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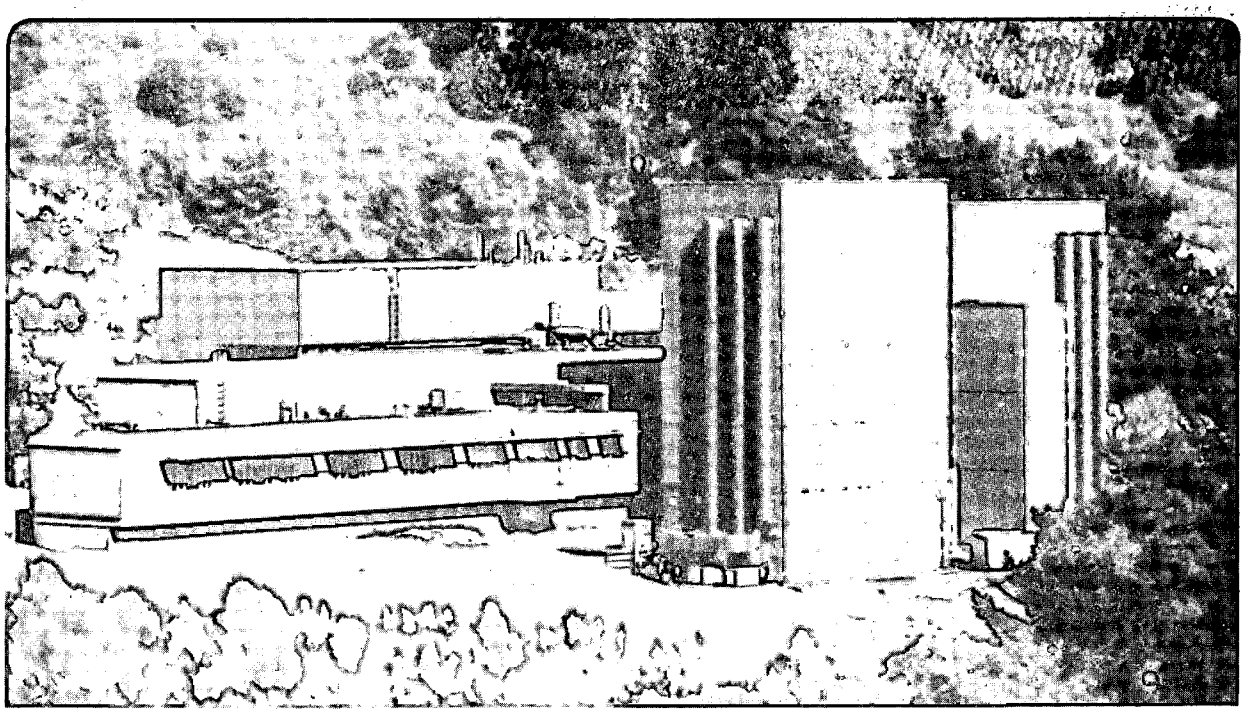

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THE FORMATION OF HEXAGONAL SILICON AT TWIN INTERSECTIONS

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Introduction

The geometric configuration of intersecting twin bands has been considered in the past in the context of dislocation mechanisms and deformation behavior(1,2,3). It is generally found that a twin band is an effective barrier to the propagation of another, noncoplanar twin band. However, under conditions of sufficiently high local stress twin intersections are possible, subject to conditions of continuity(1). Mahajan and Chin have examined the structure of a plane-strain deformed Co-8wt%Fe single crystal by optical and transmission electron microscopy(4,5). Their observations showed that intersecting twins gave rise to highly complex local deformation structures. Analysis of their TEM data led to the conclusion that the strain in the region of intersection was accommodated either by slip or by (secondary) twinning.

The problem of intersecting twins has gained renewed interest with the recent hot-indention experiments in silicon(6,7,8) where the deformation conditions are similar to those in Mahajan and Chin's work. The deformation microstructure consists of twin bands and planar ribbons of hexagonal Si radiating from the area of the indent(6). Although at high pressures silicon forms in several different crystal structures, only the diamond-cubic structure is stable at atmospheric pressure(9,10). Thus the diamond-hexagonal structure that forms during hot indentation of single crystals is a metastable modification. Recent research established its crystallography by means of high-resolution electron microscopy(7). In particular it was shown that the transformation from the diamond-cubic to the diamond-hexagonal structure was of a martensitic nature(8). It has been postulated that the formation of hexagonal Si in the deformation zone is related to multiple twinning(8), and a detailed crystallographic model for this transformation has been proposed(11). One feature of this model is the hypothesis that under strict plane strain conditions the region of twin intersection will be forced into hcp stacking in order to accommodate the strain of the crossing twin. While the observed crystallography of the hexagonal phase is in excellent agreement with this model, no *direct* evidence for this mechanism has been observed to date. The present note reports such an observation by high resolution electron microscopy.

Results

A schematic <011> projection of an fcc crystal is shown in Fig.1, where one twin band (Fig.1a) is being crossed by another twin band (Fig.1b). From this figure it is apparent that for compatibility the region of twin intersection must undergo a shear of the same

magnitude (0.707) as the twinning shear. It can be shown that in the crossed twin the shear plane is of the {511} type and the shear direction is <255>(8). The lattice planes represented by lines in Fig.1 are the close packed {111} planes and the atomic positions are at the nodes of the lattice. In the region of intersection the homogeneous shear has changed the ABC stacking of the horizontal close packed planes to AAA stacking. The simplest option for the crystal to avoid this high-energy stacking sequence is to shuffle every other atomic layer to form ABAB hexagonal stacking. Thus the region of intersection undergoes a cubic to hexagonal transformation with the basal planes coherently matched with the horizontal close packed planes in the crossed twin. In this model the accommodation shear is homogeneous (apart from the shuffle) and lies entirely in the plane of the strain.

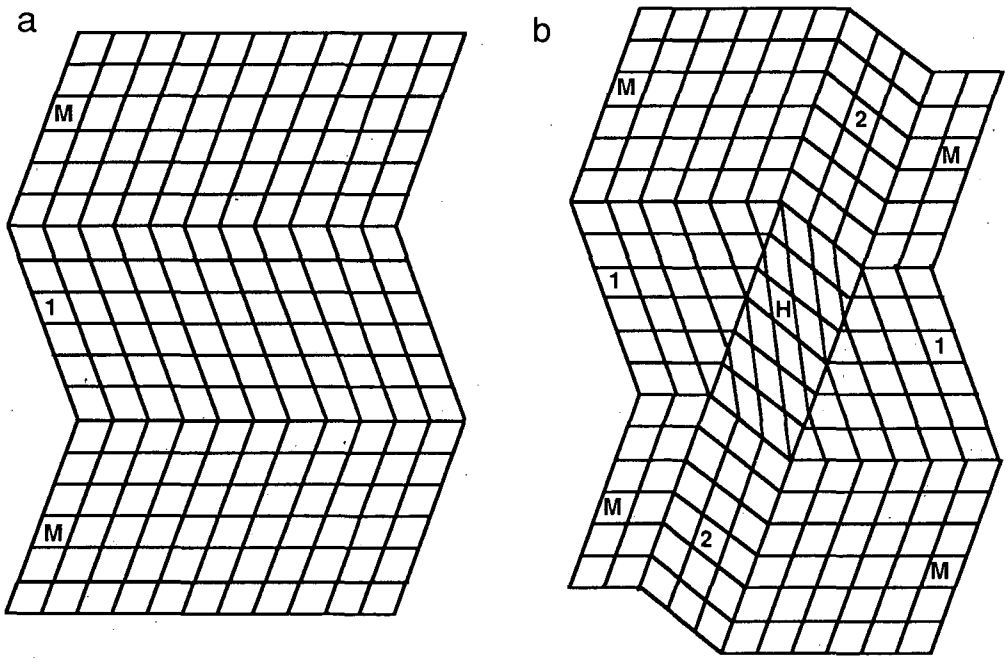

Fig. 1 Schematic diagram showing single twin in (a) being intersected by a second twin in (b). Strain accommodation causes the region of intersection to transform to hexagonal stacking. Matrix labelled M, twins labelled 1 and 2, hexagonal phase labelled H.

Fig. 2 shows a high-resolution micrograph of a silicon single crystal that was hot-indented at 400°C. Two intersecting twins 1 and 2 are oriented the same as in the schematic. The region of intersection clearly shows a perfect hexagonal stacking sequence in agreement with the model. Twin 2 tapers as it crosses twin 1 from the top right to the bottom left of the micrograph, emerging as a single stacking fault below twin 1. Thus the tapered end must contain the twinning dislocations, or their <255> equivalent at its interface with twin 1. It is clear from the local structure of twin 1 at the lower part of the intersection that some form of dislocation reaction has taken place in this region. As a further point of interest note the stacking fault parallel and to the right of twin 2. Instead of traversing twin 1 straight it is deflected by it. This means that the stacking fault was present before the formation of twin 1. It must also be mentioned that most twin intersections examined were more complex than the example shown in Fig. 2. A commonly observed feature was the spreading of a well-

defined twin band into several stacking faults or narrower bands on crossing another twin and a localized, irregular change in the orientation of the crossed twin. These observations attest to the difficulty of strain accommodation at twin intersections.

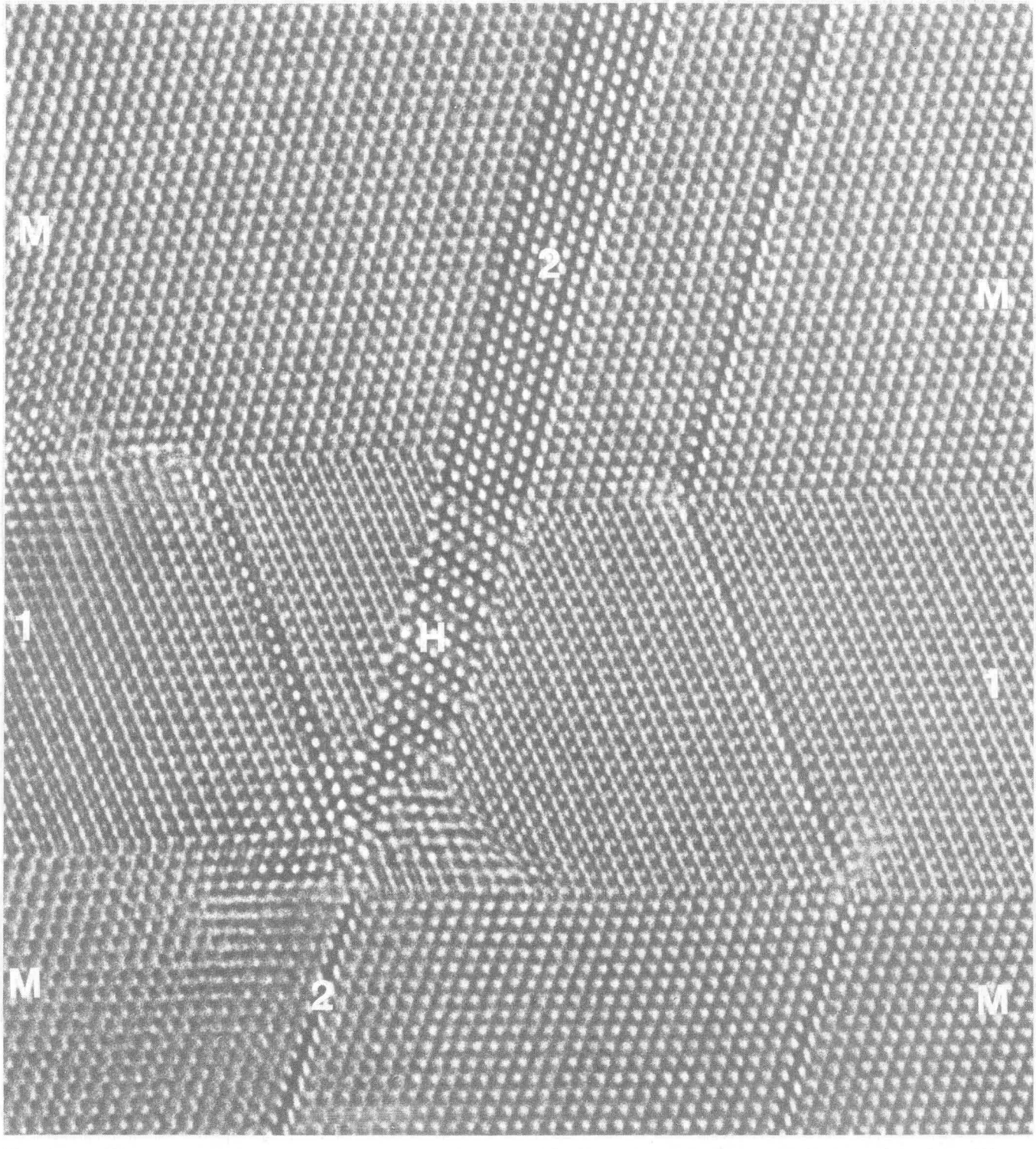

Fig. 2 High resolution micrograph taken at 800kV of two intersecting twins in silicon single crystal indented at 400°C. Matrix labelled M, twins labelled 1 and 2, hexagonal phase labelled H. A slight crystal misorientation is responsible for the variation in the images of the matrix and the two twins. (XBB 880-9626)

A more detailed account of the experimental observations on ribbons of hexagonal Si, its associated crystallography and dislocation mechanics is being submitted for publication elsewhere(11). However, the model for the strain accommodation at intersecting twins, here confirmed for silicon, is likely to be of more general applicability, and further confirmation is presently being sought in fcc-based materials of low stacking fault energy.

Acknowledgement

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