
For the description of chemical ordering in models of metallic glass alloys, or for following local order changes on annealing, sensitive three-dimensional structural characterisation methods are necessary. We discuss here the merits or otherwise of three proposed methods.

(1) In the Voronoi polyhedron construction, the volume occupied by an N-atom model is partitioned into N non-arbitrary polyhedra, each containing all points in space closer to a given atom centre than to any other. The occurrence of certain polyhedron types has been used in discussing the validity of icosahedral models of single-component glasses (eg Barker et al, Nature 257, 1200(1975)) and to identify crystalline nuclei (Tanemura et al, Prog. Theor. Phys. 58, 1079(1977)). However, there is uncertainty in relating a given polyhedron type to a familiar real space structure, although the reverse procedure (real cluster to polyhedron) is fairly clear. Using an interactive computer graphics system, we have examined visually the polyhedra occurring in random packing glass models, and the changes in polyhedron topology consequent upon certain real space distortions followed. Some of the ambiguities observed in currently-made Voronoi real space identifications will be presented.

(2) The Radical Plane Polyhedron. As the Voronoi construction places dividing planes midway between atom centres, its application to assemblies of different-sized atoms results in dividing planes that intersect the bounding surfaces of the larger atoms. Too much volume is thereby allocated to the smaller component, too little to the larger and the polyhedron topology is liable to distortion. This problem is completely overcome by generalising the Voronoi procedure: the resulting radical plane construction (Fisher et al, Neues Jahrb. Min. Monat. 227(1971)) places the dividing plane in a position which takes account of the different radii yet remains rigorous. For touching or overlapping atoms, the plane is the common tangent and common chord respectively. Applications of the method to differently-constructed models of amorphous PdSi (Gaskell, J. Non-cryst. Sol. 32, 207(1979)) and FeB (Boudreaux and Gregor, J. Appl. Phys. 48, 5057(1979)) will be described.

(3) Interaction Correlation Functions. Bernal (Proc. Roy. Soc. A284, 285(1964)) identified two types of "canonical hole" in hard sphere random packing: of these, the tetrahedron and octahedron were dominant (75% by volume). In relaxed soft sphere models, however, the three other polyhedra are squeezed out, and it becomes possible to describe the assembly in terms of a packing of (distorted) tetrahedral and octahedral building blocks. A close-packed crystal structure can be described also as an assembly of the same building blocks, although more perfect and arranged in a regular, periodic manner. Thus if we regard the soft sphere random packing as an idealised glass, the possibility arises of a unified description of both non-crystalline and crystalline packed structures. Two aspects of such a possible description are discussed. First, partial correlation functions between like and unlike interstices indicate how the two types of building block are arranged in different glass models. Secondly, the power of a description of local ordering in terms of the arrangement of interstices about atom centres is compared to the much less sensitive Voronoi polyhedron approach.