The 'Atomix': a teaching model of atomic structures in solids and liquids

by W. A. Miller and G. C. Weatherly

The *Atomix* * (pronounced atom-mix rather than atomics), is both a fascinating toy and a remarkably good dynamic model of atomic arrangements in simple materials. It consists of a 127 mm (5 in.) square acrylic moulding 25·4mm thick, containing a shallow square-well inset of precise depth. The well contains 6000 × 1mm diameter ball bearings which can be made to move quite dramatically by tilting, tapping, rotating or vibrating the tray, causing the 'atoms' to assume some interesting close-packed structures (Fig. 1). The device was designed by a Montreal artist who was intrigued by the aesthetics of its geometrical patterns and by its link with science as well as art. Its intrinsic interest to materials scientists in addition to its potential value as a teaching aid has prompted the writing of this article. We outline briefly below some of the more obvious applications of this model.

Crystalline close packing

When oriented such that the well containing the ball bearings is in a vertical plane, the spheres assume positions of planar close packing in response to gravity. The *Atomix* is of course useful to compliment the classical Bragg-Nye soap bubble model: although both models exhibit many of the same features, the *Atomix*, for example, is unsuited at present to show interstitial or substitutional impurities, while it is somewhat superior to the soap bubble model in demonstrating rapid atomic motion and in its simplicity and portability. The model readily displays grain boundaries, triple junctions, and after shaking, the phenomena of recrystallisation and grain growth. Careful rotary manipulation of the device to cause slow growth can result in the formation of a single 'crystal' (Fig. 2).

The 'crystals' almost always contain defects, some of which represent defects in real crystals quite nicely, (see Fig. 1 and 2). Vacancies are most common, although di-, tri- and other vacancy clusters are also observed, some of which are stable, while others either collapse or, with suitable manipulation, migrate to the free surface. Single vacancies on the other hand are completely stable. Isolated edge dislocations are rare, but they are sometimes observed to be associated with stacking faults which occur frequently (see the upper right hand corner of Fig. 1).

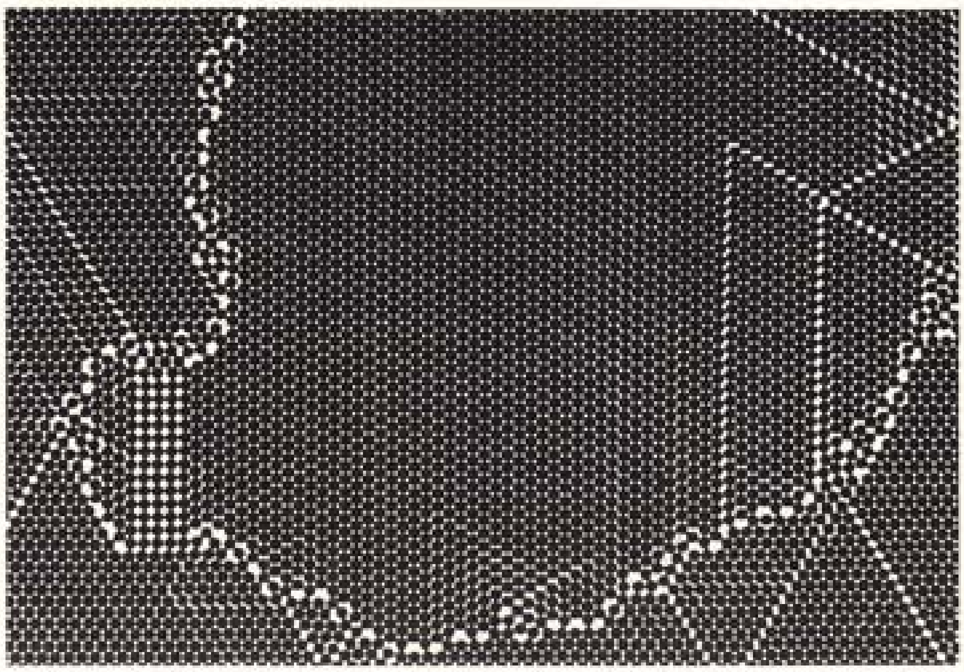
Square packing and stacking faults

'Crystals' are nucleated by the flat edges of the well, but these edges are separated by angles of 90° in comparison to the 60° angles between the close packed directions of a stable single crystal. The model often accommodates this orientation difference with stacking faults in preference to grain boundaries (Fig. 2), the faults consisting of a layer of AA stacking within an AB grain (one also finds faults in which the stacking sequence is not AA or AB but exhibits some intermediate arrangement). Light tapping of the container causes these faults to move very rapidly, generally at a rate which is too fast to permit detailed atom movements to be observed. The stacking faults often terminate within a grain at a dislocation or at other intersecting faults (Fig. 1). The atomic configuration at such faults is best observed by slowly tilting the model toward the horizontal plane and viewing along the rows of 'atoms'.

The AA stacking sequence is often extended, resulting in a 'grain' which has a square packing arrangement (Fig. 1). This 'simple cubic phase' is often found near the free surface and is thought to be associated with the repulsion between spheres in consequence of electrostatic charges developed between the ball bearings and the plastic container. The static electricity can also stabilise an extensive vapour phase (Fig. 2) —when the model has not been used for a prolonged period this effect is not pronounced, however it can be accentuated by vigorous shaking for several seconds before 'growing a crystal'.

Liquids

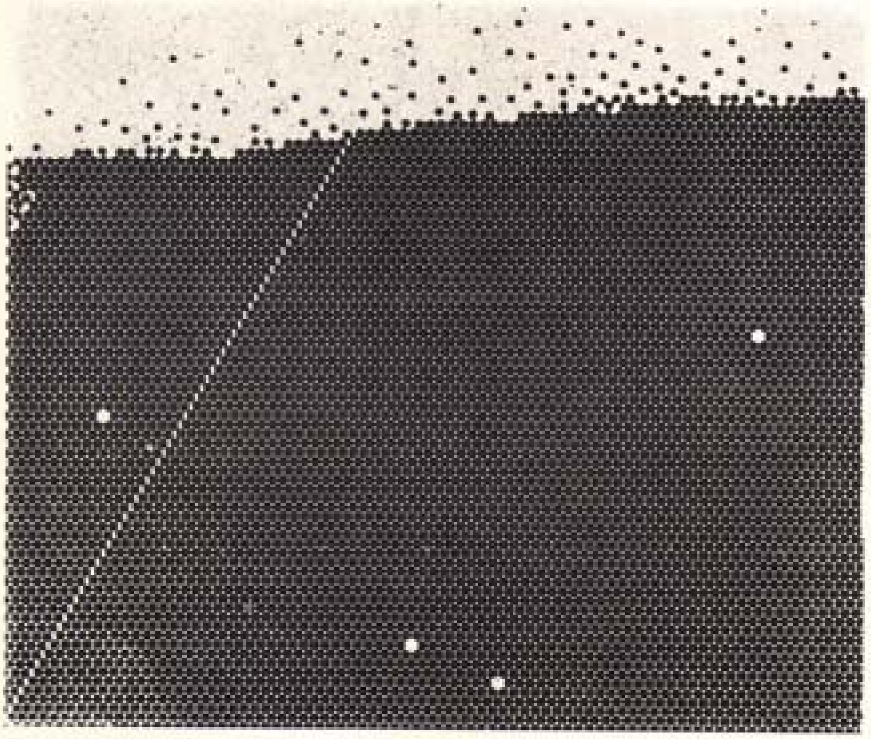
The *Atomix* can be used to demonstrate the Bernal model of simple liquids, *ie*. an irregular close-packing of spheres. To do this, the model is used in the horizontal plane and the spheres are made to occupy the central region of the well, away from its



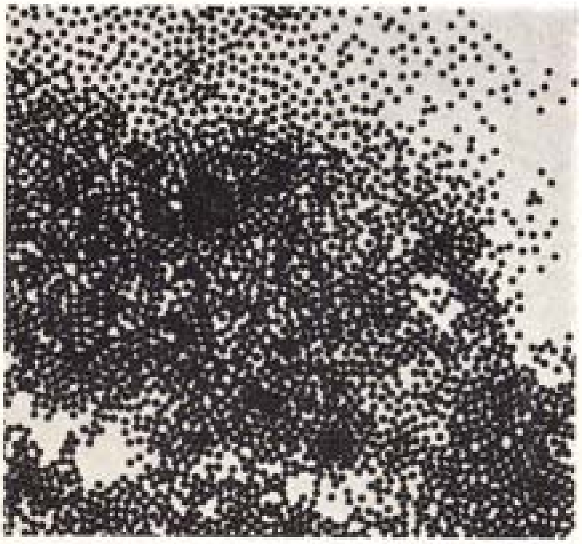
1 A packing pattern showing grain boundaries, stacking faults and interphase boundaries. The non-spherical appearance of the atoms results from shadows cast in photography.

* Trademark of Emotion Productions Inc., Montreal, Canada; designed by Francois Dallegret.

The authors are with the Department of Metallurgy and Materials Science, University of Toronto.



2 A single crystalline packing containing only one stacking fault (which originates at a corner of the well) and four vacancies.



3 A loosely packed configuration which represents a crystal melting. The flat well bottom makes it difficult to 'melt' the solid completely without forming an excessively loosely packed liquid.

flat edges (see Fig. 3). This effect is best demonstrated after the model has been left stationary for some time, because the electrostatic repulsion between the spheres prevents close packing. Electrostatic attraction between the container and the spheres also has a disruptive effect on the simulated liquid, in that the balls become stuck to the flat edges which can then stimulate rapid crystal growth. Liquid structures commonly display five-fold co-ordination in the horizontal plane, and are most readily observed by using the model over a light box.

Interfaces

The model is also useful for demonstrating the structure and some of the properties of a variety of interfaces. We have previously referred to grain boundaries, stacking faults and interphase boundaries, but it is also worth mentioning that solid-vapour and solid-liquid interfaces can be represented strikingly. With the model in the vertical position, the free surface becomes a solid-vapour interface. The 'vapour pressure' can be controlled to some extent by varying the electrostatic charge. If the model is slowly rotated about a horizontal axis, the role of steps at faceted interfaces in either crystal growth or dissolution becomes obvious (see the interface in Fig. 2). Rapid motion across the interface during rotation, accompanied by many near-elastic collisions between surface atoms, clearly simulates the process of surface diffusion. On the other hand, with the model near to the horizontal position, the solid-liquid transition can be made to occur, in which case the crystal 'melts' with an atomically rough surface.

Projection

The model can be projected on to a screen using an overhead projector, making it useful as a lecture demonstration device. Provision should be made for projection in both the horizontal and vertical orientations, allowing freedom for rotation to demonstrate the various kinetic aspects of the model. Slow-motion photography could also be usefully employed to study the mechanism of some of the more rapid processes.

Suggestions for improvement

The principal weakness of the *Atomix* is its inability to demonstrate a shearing mechanism, such as is easily provided in the Bragg-Nye soap bubble model. A more elaborate model could of course be produced to incorporate this capability. Another worthwhile modification would be to produce a second version with a circular well in order to reduce the occurrence of the AA stacking faults which are not representative of close packed structures. Finally, a third modification employing roughened edges would be useful for demonstrating liquid behaviour, although it is probably necessary to retain the flat well bottom, which in itself tends to promote 'crystallisation.'

While improvements are desirable, it is clear that much of the appeal of the *Atomix* is a result of its simplicity: a teacher may bring it to his lecture in his coat pocket. There are other more complicated and expensive atomic models on the market, yet to our knowledge none have this feature. 'Improvements' at the expense of simplicity may therefore be of doubtful value.

Availability

Information on the *Atomix* is available through Emotion Productions Inc., 4825 St. Catherine St. W., Montreal 215, Quebec. The Canadian price for a single unit is $30·00.