

LETTERS TO THE EDITOR

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About the diffuse absences and the diffuse planes due to the atomic size effect

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In a recent contribution, Butler, Withers & Welberry (1992) report the observation and explain the origin of a characteristic modulation of the diffuse intensity observed in the diffraction patterns of crystals of some disordered oxide alloys displaying an atomic size effect. This modulation consists of lines with no intensity passing through the diffraction spots, each flanked by two diffuse satellite lines with an excess of intensity; these lines are in fact the traces of reciprocal diffuse planes. In §4 of their paper, the authors, who explain this distribution by the lattice distortions resulting from the size effect, ask themselves the following question: 'Why then have diffuse absences of this kind, which are natural manifestations of these distortions, not been reported previously?'. However, this question is irrelevant, since a similar modulation has already been reported and explained in the same terms. Glas, Hénoc & Launois (1985) were the first to report the presence of pairs of satellite planes of diffuse intensity passing on each side of the spots (except 000) of the electron and X-ray diffraction patterns of $\text{In}_x\text{Ga}_{1-x}\text{As}$, a III-V pseudo-binary semiconducting alloy where In and Ga, whose covalent radii differ by about 14%, share without ordering the column III sublattice of the sphalerite structure. These planes are all normal to the direct-space $\langle 110 \rangle$ directions, which join the nearest neighbours on each sublattice, and persist at low temperature. The intensity in the planes is itself modulated, producing in particular characteristic 'double-corner' maxima near the spots in the diffraction patterns. Glas, Hénoc & Launois also reported that similar planes exist for $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$, but not for the $\text{Ga}_x\text{Al}_{1-x}\text{As}$ alloys, which are the only pseudo-binary III-V alloys without atomic size effect. More recently (Glas, 1989; Glas, Gors & Hénoc, 1990), we reported the observation of the same features in all the III-V alloys we examined by electron diffraction (except again $\text{Ga}_x\text{Al}_{1-x}\text{As}$) and we detailed

the tilting experiments revealing the planar nature of the diffuse intensity. In the same papers, we calculated the diffraction patterns of large three-dimensional simulated crystals of disordered $\text{In}_x\text{Ga}_{1-x}\text{As}$ and $\text{In}_x\text{Ga}_{1-x}\text{As}_y\text{P}_{1-y}$. These calculations took into account all the static atomic displacements from the sites of the average lattice resulting from the difference in size of the atoms sharing a common sublattice; the displacements were calculated by using a valence force field model. Note that Butler, Withers & Welberry (1992) simulate only two-dimensional crystals and that our model includes bond-angle distortions as well as preferred distances between pairs of atoms. Our calculations reproduced the satellite planes separated by a gap previously observed and the characteristic double-corner shape of the diffuse distribution around the $pq0$ spots with $|p| \neq |q|$. We concluded that these planes were due to 'the correlation, mainly along the $\langle 110 \rangle$ directions, of the atomic displacements produced in its vicinity by any atom of the mixed sublattice(s)'. The results of Butler, Withers & Welberry (1992) thus confirm our previously published results.

References

- BUTLER, B. D., WITHERS, R. L. & WELBERRY, T. R. (1992). *Acta Cryst.* **A48**, 737-746.
- GLAS, F. (1989). *Microscopy of Semiconducting Materials 1989*, Institute of Physics Conference Series No 100, edited by A. G. CULLIS & J. L. HUTCHISON, pp. 167-172. Bristol: Institute of Physics.
- GLAS, F., GORS, C. & HÉNOC, P. (1990). *Philos. Mag.* **B62**, 373-394.
- GLAS, F., HÉNOC, P. & LAUNOIS, H. (1985). *Microscopy of Semiconducting Materials 1985*, Institute of Physics Conference Series No. 76, edited by A. G. CULLIS & D. B. HOLT, pp. 251-256. Bristol: Adam Hilger.