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A floating magnet model for simulating metals and alloys

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A floating magnet model [5, 6] originally devised for simulating effects in superconductors has been modified to simulate metal and alloy lattices*. The model shows grain boundaries, edge dislocations and point defects in the metal lattice, demonstrating the pinning of dislocations by impurity atoms and the drift of impurities to grain boundaries. Although the alloy was disordered for most concentrations, a stable ordered square lattice was formed readily at equal proportions of the two atoms. Defects, particularly dislocations, were more complicated in the ordered alloy than in the simple metal.

1. Introduction

The first and best known of the models for simulating crystal defects is the bubble raft model [1-3]. Another model devised more recently is the "Atomix" ball bearing model [4]. Both have their advantages and disadvantages. The bubble raft is, for example, very good for simulating shearing mechanisms, which cannot be demonstrated successfully in the ball bearing model. The ball bearing model, on the other hand, can demonstrate solid-liquid and solid-vapour interfaces which the bubble raft cannot. A third model, the floating magnet model, devised by Rose-Innes and Stangham [5] to stimulate the fluxon lattice in superconductors, can also be used to simulate crystal defects, and it is this application of this model that is considered here. A disadvantage of this model is that it provides only repulsive forces between the atoms, unlike the bubble raft model where there are both attractive and repulsive forces. However, it can show features such as grain-boundary migration, which are not so clearly shown in the bubble raft model and, what will be of greatest concern here, it can very easily be used to simulate effects in alloys.

2. Details of the model

The atoms were simulated by magnetized hard steel pins, attached to floats of expanded polystyrene, floating in a dish of water. The pins were suspended vertically, so that there was a mutual repulsive force between them. An effective attractive force between the pins was provided by reaction from the sides of the dish where pins were prevented from going any further. Sodium nitrite was present in the water to stop the pins rusting, and detergent was used to reduce surface tension. In the particular model used here there were 640 large atoms (pins 25 mm long) attached to white floats, and 320 small atoms (pins cut down to 15 mm) attached to floats with black centres. The dish measured 450 mm × 550 mm. Further details of the model are given in earlier work [5, 6]. Effects described here are best seen by time lapse photography, speeding-up the action about 50 times.

3. Simple metal

Photographs of the model for the pure metal (of large atoms) are shown in Fig. 1. There is a triangular lattice, as is also seen in both the bubble raft and the ball bearing models, as this represents the closest packing in a two dimensional lattice.

Grain boundaries (Fig. 1a) arose through trying to fit a triangular lattice into a rectangular dish, the atoms liking to take up an orientation so that the close packed lines were parallel to the sides of the dish. Both orientations for the main grain were possible (parallel to the long or short sides of the dish), although the orientation generally preferred was that parallel to the long side. Grain boundaries could be made to migrate by creating vacancies and interstitials within a

*A ciné film of the model has been made and is available for loan.

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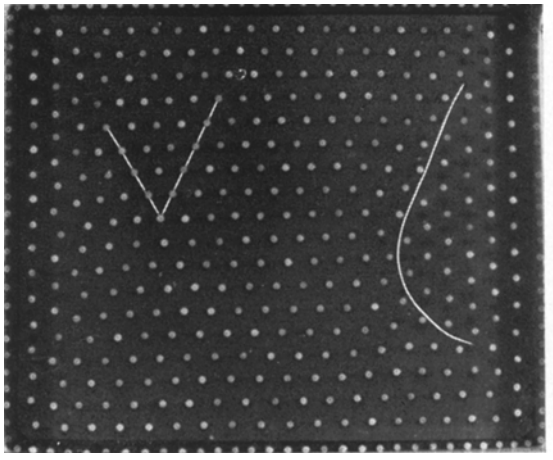

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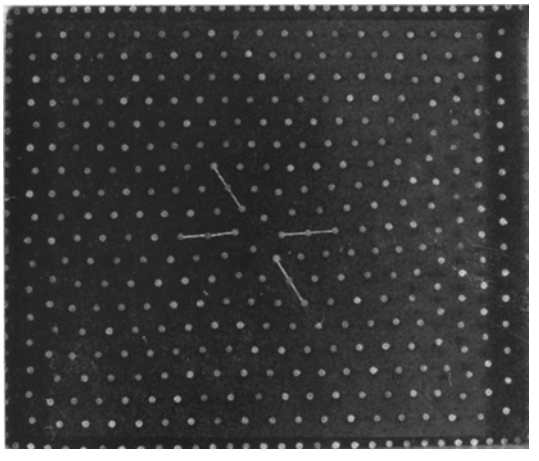

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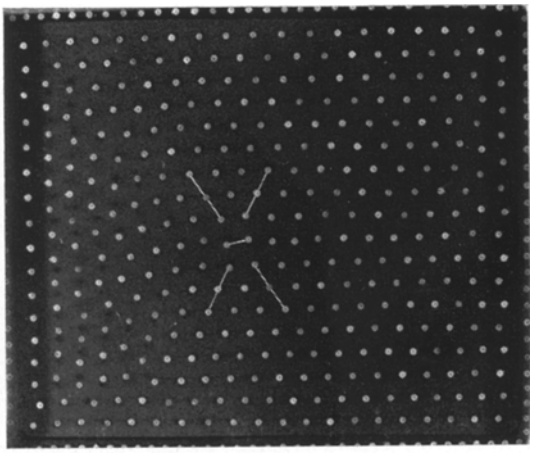


(c)

Figure 1 Simple metal. (a) Grain boundaries and edge dislocation (centre left), indicated by the position of the extra half planes. (b) Shared vacancy (centre), at intersection of lines shown. (c) Shared interstitial (centre). The interstitial atoms are indicated by O–O.

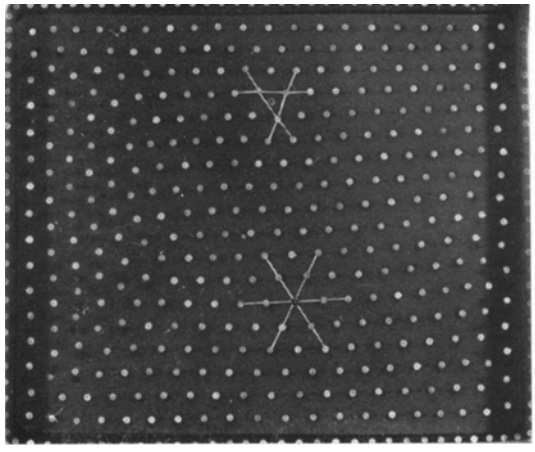
few spacings of the grain boundary, or by otherwise disturbing the lattice (e.g. by blowing on the surface of the water). The grain-boundary motion was somewhat unpredictable, as the grain boundary could move in either direction, sometimes very quickly. In one particular case, when the initial configuration was with the main grain parallel to the short sides of the dish, the grains parallel to the long sides were persuaded to grow towards the middle of the dish. The final stages of the growth, causing these two grains to meet and then spread out through the rest of the dish, was accomplished very quickly, and once the process had been initiated no further external disturbance of the lattice was required to complete it. Similarly, before this had been achieved the grains growing from the long sides were on occasion seen to collapse quickly and unpredictably.

Edge dislocations readily appeared in the lattice (see Fig. 1a), although they tended to be unstable, and drifted towards grain boundaries. They could, however, be strongly pinned by impurity atoms (see below). The dislocations had the characteristic shape for dislocations in triangular lattices as observed also in the bubble raft and ball bearing models, that is, with two extra lines of atoms at 60° to one another.

Fig. 1b shows a shared vacancy, and Fig. 1c a shared interstitial. Point defects in the model always had this shared form (except when first created by removing an atom from the dish or adding an extra one). This is in contrast with the simple vacancies seen in the bubble raft and ball bearing models. Neither vacancies nor interstitials were very stable, tending mutually to annihilate or to drift to grain boundaries or dislocations where they were absorbed.

4. Impurity atoms

Two kinds of impurity atom were used in the matrix lattice of the large white atoms. These were the smaller atom described above, and marked with a black dot on a white background, and larger atoms (coloured black) made by sticking two of the pins used for the white atoms through the same float. When added in small quantities the larger atoms took the place of the



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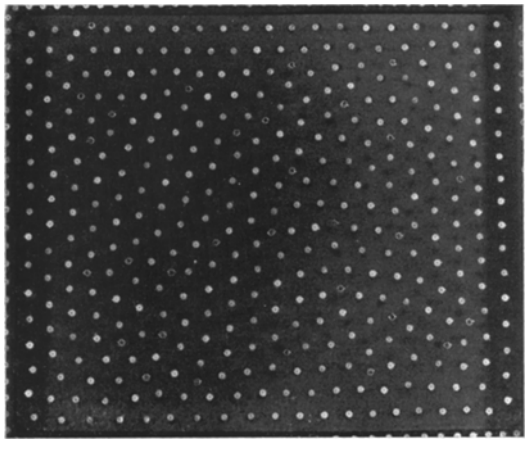

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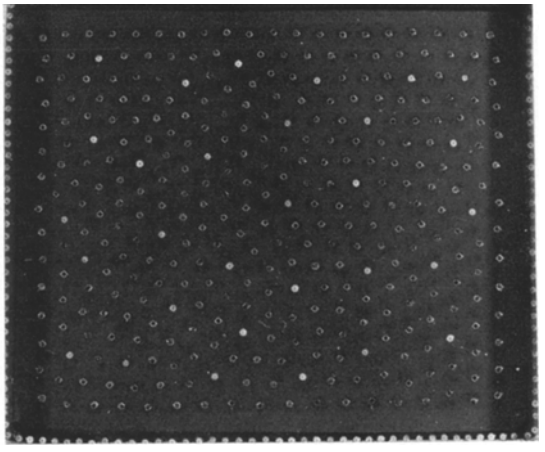


(c)

Figure 2 Addition of impurity atoms. (a) One smaller atom ⊙ occupying an interstitial site and one larger atom ●, occupying a substitutional site. (b) Alloy "white 10 at. % black". (c) Alloy "black 10 at. % white".

ordinary white atoms, but the smaller atoms went into solution, occupying interstitial sites (see Fig. 2a). Both kinds of impurity atom were effective at pinning dislocations. Dislocations tended to drift towards the impurity atoms, and in some cases the addition of a large impurity atom could cause a dislocation to be nucleated at a grain boundary, and then drift towards the impurity atom.

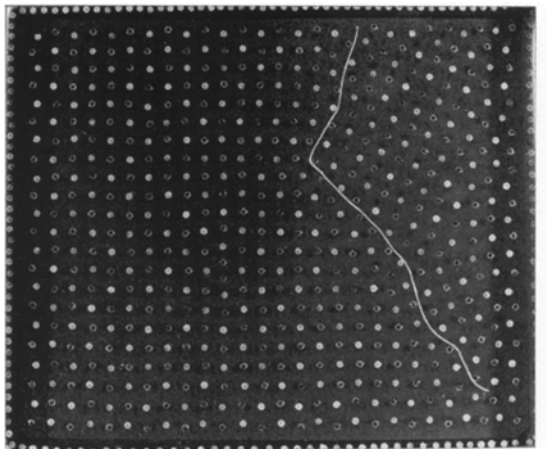
The effect of impurity atoms on grain boundaries was equally impressive. Both kinds of impurity atom drifted towards the grain boundary, the small atoms more easily than the large ones, but there was a tendency too for the grain boundary to move towards the impurity atom. The model generally allowed grain boundaries to move more easily than is probably true in real metals. The impurity atoms remained firmly pinned at the grain boundaries, and on removal of the impurity atoms the grain boundaries were seen to readjust their shape.

5. Disordered alloys

As the concentration of impurity atoms was increased disorder set in. Fig. 2b and c show the alloys "white 10 at. % black" and "black 10 at. % white" respectively. In these cases a fair degree of order is still visible, the large white atoms substituting the matrix black atoms in the first case, but the smaller black atoms showing preference in some instances for interstitial sites in the matrix of the larger white atoms. However, as the concentrations were increased the order disappeared.

6. Ordered alloy

At equal quantities of black and white atoms an interesting thing happened. There were two stable phases for the alloy – a disordered phase, and an ordered phase with a square lattice formed by alternate black and white atoms (see Fig. 3). Symmetry suggests that this ordering gives a lower energy state, but this depends on the relative sizes of the atoms. Clearly if the atoms were very nearly the same a triangular lattice would predominate, and if one set of atoms were very much smaller than the others, the small ones would just occupy interstitial sites in the matrix formed by the large atoms. Sym-



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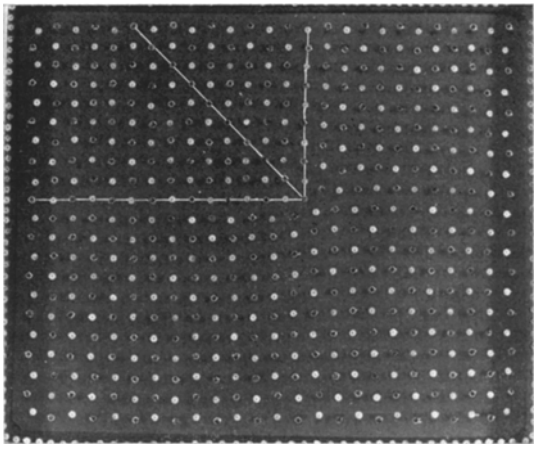

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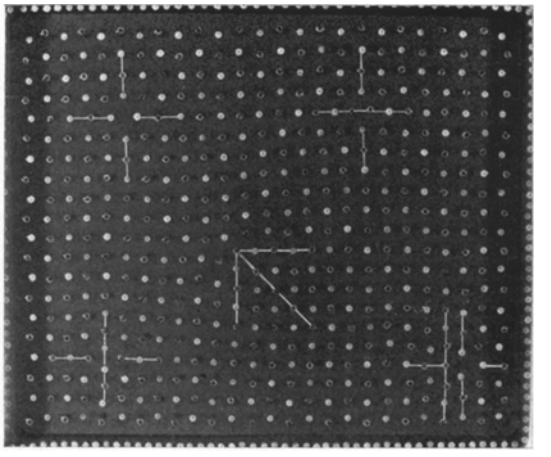


(c)

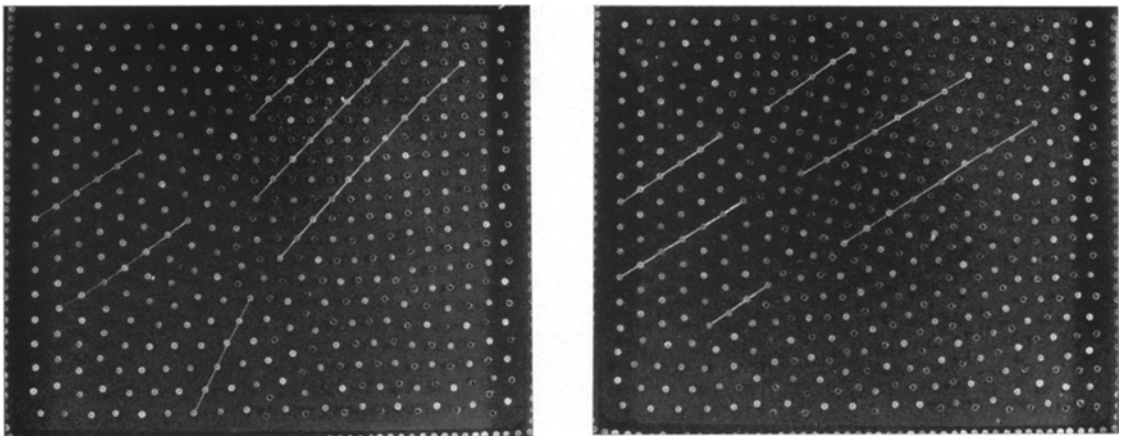
Figure 3 Ordered alloy. (a) Grain boundary (top right). (b) Edge dislocation (centre). The lines at right angles give the position of the extra half planes. The line at 45° to these shows the single half plane that is seen if the true unit cell is taken (just one kind of atom). (c) Edge dislocation (centre). Black atom removed from bottom right and placed bottom left, leaving a shared black vacancy (bottom right) and a shared black interstitial (bottom left). White atom removed from top left and placed top right, leaving a shared white interstitial (top right), and a rather complicated shared white vacancy (top left).

metry also suggests that it should be possible to produce a honeycomb lattice at concentrations 2:1, 1:2 of the atoms. With the sizes of pins used in the present mode, however, no such lattice could be obtained, but this could probably be achieved if pins of more similar sizes were used.

Examples of grain boundaries are shown in Fig. 3a. These show no surprising properties. The most interesting defects were edge dislocations. Normally in a binary ordered alloy (e.g. β-brass) one would expect to see a pair of dislocations separated by an antiphase boundary [7]. In the model, however, single dislocations were seen with a more complicated structure. An example is shown in Fig. 3b. This seems to show two extra lines of atoms at right angles to one another. If, however, it is viewed from the true unit cell (e.g. just the white atoms), forming a lattice at 45° to the dish, a conventional square lattice dislocation is seen with only one extra line of atoms, and it is in a direction perpendicular to this that the dislocation moves. Motion of the dislocation is quite complicated since reordering of atoms is necessary at the dislocation core.

Point defects in the lattice often looked quite complicated (see Fig. 3c). Removal of a black atom produced a simple black vacancy, but addition of a black atom produced a shared black interstitial. Removal or addition of a larger white atom produced rather greater lattice distortion, but examination of the lattice formed by just the white atoms shows that these are basically shared vacancies and shared interstitials.

Fig. 4a shows the phase boundary between the "white 50 at. % black" alloy and the pure "white metal". What is particularly interesting here is is that when the lattice had been disturbed by blowing lightly on the surface of the water, the model settled down so that the lines of the white atoms in the alloy were parallel to those in the



(a) (b)

Figure 4 Phase boundary between pure metal and ordered alloy. (a) Before disturbing the lattice. (b) After disturbing the lattice. The lines show the lines of white atoms matching up after the lattice has been disturbed.

pure metal (see Fig. 4b), which is perhaps extra evidence for the coincident lattice site theory.

Acknowledgements

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