analysis can be formulated with a separate dimension for temperature with no consequent error in the solution[15].

FRANCIS COLLINS
E. R. BROWNSCOMBE

Atlantic Richfield Co.,
Dallas, Texas.

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Fine Structure in the Radial Distribution Function from a Random Packing of Spheres

EARLIER, we reported[1] the radial distribution function from a random packing of spheres covering the range of sphere separations from 1·0 to 1·3 diameters. Inspection of the data indicated some possible fine structure in the distribution function. The results supplemented those of Bernal[2] and Scott[3] which covered a far larger separation range.

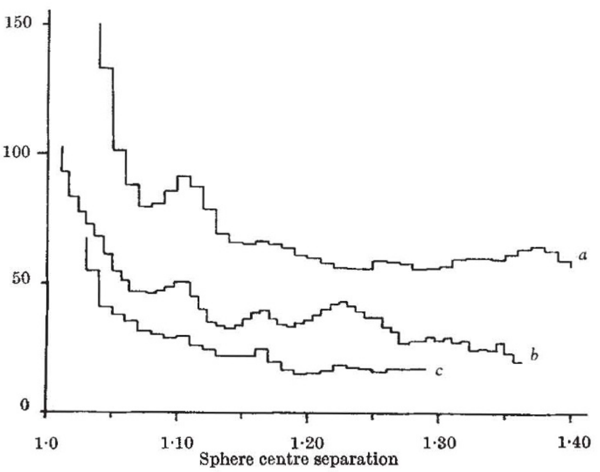

Fig. 1. Radial distribution function histograms. *a*, Scott; *b*, Mason and Clark; *c*, Bernal.

The data were processed by taking two successive running three-fold averages over the original histogram of the radial distribution function. The original co-ordinates of Scott were brought to the same form and together with Bernal's results were subjected to a similar averaging treatment. The three sets of results are shown in Fig. 1. The "number of pairs" varies as the total number of spheres in the packing and the width of the histogram columns. To avoid confusion between the results, they have not been normalized. Three possible peaks appear at separations of 1·105, 1·165 and 1·225 diameters. The peak at 1·225 diameters is apparently shifted on the results of Scott. This structure may be explained by the existence of certain arrays of spheres in the packing. For example, if a unit of seven spheres is considered, five of which form a ring around the equator of two touching spheres, a small gap must exist between two spheres of the ring (Fig. 2*a* and *b*, 5–6). The sphere centre separation of this gap has been calculated as $\frac{4\sqrt{2}}{3\sqrt{3}} = 1{\cdot}0886\ldots$ diameters.

If another ring of five spheres is added to this first ring such that each sphere touches two adjacent spheres of the ring as well as one of the central pair, then five gaps are observed between these added spheres. Three of the gaps can be shown to be caused by a sphere centre separation of 1·0886 diameters (Fig. 2*c*, 12–8, 8–9 and 9–10), but the other two are greater. They are larger because one member of the new ring occupies a site above the original small gap and is therefore slightly below the plane of the other four new spheres. The sphere centre separation for these larger gaps can be shown to be $\frac{5}{\sqrt{19}} = 1{\cdot}14707$ ... diameters (Fig. 2*c*, 10–11 and 11–12).

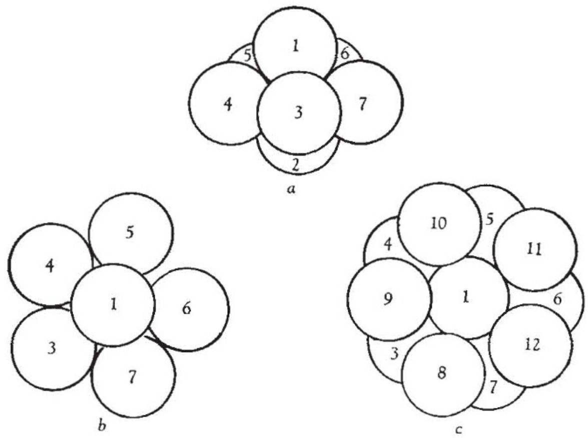

Fig. 2. Configurations containing small gaps.

These separations agree approximately with the first two small peaks of Fig. 1, but both are smaller than the actual separation peaks. It requires at least seven spheres and fifteen contacts to form the smallest gap. If one small separation is introduced somewhere in the fifteen contacts, then it is found that in five cases the 1·0866 diameters separation is reduced whereas in ten cases it is increased.

For the 1·14707 diameter separation it requires at least nine spheres and twenty-one contacts to form a configuration where the separation is possible. If each of these contacts is opened in turn it is found that five have little effect, six close the separation and ten open it. A rigorous reasoning is more difficult than in the first case because there are two 1·14707 separations in the new layers but in general a small gap introduced into the structure appears more liable to open the two main separations than to close them.

Gaps of 1·14707 could propagate still larger gaps in a similar manner which might account for the possible peak at 1·225 diameters.

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G. MASON
W. CLARK

School of Physics,
Bristol College of Science and Technology.

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