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A Hard-Disc System: Structures of a Close-Packed Thin Layer*

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Abstract

The possible structural transitions between n and $(n-1)$ thin layers of hard discs are considered. The apparently obvious homogeneous transition postulated on the basis of $n = 2$ is shown by an analogue experiment not to be the general solution. It is argued that the maximum density is retained by a 'Δ-form' transition which minimizes the density deficit at the boundary walls, and can be referred to different sections of a two-dimensional close packing.

Close-packed structures have been extensively studied over many years, both for their intrinsic geometrical interest, and as models of real crystalline and non-crystalline systems (Rogers, 1958; Bernal, 1964; Finney, 1971*a*,*b*, 1977). The effects of the boundary are frequently significant, either as artefacts to be removed (Finney, 1971*a*; Bernal, 1964) or as an essential aspect of the system to be modelled, *e.g.* the crystal–melt interface (Visscher & Bolsterli, 1972; Bonissent & Mutaftschiev, 1977; Bonissent, Finney & Mutaftschiev, 1977).

In two dimensions, the perfect triangular lattice has been proved (Fejes Tóth, 1963; Coxeter, 1961) to be the densest possible structure for an infinite ($\infty \times \infty$) hard-disc assembly. The theorem is, however, not valid in the case of a thin layer, where the non-negligible influence of the limiting walls must be taken into account. We consider here the peculiar case of a thin layer of hard discs contained between two infinite, flat, hard walls.

We formulate the problem as follows. Let D be the separation of two infinite hard walls as shown in Fig. 1. Let σ be the diameter of hard discs, which are to be packed within the box (to simplify the notation we put $\sigma = 1$). We now ask the question: what is the densest structure achievable throughout the whole range of thickness $1 \le D < \infty$?

The lower limit of $D = 1$ is essentially trivial, the densest structure being a close-packed row of discs (Fig. 2*a*). In addition to this being the densest packing in one dimension, it can be usefully thought of as a section of a maximum-density two-dimensional hexagonal close-packed structure taken parallel to the 10 'plane' (line). Similarly, for $D = (1 + \sqrt{3}/2)$ we would expect the solution to be that shown in Fig. 2(*b*). This is obtained by a parallel deposition of a second close-packed row of discs and is again a section of the hexagonal lattice cut parallel to 10, but of thickness $(1 + \sqrt{3}/2)$. Extending to greater thicknesses, there exists a set of discrete values of D,

$$D_o(n) = 1 + (n-1)\sqrt{3}/2, \quad n \ge 1, \qquad (1)$$

for which the box can be filled with strips of the perfect triangular lattice. The density ρ^* of such a structure, defined as the ratio of the area covered by the discs to the area occupied by the layer, depends on the number of rows and is given by

$$\rho_o^*(n) = \frac{\pi}{4} \frac{n}{1 + (n-1)\sqrt{3}/2}, \quad n \ge 1, \qquad (2)$$

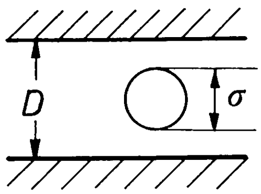

Fig. 1. Geometry of the thin layer.

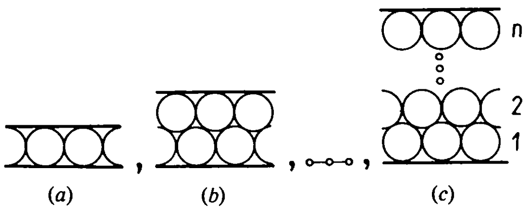

Fig. 2. Close-packed structures occurring at $D = 1 + (n-1)\sqrt{3}/2$.

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which in the limit $n \to \infty$ reaches the expected value $\pi\sqrt{3}/6$ characteristic of the perfect ($\infty \times \infty$) triangular lattice.

Equations (1) and (2) define a set of points in the ($\rho^* - D$) plane, marked as heavy dots in Figs. 3 and 5. We now require to examine the possibility of connecting these points in a continuous way for intermediate values of D. One approach is to consider possible deformations of the above-described simple structures as D is changed. We start with the simplest cases and by induction try to extend to more complex ones, with interesting results.

Compression of the two-row dense structure occurring at $D_o(2)$ (A_1 in Fig. 3) normal to the two infinite walls leads inevitably through a density minimum (B_1) to the row structure C_1. This deformation meets the required condition of density continuity, and connects the $D_o(2)$ and $D_o(1)$ solutions. We note also that the structure B_1 (occurring close to the minimum-density point) can be considered as a thin section of thickness $(1 + 1/\sqrt{2})$ cut from a square primitive packing parallel to the 11 line, removing all discs intersected by the walls.

When considering the apparently analogous deformation of the perfect three-row layer (A_2 in Fig. 3), we come to difficulties. Again the structure passes through the low-density square lattice section at B_2, but *ceases to exist below* $D = 2$, where it reaches its metastable final state (C_2 in Fig. 3). This state is also related to the two-dimensional infinite closest packing being a section of thickness 2, cut parallel to the 11 line. The orientation is, however, unfavourable for a high density, a relatively large area being left empty upon removal of those discs intersecting the walls.

Similar difficulties arise when considering analogous deformations of higher-row structures. Moreover, the behaviours of even- and odd-row structures appear rather different and, for $n > 3$, $D_o(n-1)$ appears inaccessible from $D_o(n)$.

Thus, apart from the special case of $D_o(2) \to D_o(1)$, these homogeneous deformations through a square lattice section appear not to provide satisfactory solutions.

An unexpected alternative is provided by a very simple analogue experiment in which a set of ball bearings placed on a flat surface is pressed between two parallel rulers. Instead of the homogeneous deformation discussed above, the layer transforms into a structure made up of regions of densely packed triangular lattice (Fig. 4) which slide past each other until a new $(n-1)$-row perfect triangular lattice section is formed at $D_o(n-1)$.

The density of such a 'Δ-form' structure is given in general by

$$\rho^*(n, D) = \frac{\pi}{8}\,\frac{n(n-1)}{D\left\{\dfrac{n-2}{2} + [1 - |D - 1 - (n-1)\sqrt{3}/2|^2]^{1/2}\right\}}, \quad (3)$$

where $D \in [D_o(n-1), D_o(n)]$ for $n > 2$. The density thickness variation is shown in Fig. 5. This experimentally observed Δ-form structure fulfils our requirement of continuity and is consistent with the discrete solutions at $D_o(n)$. Its density is also higher than that of the postulated homogeneous deformations.

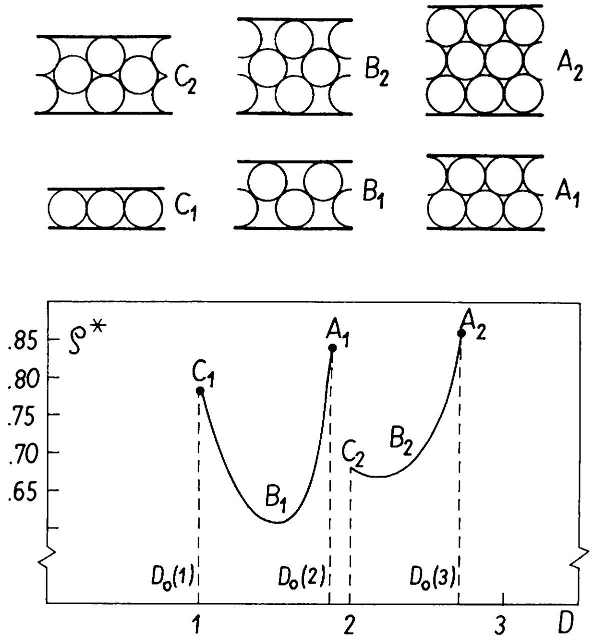

Fig. 3. Postulated homogeneous deformation and its density.

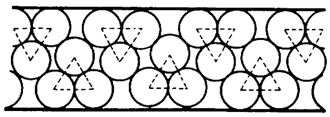
Fig. 4. Schematic view of the Δ form.

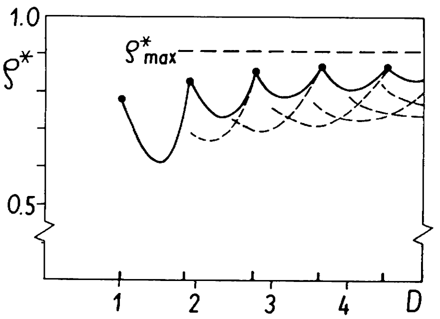

Fig. 5. Density of the Δ form (solid line). For comparison the density of the homogeneous deformation is also plotted (broken line).

We have been unable to prove to our satisfaction that the Δ form provides the maximum-density structure for intermediate values of D. The theory of packing in two dimensions is insufficiently advanced to be able to assert rigorously that some other – perhaps more homogeneous – structure *not containing close-packed regions* cannot be found with a density greater than the minimum observed during the $D_o(n) \rightarrow D_o(n-1)$ transition, although considering the much lower minimum density through which the simple homogeneous deformation passes (Figs. 3 and 5), the existence of such a structure appears very unlikely. Restricting ourselves to a mechanism involving the slippage of close-packed regions, however, the Δ form appears to fulfil the condition of maximum density during the transition. The domains of close-packed structure in each Δ form are the maximum possible for a transformation from $D_o(n) \rightarrow D_o(n-1)$ which also provide the minimum degree of mismatch at the domain edges, and which thus give a maximum density in the intermediate region. The total length of the fault line should be a minimum, and allow regular slippage; this rules out irregular routes for the fault line, which would either open up large gaps (possibly full vacancies) or lock the transitional structure in an intermediate position.

We can now reassess the previous discussion of the homogeneous deformation with interesting results. Referring again to Fig. 3, it becomes clear that for $D_o(2) \rightarrow D_o(1)$ the homogeneous deformation and Δ-form structures are identical. Thus, for $D_o(3) \rightarrow D_o(2)$, the Δ form might be considered as a homogeneous deformation of the *largest close-packed domains which the transformation can accommodate*. The width of the largest close-packed domain is evidently identical to $D_o(n-1)$.

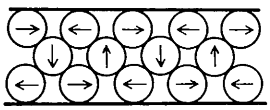

Fig. 6. Collective movement leading from the homogeneous to the Δ form.

Further consideration of the homogeneous deformation demonstrates it to be unstable (at least in the early stage of its development) when subjected to the specific cooperative movement shown in Fig. 6 which transforms the homogeneous form into the Δ structure of higher density.

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