Comment on "Structure of Rapidly Quenched Al-Mn"

In a recent Letter,[1] Bancel *et al.* presented high-resolution x-ray scattering data of icosahedral Al-Mn quasicrystals. In the analysis of their experiments, these authors assign Miller indices to the peaks, referring to six "fundamental" vectors in reciprocal space. By icosahedral symmetry, the directions of these vectors are essentially fixed; the lengths, however, are not uniquely determined by the scattering data.[1] In the following, we shall argue that it is appropriate to use a different set of fundamental vectors.

To make our point clear, we first compare with ordinary crystallography. Associated with any basis generating the Bravais lattice of a crystal, there is a unique dual basis in reciprocal space. Thus, knowledge of this basis of the reciprocal lattice yields immediately the size of a primitive unit cell in direct space.

For icosahedral quasicrystals, the situation is very similar. The general belief is[2-6] that these are composed of two kinds of rhombohedra which are arranged quasiperiodically. Such quasicrystals can be generated most elegantly by a projection method.[3-6] All rhombohedra are then projections of three-cells of a six-dimensional (6D) cubic lattice onto a suitably oriented 3D (physical) subspace. From this projection method it is very easy to derive the Fourier spectra.[4-7] If $\mathbf{q}$ is any lattice vector of the reciprocal 6D cubic lattice, and $\mathbf{q}=\mathbf{q}_{\parallel}+\mathbf{q}_{\perp}$ its decomposition into components parallel and orthogonal to the physical subspace, then there is a δ-function peak at $\mathbf{q}_{\parallel}$, and its intensity is related to $\mathbf{q}_{\perp}$: roughly, the smaller $\mathbf{q}_{\perp}$, the stronger the peak. Therefore, if $\{\hat{\mathbf{e}}_i\}$ are the projections of the six basis vectors of the 6D reciprocal lattice, the δ peaks are at positions $\mathbf{q}_{\parallel}=\sum m_i\hat{\mathbf{e}}_i$, $m_i\in\mathbf{Z}$, and it is most natural to choose $\{\hat{\mathbf{e}}_i\}$ as the set of fundamental vectors in reciprocal space. As in ordinary crystals, from $\{\hat{\mathbf{e}}_i\}$ one can recover the size of the cells in direct space. Here, we get $a=\pi/q_0$, where q_0 is the length of the fundamental vectors and a is the edge length of the cells in direct space. This differs by a factor of 2 from the corresponding relation for cubic crystals, which comes from the fact that there are two projections involved, giving both a factor of $\sqrt{2}$.[4]

The task now is to find a basis $\{\hat{\mathbf{e}}_i\}$ such that the calculated intensities of the peaks are compatible with the observed ones. In Ref. 1 the strongest peak was fitted to a fundamental vector. This is not compatible with the calculated intensities, however. Since the intensity of a peak is large for small $\mathbf{q}_{\perp}$, there are nonfundamental peaks that are much stronger than the fundamental ones. Our proposal is to identify the strongest peak (with frequency 2.896 Å^{-1}) with the vector $(2\bar{1}111\bar{1})$, where our Miller indices refer to a basis proportional to that of Ref. 1. This vector has length $(2+\sqrt{5})q_0$, and since $|\mathbf{q}_{\perp}|=(-2+\sqrt{5})q_0$ (see, e.g., Ref. 4) the corresponding peak is stronger than a fundamental one. Therefore, this choice is certainly more appropriate than the one of Bancel *et al.*[1] Indeed, the calculated intensities based on our indexing are all compatible with experiment, i.e., the relative strengths of the peaks agree qualitatively. Moreover, the length of the rhombohedral cells turns out to be $a=4.60$ Å, which seems to be a reasonable value (then, of course, each cell would contain several atoms). The indexing of Ref. 1, however, would lead to an unphysically small value $a=1.08$ Å. We also have looked for other possible indexing schemes, but did not find a satisfactory solution.

In conclusion, we have pointed out that by an appropriate indexing of the peaks it is possible to determine the size of the rhombohedral cells from the experimental data of Bancel *et al.*[1] This information is most important for the determination of the decoration of these cells with atoms.

We would like to thank H. U. Nissen and T. Ishimasa for helpful discussions.

Note added.—After submitting this Comment we became aware of two further references. Elser[8] also discusses the indexing problem and comes to the same conclusions. Portier *et al.*[9] also determine the lattice constant to be 4.6 Å.

F. Gähler and J. Rhyner
Theoretische Physik
Eidgenössische Technische Hochschule–Hönggerberg
CH-8093 Zürich, Switzerland

(Received 12 July 1985)
PACS numbers: 61.55.Hg, 61.50.Em

[1]P. A. Bancel *et al.*, Phys. Rev. Lett. **54**, 2422–2425 (1985).
[2]D. Levine and P. J. Steinhardt, Phys. Rev. Lett. **53**, 2477–2480 (1984).
[3]P. Kramer and R. Neri, Acta Crystallogr. A **40**, 580–587 (1984).
[4]V. Elser, Acta Crystallogr. A (to be published).
[5]M. Duneau and A. Katz, Phys. Rev. Lett. **54**, 2688–2691 (1985).
[6]P. A. Kalugin, A. Yu. Kitaev, and L. S. Levitov, Pis'ma Zh. Eksp. Teor. Fiz. **41**, 119–121 (1985) [JETP Lett. **41**, 145–149 (1985)].
[7]R. K. P. Zia and W. J. Dallas, J. Phys. A **18**, L341–L345 (1985).
[8]V. Elser, Phys. Rev. B **32**, 4892 (1985).
[9]R. Portier, D. Shechtman, D. Gratias, and J. W. Cahn, J. Microsc. Spectrosc. Electron. **10**, 107–116 (1985).

