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## RAMAN SPECTROSCOPY OF STRUCTURAL DEFECTS RELATED WITH SILVER ATOMS IN SILICON

**Abstract.** Vibrational and structural properties of silicon doped with silver atoms were investigated using Raman spectroscopy. It has been established that the introduction of silver atoms in silicon increases the interatomic distance in the crystal lattice, which, in turn, shifts the positions of the vibration peak to lower ones.

**Keywords:** Raman Spectroscopy, silver, interstitial and substitutional defects.

**Introduction.** It is known that the technological route for the manufacture of almost any semiconductor device is accompanied by various cycles of low- and high- temperature treatments, which inevitably leads to the formation of various kinds of structural defects and impurity centers, as well as to the degradation of device parameters. The degradation of the device parameters based on silicon structures to some extent depends on uncontrolled impurities – oxygen, carbon, metals that are in the silicon wafer or introduced during the manufacture of devices. Of all the contact impurities (Cu, Al, Au, Ag, etc.) – silver is one of the available metals [1].

It is known from theory that the diffusion mechanism allows impurity atoms to be in two states: i) S-

substitutional atoms; ii) I-interstitial states (fig. 1). For example, the authors Rollert et al. [2] showed that the overwhelming majority of Ag impurity atoms are present at interstitial sites ( $Ag_i$ ); and that substitutional silver ( $Ag_s$ ) either does not occur or occurs only in very low concentrations. Using EPR studies, the authors of [3] identified this isolated  $Ag_i$ , which represents only a small fraction of the total amount of impurity silver atoms present. Today, there is no clear picture of the microscopic structure of defects related with silver atoms in silicon. Thus, the topic of this work is relevant and promising in terms of using its results.

In this paper, the surface states of silver atoms in silicon are considered by Raman spectroscopy.

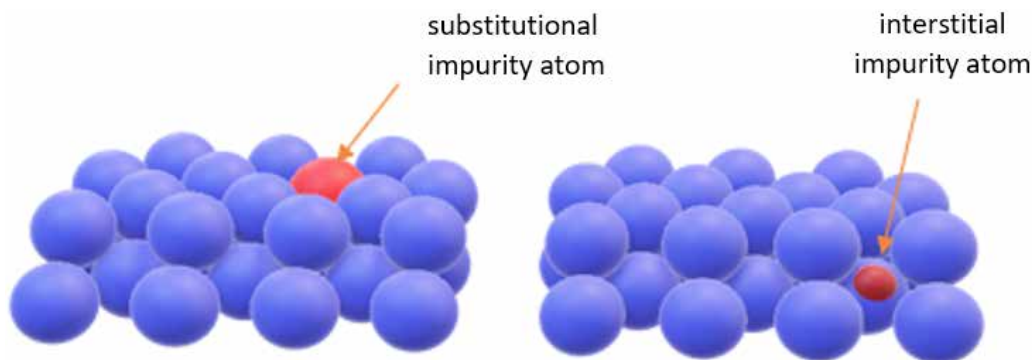


Figure 1. Distribution of impurity atoms in silicon crystal

**Experimental technique.** Samples of n-type silicon ( $\rho = 7.5 \Omega \text{ cm}$ ,  $N_D \approx 6 \cdot 10^{14} \text{ cm}^{-3}$ ) grown by the Czochralski method were selected for measurement. Doping of the silver impurity was carried out by the diffusion method at a temperature of  $1200^\circ\text{C}$  for 2–10 hours. The complete solubility of silver atoms in silicon at this temperature is achieved up to  $\sim 6.5 \cdot 10^{15} \text{ cm}^{-3}$ . Raman spectra were obtained on an Ocean Optics QE65 Pro spectrometer with a 785 nm laser and an integration time of 500 ms.

Raman spectroscopy has proven to be a key experimental technique due to its ability to identify structural and electronic effects in non-destructive measurements. Raman spectroscopy, a fast and convenient method for study of the vibrational and structural properties of materials, is widely used to investigate the structures of crystalline and amorphous silicon semiconductors [4]. Raman scattering can measure changes in vibrational frequencies induced by the microstructure or the presence of local deformations, which can be produced by distortion of the bond angle. In this paper, the surface states of

silver and gadolinium atoms in silicon are considered by Raman spectroscopy. Raman spectroscopy studies vibrational energy levels by looking at the energy difference between laser light incident on the sample and the rare photon scattered inelastically via the Raman effect. This energy difference, known as the Raman shift, is reported in energy units called wavenumbers ( $\text{cm}^{-1}$ ).

The following equation shows how to calculate a Raman shift,  $\Delta\nu$ , in  $\text{cm}^{-1}$  using the laser wavelength ( $\lambda_0$ ) and a Raman peak wavelength ( $\lambda_x$ ) in nm:

$$\Delta\nu_x (\text{cm}^{-1}) = \left( \frac{1}{\lambda_0 (\text{nm})} - \frac{1}{\lambda_x (\text{nm})} \right) \times \frac{10^7}{\text{cm}}$$

**Results and its discussion.** The Raman spectra of the light of the initial sample Si<P> and doped with silver atoms Si<Ag> are shown in (fig. 2. and fig. 3).

The Raman spectrum of Si exhibits a high peak in the region  $519\text{--}521 \text{ cm}^{-1}$  with a FWHM of  $8\text{--}12 \text{ cm}^{-1}$ . Intensity of first-order scattering due to optical phonons (TO, LO) at the central point  $\Gamma$  of the Brillouin zone.

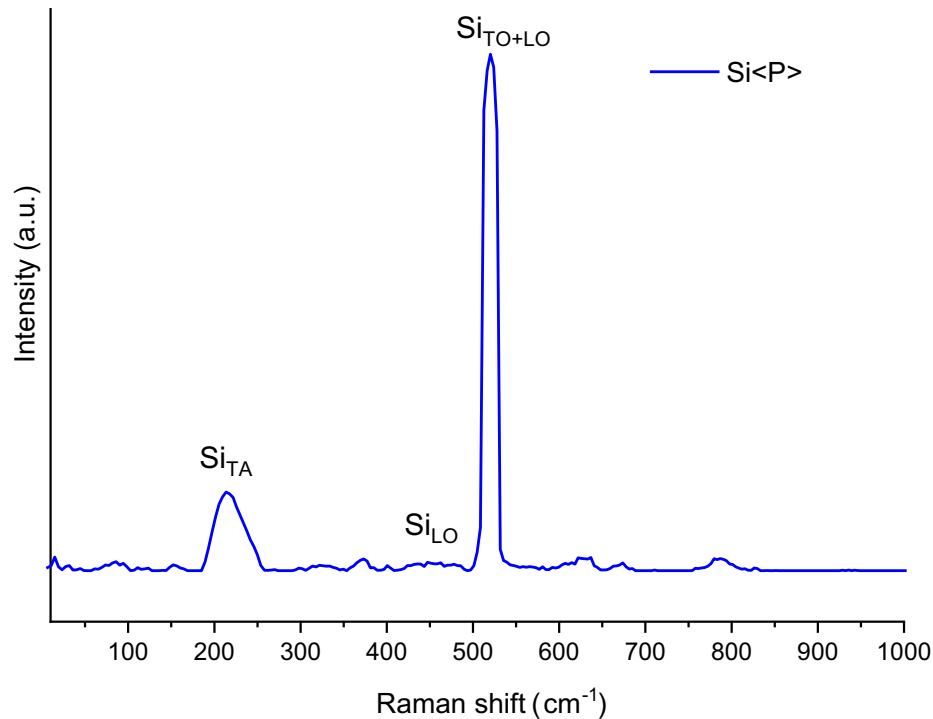


Figure 2. Raman shift of initial silicon. Modes:  $\text{Si}_{\text{TA}} - 215 \text{ cm}^{-1}$ ,  $\text{Si}_{\text{LO}} - 412\div 494 \text{ cm}^{-1}$ ,  $\text{Si}_{\text{TO+LO}} - 521 \text{ cm}^{-1}$

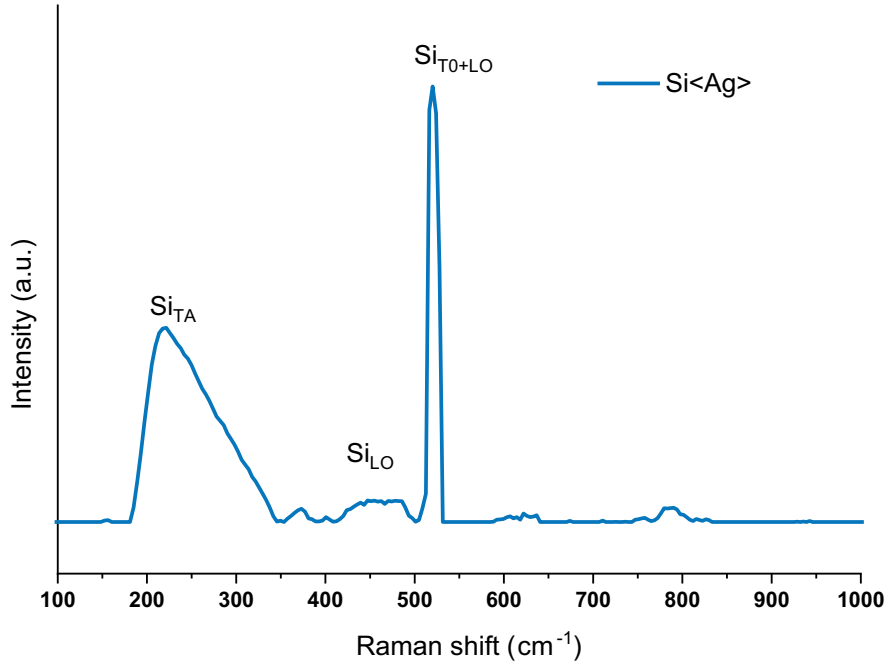


Figure 3. Raman shift of silicon doped with silver atoms. Modes:  
 $Si_{TA} - 221 \text{ cm}^{-1}$ ,  $Si_{LO} - 414 \div 504 \text{ cm}^{-1}$ ,  $Si_{TO+LO} - 520 \text{ cm}^{-1}$

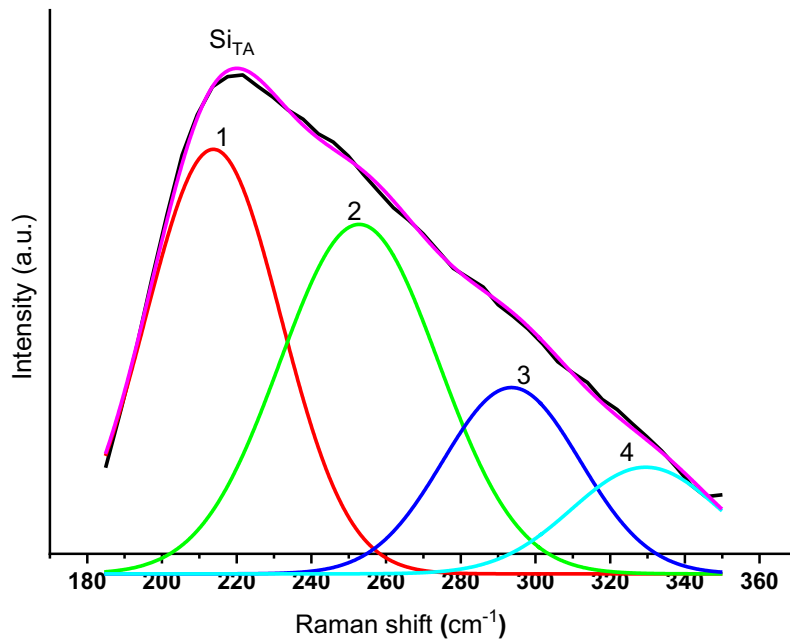


Figure 4. Gauss distribution of acoustic mode (TA) of Si<Ag>  
 sample: 1–214 $\text{cm}^{-1}$ , 2–253  $\text{cm}^{-1}$ , 3–294  $\text{cm}^{-1}$ , 4–330  $\text{cm}^{-1}$

In contrast to the main peak, one can observe scattering by acoustic phonons at  $221 \text{ cm}^{-1}$  (2TA). The authors of [5] attribute such oscillations to the intrinsic Si interstitial defect. As can be seen from

the fig.3, further doping of n-Si single crystals with silver impurity atoms leads to some change in the Raman spectra. When comparing the Raman spectra of the Si<P> and n-Si<Ag> samples, it can be seen

that after doping with Ag atoms, some of the silicon atoms ( $\text{Si}_s$ ) leave the crystal sites, which leads to a slight decrease in the intensity of the fundamental vibration (TO) at  $520 \text{ cm}^{-1}$ .

Compared to the acoustic phonon peak of the second order of the Si<P> sample at  $221 \text{ cm}^{-1}$ , which describes the interstitial nature of the crystal [5], the corresponding Raman peak in the Si<Ag> sample has an increased intensity, its line width is broadened, and the line shape becomes asymmetric with a small tail on the low energy side extending to  $346 \text{ cm}^{-1}$  (Fig. 3). The Gaussian distribution of this peak showed several scattering peaks at 214, 253, 294,  $330 \text{ cm}^{-1}$ , which is shown in (fig. 3). Analyzing the results of many publications

[2; 5], this modification can be explained by an increase in the concentration of interstitial defects ( $\text{Si}_i$ , Ag,  $\text{SiO}_2$ , etc.) after silver doping in silicon, which is caused by an increase in the intensity of the  $221 \text{ cm}^{-1}$  peak.

**Conclusion.** Thus, the processes of Raman scattering of light in silicon doped by diffusion with silver impurities have been studied. It has been shown that an increase in the concentration of interstitial defects in silicon doped with silver atoms leads to an increase in the intensity of the  $221 \text{ cm}^{-1}$  peak. It was also found that in this mode at  $221 \text{ cm}^{-1}$  have four components with Raman shift at 214, 253, 294,  $330 \text{ cm}^{-1}$  which can form nanodefects with self-interstitial impurities of silicon.

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