuse intensity along a line in reciprocal space, using an unrealistically large and very slowly decaying strain in Al around a Cu plane. In a real material this strain must oscillate but, be that as it may, they show that a very large Warren short-range parameter, α_0 , results, instead of the theoretical value of unity. (This is the area under the curves in their Figs. 2–6, excluding the region near $g=0$, which cannot be reached experimentally.) Why then are there several reported investigations in which the values are within a few percent of unity? The answer is quite simple. Bubeck & Gerold synthesize and analyze the intensity *only* along a line. This requires that they have data out to 600 or further to perform the separation, where size defects dominate and large errors can be expected in the separated intensity due to local order. Practitioners, however, make measurements in a restricted volume in reciprocal space, using symmetry to obtain the necessary regions for the separation.

In fact, the effects of atomic displacements on these techniques have already been thoroughly evaluated and discussed in the literature. It has been shown that there are indeed problems with the Borie–Sparks procedure when there is clustering and the displacements are

appreciable (Hayakawa, Bardhan & Cohen, 1975) but that this is not the case with the Georgopoulos–Cohen procedure (Georgopoulos & Cohen, 1977).

If the strains are enormous, a region close to the origin might be helpful, as the authors suggest, but if both transmission and reflection geometries are required, there can be many problems in sample preparation and in determining the absolute scale.

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