Letters

Icosahedral Symmetry

In his recent article "Icosahedral solids: A new phase of matter?" (27 Nov., p. 1242), Paul J. Steinhardt includes a section entitled "The case against conventional crystallography," in which he presents several arguments to support his contention that the evidence rules out the models of the so-called icosahedral quasicrystals of $MnAl_6$ and many other intermetallic compounds as icosahedral twins of conventional crystals. These include my own model (*1*), which was based on a cubic 820-atom crystal with eight icosahedral 104-atom clusters at the β-tungsten positions in the cubic unit of structure. I believe that Steinhardt's arguments are invalid.

With my model (*1*) the cubic crystals are so oriented with respect to a fivefold axis of the icosahedral quasicrystal grain that only *hh*0 primary reflections would occur on the fivefold-axis electron-diffraction photographs, with possibly a few other planes adventitiously in orientations permitting primary diffraction. I suggested (*1*) that some of the spots on the photographs are produced by double diffraction. Steinhardt states that double diffraction does not occur to any significant extent with x-rays and that "these peaks have been clearly observed in several independent powder x-ray experiments. . . . As a result, the specific models proposed thus far by Pauling have been ruled out."

I believe this conclusion is based on the fallacious assumption, as expressed by Steinhardt, that "Any peaks added by multiple electron scattering should not be found with x-rays." The presence or absence of an electron, x-ray, or neutron diffraction maximum (a peak) depends not only on the structure factor of the plane but also on the technique. Failure of a plane to produce a peak or spot is usually the result of a geometrical relation between the incident beam and the plane such that the Laue-Bragg conditions for diffraction are not satisfied. With monochromatic radiation and a stationary crystal in an arbitrary orientation, no plane can be expected to diffract. In the original Bragg technique and in the various rotating-crystal techniques, the crystal rotates into orientations satisfying the diffraction conditions. With my model of icosahedral twinning, the cubic crystallites are oriented to permit primary *hh*0 diffraction, and with my model of decagonal twinning they are oriented to permit all *hk*0 to show primary diffraction, giving a fivefold-axis electron-diffraction photograph with many more spots (*1*). In the case of powder photography, there are for each plane some minute crystals with the proper orientation to permit diffraction, and accordingly peaks can occur that are ruled out for the stationary-crystal technique.

I shall not discuss Steinhardt's other arguments against the twinning model except to say that in my opinion they are all invalid. I have discussed some of them in other papers, mainly not yet published (*2*).

On the other hand, there is an increasing body of evidence supporting the twinning model. For example, the icosahedral quasicrystal Al_6CuLi_3 gives a fivefold-axis electron-diffraction pattern like that of $MnAl_6$, but with a shrinkage in scale by 10%. I have analyzed the x-ray precession photographs of this substance and have found that the cubic unit of structure is larger than that of $MnAl_6$, with 1088 atoms, eight 136-atom icosahedral clusters, in the β-tungsten positions in place of the eight 104-atom clusters of $MnAl_6$. Also, I have found for decagonal Mn_2Al_7, Fe_2Al_7, and $(Mn_{0.7}Fe_{0.3})_2Al_7$ an orthorhombic unit with $a = 32.86$ Å, $b = 31.23$ Å, and $c = 24.80$ Å containing 16 104-atom icosahedral clusters in positions slightly distorted from those for $MnAl_6$. I have also found tetragonal structures for octagonal quasicrystals.

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REFERENCES AND NOTES

1. L. Pauling, *Phys. Rev. Lett.* **58**, 365 (1987).
2. ——, *ibid.*, p. 2120. In this paper the shift in positions of the spots is discussed.

Response: A viable multiple twinning model must explain the diffraction peaks observed in icosahedral solids in terms of the diffraction peaks of the twin crystallites. For any given model, the peaks can be divided into two classes. "Primary" peaks are ones that also appear in the diffraction patterns of one or more of the individual crystallites (*1*). "Secondary" peaks do not appear in the pattern of any one crystallite; they are only observed if there is multiple scattering (also called double diffraction) from two or more crystallites in succession.

Many multiple twinning models, including Pauling's, explain the peaks observed in electron diffraction from icosahedral alloys as a combination of primary and secondary peaks. A test for multiple scattering is to replace electron diffraction experiments from a single grain with x-ray diffraction from a powder containing many small grains. The glib explanation given in my article is that significant multiple scattering is not expected in powder x-ray experiments because x-rays scatter much more weakly than electrons. "Yet, the peaks have been clearly observed in several independent powder x-ray experiments." This represents a serious blow for multiple twinning models. Although the approach is a conventional one for crystallographers, such a compact statement does not include the full logic of the argument. Since Pauling suspects that the argument is fallacious, I welcome the opportunity to discuss the issue in further detail.

The key features that distinguish powder x-ray from electron diffraction experiments are (i) in powder experiments, the scattering is from many small (1 to 10 micrometers in diameter), randomly oriented grains, whereas the scattering is typically from just one grain in electron diffraction; and (ii) the x-ray scattering length (*2*) is comparable to the entire sample thickness—orders of magnitude greater than the dimensions of a single grain—whereas the electron scattering length is less than the dimensions of a single grain. Primary peaks in powder x-ray diffraction come from the sum of the scattering from the individual grains. Because of the weak scattering of x-rays, the probability of scattering from any one grain is small; but there are many grains in the sample.

Multiple scattering contributions to secondary peaks are highly suppressed. First, the probability of multiple scattering within any single grain is extremely small because the grain size is small compared with the x-ray scattering length. Second, the probability of multiple scattering between two fortuitously oriented grains in the pulverized sample is not only small; but, if one averages over all possible relative orientations and positions of the grains, the sum over all multiple scatterings produces a smeared out "diffuse background" rather than a sharp secondary peak.

According to the quasicrystal model, all of the peaks observed in electron diffraction are primary peaks and should also be observed in a powder x-ray diffraction pattern with sufficient sensitivity. According to multiple twinning models like Pauling's, some peaks are secondary and, hence, should be greatly suppressed in amplitude in powder x-ray experiments. In the specific model of Pauling, the primary and secondary peaks are clearly delineated.

The experimental results for icosahedral solids are very clear, even more decisive than I described in my article. The electron diffraction peaks predicted to be secondary are unambiguously observed in powder x-ray experiments. In fact, they are significantly more intense than the peaks predicted as being primary in multiple twinning models. While, in principle, dynamical interference effects can produce enhancements of secondary peaks in large single crystals of some materials, it is very difficult to explain why such an effect is observed in powder samples from a wide variety of icosahedral alloys prepared by many different methods. It is much more natural to conclude that all of the peaks are primary as the icosahedral quasicrystal model predicts.

I should emphasize that, while Pauling's model requires some of the observed peaks to be secondary, other multiple twinning models utilizing larger unit cells may not have this requirement. I refer the reader to the original article for a description of other experimental evidence against generic twinning models. Also, I disagree with Pauling's statement concerning further evidence in favor of twinning. The evidence that he cites does not distinguish between the models, since it is equally consistent with a larger crystal unit cell or a larger quasicrystal unit cell.

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NOTES

1. Multiple scattering may contribute to the observed intensity of primary peaks, but the peaks would have nonzero intensity even in the absence of multiple scattering.
2. The scattering length is the distance over which half of the x-rays are coherently, elastically scattered out of the primary beam.

Technology Transfer

While I would agree with James Johnson (Letters, 29 Jan., p. 450) that "technology transfer" has been the subject of much faddism both inside and outside universities and it often is misidentified, particularly by politicians, as the magic bullet to solve all our industrial competitiveness problems, I must disagree with his assessment that major research universities should not play a role.

First, universities have always been the source of the most fundamental form of technology transfer—the education of students, both full and part time, who move their knowledge directly into business and industry. After all, technology is not a thing to be packaged and sent as an industrial CARE package. To quote Robert H. Waterman, Jr., "Technology is housed in the skills of people" (*1*).

Second, while perhaps there was a time when universities did basic research and industry did the applied research and development, we now find that in most areas of research this distinction just does not work. Industry now knows that the economic half-life of a new technology in the marketplace is so short it cannot just wait for the thorough but slowly revealed university research. This is one reason why university-industry collaborative research continues to grow in popularity. Of course this is also "technology transfer."

Finally, it is recognized that attempts to provide active technology transfer from university to industry can be somewhat of a failure if incorrectly organized. In our industry-driven program, as is true in a number of others around the country established by major research universities, we have a team of "impedance matchers" to work directly with industry to provide the needed one-on-one approach. These regionally located technology consultants are all "degreed" engineers with substantial industrial experience. It is their job to understand each company's needs and apply the proper resources, be it their own knowledge, that of university faculty, that of a university facility, or even that of an outside resource. We have found the vast majority of our faculty very willing to participate in this stimulating effort, even without salary incentives; and they are directly involved in close to 50% of our assistance efforts.

I certainly do not suggest that university research should just dance to industry's tune, but in today's environment a research university that ignores industrial interfaces will sooner or later find itself inconsequential to its community.

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REFERENCES

1. R. H. Waterman, Jr., in R. N. Foster, *Innovation: The Attacker's Advantage* (Summit, New York, 1986), p. 17.

Erratum: The last sentence of the fourth paragraph of Devra Lee Davis' letter "Paleolithic diet, evolution, and carcinogens" (18 Dec., p. 1663) contained errors. It should have read, "Moreover, the range of early diets was extensive, from protein-rich diets of far northern peoples to the plant-dependent diets of the Kalahari hunters and gatherers."

Erratum: In the report "Stimulation of heterotrophic microplankton production by resuspended marine sediments" by Sam C. Wainright (18 Dec., p. 1710), two articles should not have been included in reference 2. These are G. T. Rowe, C. H. Clifford, K. L. Smith, Jr., P. L. Hamilton, *Nature (London)* **255**, 215 (1975) and S. W. Nixon, C. A. Oviatt, S. S. Hale, in *The Role of Terrestrial and Aquatic Organisms in Decomposition Processes*, J. M. Anderson and A. MacFadyen, Eds. (Blackwell, Oxford, England, 1976), pp. 269–283.