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Effect of weak magnetic field on structural arrangement of extrinsic oxygen atoms and mechanical properties of silicon monocrystals

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Abstract. IR spectroscopy study is indicative of the change in the relative concentration of interstitial oxygen in silicon monocrystals after their treatment by using the magnetic field. This is an evidence of a considerable effect of magnetic field on the defect structure of the investigated crystals.

Keywords: silicon, magnetic field, IR spectroscopy, oxygen precipitates, interstitial oxygen, microhardness.

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1. Introduction

In recent years, a lot of works concerning the effect of magnetic field on the state of the defect-extrinsic structure of nonmagnetic materials were performed when explaining the physical mechanisms of this effect of weak magnetic field on nonmagnetic crystal structure, most of researchers chose the model of spin-dependent reactions. The main idea of this model is that magnetic field revokes the restraints on some electron transitions, *i.e.* makes the intercombination transitions possible in the "radical pair" formed by structural elements in a certain spin configuration (for example, singlet or triplet) [1–3]. Magnetically stimulated evolution of electron spins of the extrinsic centers has an influence on the behavior of the crystal defect structure. It is necessary to note that though there is a lot of experimental results in this field, definitive physical explanation of the effect of magnetic field on the monocrystals structural state is in the stage of the development yet. Besides, many questions demand additional examination. For instance, there is no information regarding the effect of magnetic field on clusters in nonmagnetic monocrystals. So, the study of the regularities of magnetic impact gives possibilities both to develop new means to control imperfections of the real monocrystals and improve the theoretical model of magnetic impact on the crystals structure.

The main purpose of this work was to determine changes of the interstitial oxygen concentration in silicon monocrystals before and after constant magnetic field treatment using IR spectroscopy (IRS).

2. Experimental

Magnetic treatments of the Si samples (the exposure of the samples to magnetic field with the induction $B = 0.17$ T) were performed for 7 days. The study of the interstitial oxygen content in the *n*-type silicon monocrystals doped with phosphorous to a level of specific resistance $\rho_1 = 2$ Ohm·cm (КЭФ-2) and $\rho_2 = 5$ Ohm·cm (КЭФ-5) was carried out using an automated IR spectrometer ИКС-25М. It is intended to the registration of the transmission and reflection spectra of solid, liquid and gas materials in the spectral range from 4200 down to 250 cm^{-1} as well as to the mathematical processing the obtained spectral data. As is well known, the intensity of the absorption band 1107 cm^{-1} is determined by the concentration of interstitial oxygen atoms in monocrystalline silicon [4]. In our experiments, the miscalculation in oxygen content calculations did not exceed 5 %. IR transmission spectra

Table. Changes of the interstitial oxygen concentration after magnetic treatment.

№	Sample	State	Oxygen concent-ration, cm^{-3}	Relative change of the interstitial oxygen concentration, %
1	КЭФ–2	initial	$7.9\cdot10^{17}$	15
		after magnetic treatment	$9.1\cdot10^{17}$	
2	КЭФ–5	initial	$6.6\cdot10^{17}$	17
		after magnetic treatment	$7.7\cdot10^{17}$	

were registered in the range of wavenumbers (ν) from 900 to 1300 cm^{-1} at room temperature.

3. Results and discussion

IR transmission spectra of some investigated samples are presented in Fig. 1.

It is known that the absorption band with the peak position 1107 cm^{-1} and full width at half maximum 33 cm^{-1} is attributed to the interstitial oxygen atoms vibrations in silicon lattice. The change of the intensity of this band as a result of magnetic field effect indicates increasing contribution of the Si–O bonds.

Analysis of IR spectra shown in Fig. 1 and similar spectra obtained for other silicon samples has given a possibility to determine the change of interstitial oxygen concentration in the Si samples after magnetic treatment. The corresponding data are listed in Table.

The data presented show that after magnetic treatment the relative concentration of interstitial oxygen in Si crystals increases. This result is in a good agreement with the well-known conjecture regarding magnetic field effect on the dissociation of chemical bonds [1, 5, 6]. According to the model conceptions from the literature, the probability of chemical bond dissociation and, therefore, structural complex with, at least, two radicals (atoms) with their spin angular moments depends on mutual orientation of the spins. Magnetic field effects on the probability of the favorable orientation appearance and shifts the “reaction” in the “radical pair” (structural complex) to the dissociation direction. The well-known scheme of the change of pair multiplicity upon intercombination transitions [2, 3, 7] can be applied to the reaction description between any types of the defects, including the paramagnetic ones. Extrinsic and point structural defects and their complexes can exemplify such defects in the crystal. To a considerable extent, spin-dependent reactions between them depend on the reagent type. In our case, Si-O-Si quasi-molecules and SiO_x precipitates can appear as “radical pairs”. As follows from the experimental data [5], the efficiency of magnetic field impact on Si monocrystals is defined by the availability of dissolved oxygen in silicon. It is known that oxygen in silicon occupies mainly the bridging position, in which its two stretching bonds are distributed between two stice Si atoms [4, 8]. While in Cz-Si, oxygen can be located not only in the form of Si-O-Si quasi-molecules but in the form of some SiO_x precipitates produced during the ingot growth process, too [4, 9]. Thus, it was shown [9] that, in some as-grown Si monocrystals, the oxygen content in the precipitate phase may achieve 20 % of the total oxygen concentration. In our assumption, the reaction with involving the radicals, forming Si-O-Si quasi-molecules and SiO_x precipitates, can lead to dissociation of their chemical bonds under magnetic field influence. In our opinion, after the mentioned bond dissociation the relative concentration of interstitial oxygen should increase. These assumptions are well

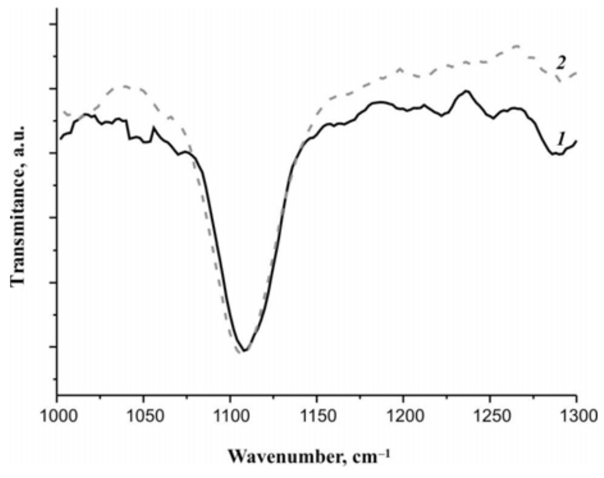

Fig. 1. IR transmission spectra of the *n*-type silicon sample before (1) and after (2) magnetic treatment.

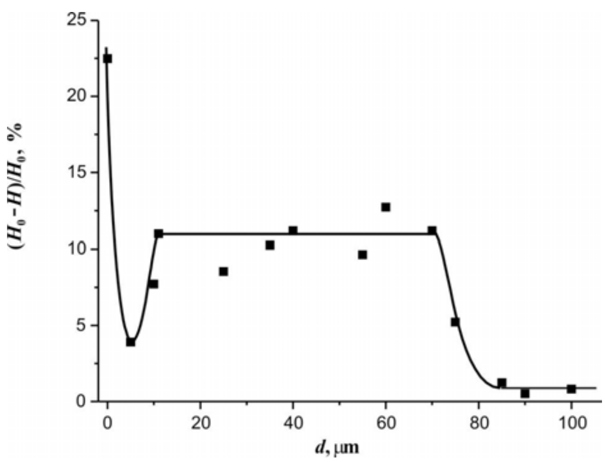

Fig. 2. Distribution of the microhardness value in the bulk of silicon samples before (H_0) and after (H) magnetic treatment.

confirmed by the results of the IRS study of structural defect subsystem in silicon crystals after magnetic treatment. Supposing that for the same time of exposure in magnetic field, the equal number of Si-O-Si quasi-molecules and SiO_x precipitates is dissociated, probably, the “addition” to the total interstitial oxygen atomic concentration in the crystals with different “biography” (different initial oxygen content, doping and residual impurities concentration) can distinguish. This assumption has been confirmed experimentally (Table).

At the same time, we have found that the changes of the structural arrangement in Si monocrystals under the influence of magnetic treatment lead to the reversible changes of their structural-dependent properties. In particular, the changes of microhardness, namely, the appearance of magnetomechanical effect were observed. It was found that, in КЭФ-2, Si monocrystal microhardness is reduced to 23 % whereas that in КЭФ-5 is reduced to 25 %.

The mentioned changes of microhardness were revealed on the surface of investigated Si samples. Using step-by-step chemical polishing in the special solution ($HF : HNO_3 : CH_3COOH = 2 : 1 : 1$), the distribution of magnetomechanical effect over the sample depth was investigated.

The dependence shown in Fig. 2 indicates complicated enough, multistage distribution of magnetomechanical effect over sample depth. So, it was established using step-by-step polishing that the change of magnetomechanical effect in depth is not monotonous. Non-monotonous variations of mechanical properties can be associated with a non-uniform distribution of the structural defects that are transformed and modified in magnetic field. The latter requires subsequent experimental verification.

4. Conclusion

In principle, the theory of spin-dependent reactions explains the changes of point defect arrangement in weak magnetic fields while experimental results allow to make a hypothesis that magnetic field modifies the reactions kinetic taking place in the subsystem of structural defects between separate defects. In our opinion, magnetic field modifies the atomic structure of oxygen-containing clusters. This is just the cause of correlated change in the structural arrangement of extrinsic oxygen atoms, IR spectra shape as well as microhardness of Si monocrystals after magnetic treatment.

So, the investigations performed indicate that the magnetic treatment of silicon monocrystals leads to the correlated change both structural arrangement of oxygen extrinsic atoms and structural-dependent characteristics, most of all microhardness.

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