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SOME REMARKS TO THE PROBLEM OF THE DISLOCATION LOOPS CREATION IN THE REGION OF INTERFACE

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Resume.- Dans ce travail, on discute des conditions de création de boucles de dislocations autour de précipités Ag₂Te-α, dans les cristaux de ZnTe. Les facteurs d'accomodation ont été calculés pour ce type de précipités. A partir de ces calculs, on discute le problème des variations de défomation entre les parties implantées et non implantées de cristaux de Si, après recuit.

Abstract.- The aim of this work is discussion on the conditions of dislocation loops created round the Ag₂Te - α in ZnTe crystals. The misfit factor for this kind precipitates has been calculated. On the base of obtained results, the problem of strain changes between implanted and non-implanted parts of Si crystals after annealing process have been discussed.

Interaction of silver impurities with the ZnTe crystal lattice were investigated by means of TEM. The crystal were doped with silver, introduced either during the crystallization process directly from the melt with an excess of tellurium or introduced by diffusion for 48h at a temperature of 900°C. Silver concentrations in both cases were similar and amounted to 3.5 x 10⁻³ wt % and 3.1 x 10⁻³ wt %. The basic defects in the first kind of crystals were precipitations. By means of microdiffraction and EDAX-system connected to JEM-200A electron microscope it was possible to establish that the investigated material contained three types of precipitations viz. pure tellurium (22%), monoclinic Ag₂Te phase (76%) and hexagonal Ag₂Te₃ phase (2%). When silver atoms were introduced into the crystal lattice by diffusion, helical dislocations and dislocation loops decorated by small precipitates were observed in the whole volume of the sample. The precipitations were identified using Moire' pattern as Ag₂Te - α phase of cubic structure. Typical dislocation loop around a precipitation is shown in figure 1. It was very interesting to explain how these loops could be created. The explanation was based on a theoretical model proposed by Weatherly /1/ and Ashby and Johnson /2/. A "critical misfit" causes the generation of dislocation loops at a misfitting precipitate. A measure of the misfit is "constrained strain" which is given by the expression :

$$\varepsilon = \frac{3k}{3k + 4G} \delta$$

where \(k\) is the bulk modulus of the precipitate, \(G\) is the shear modulus of the matrix, \(\delta\) is the "stress free strain" /3/

Fig. 1 : Scale : 200 Å

Considering a misfitting precipitate centred at the origin of a cartesian coordinate system \(X₁, X₂, X₃\) and assuming that both precipitate and matrix are elastically isotropic, the shear stress is :

$$\sigma_{xy} = -\frac{6G \varepsilon X₁X₂X₃}{R^2}$$

where \(R\) = radius of the precipitate

\(R^2 = X₁^2 + X₂^2 + X₃^2\)

A dislocation segment bulges from the precipitate-matrix interface on a slip plane on which the shear stress is the greatest. The segment is shaped roughly like a segment of a circle. Energy of the system consisting of a single misfitting precipitate of radius
The work $W$, which is done by the component $a_{1,2}$ of the stress field of the precipitate as the loop expands over the area $dS$

$$W = \int_{\text{loop}} \alpha_{1,2} b dS$$

Energy of a loop is given by the expression:

$$E = \frac{\alpha b^2 r}{4} (2\nu - 1 - \frac{8 r}{b} - 2)$$

where $r$ - radius of a loop
$b$ - Burgers vector of a loop
$\nu$ - Poisson's ratio

The creation of a dislocation loop around a precipitate relaxes the stresses around it and the total energy of the system is less. This result is obtained on condition that $\Delta E < 0$. For precipitate radii and radii of loops created around them, measured on micrographs, the misfit parameter (Fig. 2) of Ag$_2$Te-a (lattice parameter $a = 6.585\ A$) in ZnTe ($a = 6.1036\ A$) was calculated, using the above formula. This parameter has a value of 0.135, which indicates big stresses at the interface between the precipitation and matrix.

Our suggestion is that mechanism can be responsible for the creation of dislocation loops in the case of annealed boron-implanted silicon.

In the paper by W. Hubrig, J. Auleytner and M. Maciaszek /4/ we reported on changes of X-ray topographic contrast due to annealing of boron-implanted silicon. Silicon slices were investigated by means of Lang method at the boundary between implanted and non-implanted crystal parts after annealing at various temperatures. It was shown that annealing from room temperature up to $700^\circ\mathrm{C}$ causes no change of the diffracted intensity. At higher temperatures the intensity of the diffraction pattern at the boundary diminishes and about $900^\circ\mathrm{C}$ an inversion of contrast occurs. This fact can be in general explained by annealing of lattice damage and increasing incorporation of boron atoms at substitutional sites. This conclusion agrees with channeling effects measurements from Fladda et al. /5/, who found about 90% of boron atoms to be substitutional at this temperature and with our measurements of the electrical sheet resistivity, which have shown that the carrier concentration increases distinctly at $900^\circ\mathrm{C}$.

But how can be explained appearing of the inversion of the contrast in details? X-ray topographic contrast is a suitable property to follow lattice strains. Annealing of boron implanted silicon slices leads to a decrease of contrast starting at $700^\circ\mathrm{C}$ and near $900^\circ\mathrm{C}$ the observable reverse contrast refers to the appearing of tensile strains inside the implanted layer.

We think that the lattice strain will be influenced also by secondary defects generated during annealing. Bartsch et al. /6/ have shown by electron microscopy that in silicon implanted and annealed in the same manner, a high dislocation and dislocation loops density appears. Transmission electron micrographs (see figure 3 in /4/) show defect structures after 770, 900 and $1050^\circ\mathrm{C}$ annealing. Particularly at the annealing temperature $900^\circ\mathrm{C}$ large number of dislocation loops is visible. But after annealing at $700^\circ\mathrm{C}$
small boron clusters predominate. It will be interesting to examine, whether like in the case of annealed ZnTe/Ag/ crystals, the boron precipitates can be the sources of dislocation loops in silicon and if the creation of dislocation loops similar in the range of annealing temperatures 770° and 900°C eliminate the strains at the boundary between boron implanted and non-implanted crystal parts.

References

/1/ Weatherly, G.C., Philos. Mag., 17 (1968) 791.