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1960

SovietRxiv

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Abstract

Full Text

PHYSICAL CHEMISTRY

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ON THE NATURE OF THE MOSAIC STRUCTURE OF GERMANIUM AND SILICON SINGLE CRYSTALS

(Presented by Academician P. A. Rehbinder on 26 IV 1960)

At the present time the opinion that the mosaic structure is dislocational in nature is generally accepted. The simplest type of dislocation boundary between blocks is shown in Fig. 1. In this case the boundary is a wall of edge dislocations with Burgers vector b, and the angle of misorientation of the blocks θ is determined by the distance between dislocations h:

$$\theta = \frac{b}{h}. \tag{1}$$

Fig. 1. Burgers model of a block boundary

To reveal dislocations in germanium and silicon single crystals (the dislocation density is usually not higher than 10^6 cm^{-2}), etch figures are most often used. Etch figures in Ge and Si are revealed best on the (111) plane. As studies have shown ([1,2]), in crystals grown by pulling from the melt along the (111) axis, almost all dislocations are edge dislocations, with Burgers vector $a/2\,(\bar{1}10)$. In individual cases, etch figures on the polished section form lines called low-angle boundaries.

It was shown ([3]) that for such boundaries the misorientation between blocks, determined by the X-ray method, agrees well with that calculated from formula (1) (the distance between dislocations in the boundary was determined metallographically).

We investigated Ge and Si single crystals obtained by pulling from the melt along the (111) axis. The samples were plates 2–3 mm thick, cut from ingots perpendicular to the growth axis, so that the polished-section plane deviated from the crystallographic plane (111) by no more than several degrees.

Fig. 2. Schematic of the setup

Figure 2: Fig. 2. Schematic of the setup

For the X-ray investigation, Ge samples with dislocation densities in the range 10^2-10^6 cm^{-2} and Si with dislocation densities 10^2-10^3 cm^{-2} were selected. The sample with the lowest dislocation density was used as the monochromator. The X-ray investigations were carried out by the method of a two-crystal spectrometer ([4]) with a parallel arrangement (Fig. 2) of the crystals.

The principle of the method is that the sample II, on which a preliminarily monochromatized beam of X-rays is incident, is rotated through small angles with the counter fixed. The constructed···

points (for each position of the specimen), the curve of the dependence of the double-reflection intensity I on the angle of rotation of the specimen β is called the rocking curve. Since the region of reflection of X-rays by a perfect crystal is small (of the order of several angular seconds), the specimen must be rotated through angles of the order of $1'$. We made a special goniometric head ([5]), which makes it possible to carry out rotations through small angles (with an accuracy up to $0.5''$). The work was carried out on a URS-50I apparatus with a Geiger counter.

To reduce the vertical divergence of the beam, slits 3, 4 of height 0.7 mm were introduced (Fig. 2).

The width of the double-reflection curve for an ideal crystal can be calculated ([4]); for the (111) reflection of Ge and Si with Cu$-K\alpha$ radiation it is approximately $20''$ and $7''$, respectively. With an experimental accuracy of $5''$, in the case of Si one can count only on obtaining qualitative results. Therefore the main experiments were carried out on Ge specimens. Individual Ge specimens gave rocking curves with a width of about $20''$, which indicates the practically complete absence of geometric broadening.

Fig. 2. Schematic of the setup

Consequently, broadening of the rocking curve can be associated only with the mosaic structure of the specimen. Noticeable broadening of a curve with a width of $20''$ will be obtained when the blocks are misoriented by angles not less than $10''$.

The main types of experimental rocking curves are shown in Fig. 3. If it is assumed, to a first approximation, that the scattering of X-rays by different blocks is completely incoherent, then the rocking curve of a mosaic specimen is simply composed of the double-reflection curves of the individual blocks (see Fig. 3). The distances between the maxima of these elementary curves are equal to the angles of misorientation of the blocks, and from the number of rocking curves one can determine the size of the blocks.

Fig. 3. Types of rocking curves: a —ideal crystal, —mosaic crystal; —specimen with small-angle boundaries, —principle of deciphering rocking curves

Figure 3: Fig. 3. Types of rocking curves: a —ideal crystal, —mosaic crystal; —specimen with small-angle boundaries, —principle of deciphering rocking curves

Fig. 3. Types of rocking curves: *a* —ideal crystal,
—mosaic crystal; —specimen with small-angle boundaries,
—principle of deciphering rocking curves

In our experiments, Ge specimens with a random arrangement of dislocations were investigated. In a crystal with a dislocation density of the order of 10^2 cm^{-2}

it is difficult to assume the presence of a block structure within the framework of the Burgers model, since dislocations located at distances on the order of 1 mm cannot produce any appreciable misorientation of blocks. In general, it is difficult to expect that randomly arranged dislocations can produce a mosaic structure. Nevertheless, the results of the X-ray study show that at all dislocation densities Ge single crystals have a mosaic structure, and the misorientation angles of the blocks and their sizes change little when the dislocation density is varied by four orders of magnitude. This fact does not fit within the framework of the Burgers model. The experimental results are given in Table 1.

Table 1

Sample No.	Dislocation density, cm^{-2}	Block size, cm	Block misorientation	Sample No.	Dislocation density, cm^{-2}	Block size, cm	Block misorientation
2	$6 \cdot 10^2$	$8 \cdot 10^{-2}$	13″	10	$2 \cdot 10^6$	$7 \cdot 10^{-2}$	22″
6	$2 \cdot 10^4$	$6 \cdot 10^{-2}$	22″	11	$3 \cdot 10^6$	$8 \cdot 10^{-2}$	23″
9	$7 \cdot 10^4$	$9 \cdot 10^{-2}$	14″				

A study of Si samples with a small dislocation density, on the order of $10^2 \div 10^3$ cm^{-2}, showed that in silicon the block size is much smaller than in germanium. This fact also does not fit within the framework of the Burgers model, since the lattice periods of Ge and Si differ little.

It may be assumed that the discrepancy between the metallographic data and the X-ray data is connected with experimental errors. To check the method, Ge samples with small-angle boundaries were studied. The rocking curves of these samples are similar to that shown in Fig. 3 *c*. They show that, in the presence of small-angle boundaries, Ge crystals have a fragmented structure, and the misorientations between fragments agree in order of magnitude with those calculated from the distances between dislocations in the boundaries.

The experimental results indicate that the boundaries of blocks in Ge and Si, even if they are associated with dislocations, are not formed by the small-angle-boundary mechanism. Here, possibly, the role is played not by dislocations but by some other structural defects. The boundaries between fragments, however, are built of dislocations in full agreement with the Burgers model. Consequently, the nature of block and fragment boundaries is different.

Moscow Institute of Steel
named after I. V. Stalin

Received
2 III 1960

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Note: Figure translations are in progress. See original paper for figures.