Distinguishing a Quasicrystal from an Icosahedral Glass Via Lattice Imaging

Two leading models for the structure of the icosahedral phase of Al-Mn (*i*-Al-Mn)[1] are the icosahedral quasicrystal[2] (IQ) and the icosahedral glass[3] (IG). The diffraction patterns of both models agree closely with the electron-diffraction and x-ray powder patterns of *i*-Al-Mn. The observation of finite peak widths (~200–500 Å) in the powder patterns can be explained as being due to either the short-range positional order in an IG or quenched phason strains in an IQ.[4]

In spite of their similarities, the two models should be distinguishable through high-resolution lattice imaging (HRLI). First, the IG model requires rather large packing units (diameter ~10–20 Å), resolvable with HRLI, in order to obtain a diffraction pattern consistent with that of *i*-Al-Mn.[3] Second, although the locations and relative amplitudes of the most intense diffraction peaks are similar in the two models, the detailed variation of the intensities and phases across the individual peaks and from peak to peak differs and results in distinguishable HRLI. (The difference is consistent with the fact that the IG can be viewed as an IQ which is highly disordered via quenched random phason strains.[4]) We have run a series of numerical experiments comparing a 3D IG composed of icosahedra packed vertex to vertex[3] with the 3D IQ rhombohedral packing.[2] Fourier transformation of very similar sets of peaks including their phases in the two models leads to clearly distinguishable images (see Fig. 1). Significant disorder is observed in the IG over the scale of just a few icosahedra. Imaging different sets of peaks, introducing a cutoff in the diffraction peak intensities, and changing the resolution of the Fourier transform has produced similar results. Although atomic decoration of the packing units and the filling of gaps in the IG model will change details, the disorder will remain.

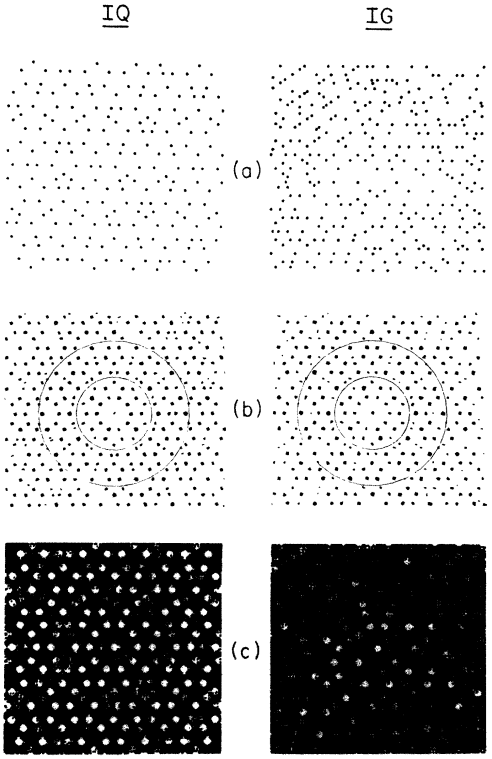

FIG. 1. Comparison of lattice imaging in IQ (left column) and IG (right column). (a) View along fivefold symmetry axis through thickness of ~9–10 icosahedra (~200 Å). Dots represent centers of icosahedra which are treated as identical point scatterers. IQ appears less dense because many icosahedra are stacked directly on top of one another. (b) Diffraction pattern along fivefold axis. An annulus of selected peaks is indicated. Note the close similarity. (Peak shapes are distorted because of the finite pixel size.) (c) Imaging from peaks in the annulus shown in (a). White represents high density.

HRLI obtained by various groups from grains of *i*-Al-Mn does not show disorder on such a short scale.[5] (Instead, much longer-wavelength phason strains are observed.[4]) This is consistent with the IQ model. To salvage the IG model one needs either larger packing units or new rules to enforce longer-range correlations between units (thus making the model closer to the IQ).

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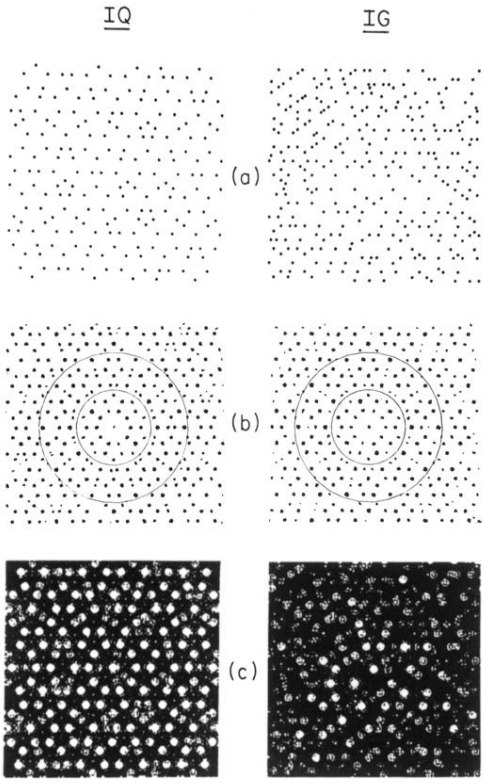
[5]See, for example, K. Hiraga *et al.*, Sci. Rep. Res. Inst. Tohoku Univ. Ser. A **32**, 309 (1985).



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