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STRUCTURE DETERMINATION AND DEFECT ANALYSIS n-Si<Lu>, p-Si<Lu> BY RAMAN SPECTROMETER METHODS

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In this work, lutetium-doped silicon samples were studied using the Raman scattering method. Registration and identification of both crystalline and amorphous phase components in the samples was carried out. There is some violation in the spectra of Raman scattering of light samples of silicon doped with lutetium in comparison with the original sample. It was found that the intensity of Raman scattering of doped samples is 2-3 times higher than the scattering from silicon. The comparison is carried out for the intensities associated with the intensities of the single-phonon line of the silicon substrate. This effect of the Raman spectra in the range 930 cm^{-1} – 1030 cm^{-1} appearing in this range is similar to the data reduction for multiphonon propagation on silicon. For the obtained images (n-Si<Lu> and p-Si<Lu>), the bands in the atomic range of combinatorial scattering have a mixed broad and oval background in the range from 623 cm^{-1} to 1400 cm^{-1}. This background can change the shape of the observed bands.
Keywords*: Silicon; Lutetium; Raman spectroscopy; Diffusion; Doping; Temperature*
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INTRODUCTION

Modern world scientific and technological progress is largely determined by the development of electronics, the achievements of which directly depend on the success of fundamental sciences, primarily solid-state physics and semiconductor physics [1]. Recent advances in these areas are related to the physics of low-dimensional structures and the creation of technologies for obtaining nanostructures with fundamentally new functionality for nano- and optoelectronics, communications, new technologies, measuring equipment, etc. Structured silicon is currently of great interest, since Si itself is an extremely promising material not only for electronics, but also for optoelectronics and solar cells [2,5]. In this regard, studies of the formation of low-dimensional objects and the study of their influence on the electrophysical, optical, photoelectric, and magnetic properties of semiconductors are topical tasks of today [4,6-8]. In the last two decades, Raman spectroscopy (Raman Spectroscopy) has been widely used to study the structure and dynamics of solids. Roman spectroscopy is one of the most powerful analytical methods, when analyzing the chemical and phase state of various objects and their structure and when researching and developing new semiconductor materials, composites, superconductors. Raman scattering has become a standard tool for studying silicon and nanostructured silicon for many years [5,13,14]. Raman studies of nanomaterials provide us with information about energy dispersion, structure, bonding, and disorder [3,16]. In this work, we present the spectra of one- and two-phonon Raman scattering of light from single-crystal silicon doped with lutetium (Lu) atoms.

MATERIALS AND METHODS

Samples of n-Si and p-Si with initial resistivity from 0.3 to 100 Ω·cm were chosen for the study. The samples were doped with Lu impurities sequentially by the thermal diffusion method. Before alloying, the samples were subjected to chemical cleaning and etching, while the oxide layers were removed from the surface of the samples using an HF solution. After thermal degassing of the samples, high-purity (99.999%) Lu impurity films were deposited on clean Si surfaces using vacuum deposition. Vacuum conditions in the volume of the working chamber of the order of $10^{-6}\div10^{-8}$ Torr were provided by an oil-free vacuum pumping system.

Before diffusion annealing, the samples were placed in evacuated quartz ampoules. The diffusion of Lu impurities into the Si bulk was ensured by heating the deposited samples in a diffusion furnace at a temperature of 1250°C for 30 hours followed by rapid cooling. To study the interaction of impurity atoms in silicon, it is necessary not only to uniformly dope the material, but also to maximize the concentration [9,10,17].

The Raman spectra were obtained using a SENTERRA II Bruker Raman spectrometer. This fully automated instrument combines excellent sensitivity with a high resolution of 4.0 cm^{-1}. Sunterra's calibration was automatic and tied to NIST standards, acetaminophen and silicon, resulting in a wavelength measurement accuracy of 0.2 cm^{-1}. The

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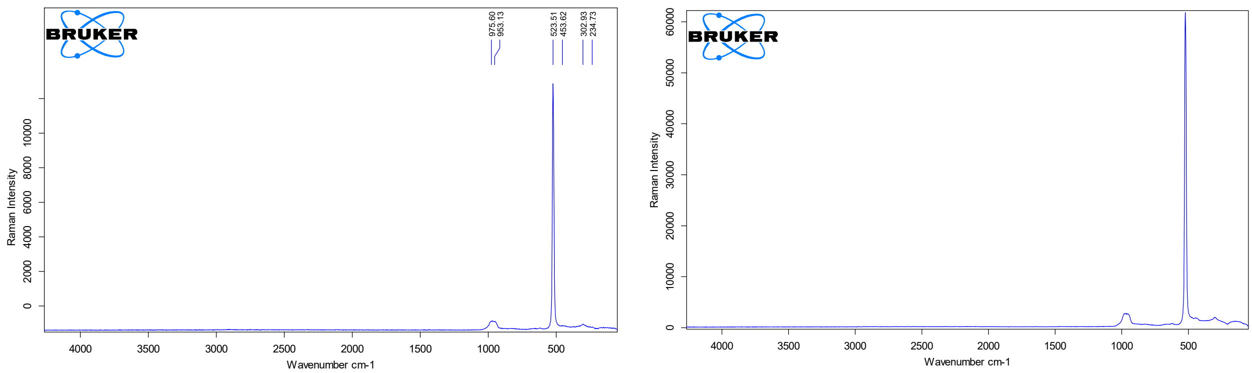
experiments were carried out with a laser with a wavelength l_0 = 532 nm, maximum power P_{max} = 25 mW, acquisition time 100 s, and summation of two spectra. This device makes it possible to obtain spectra in the range from 50 to 4265 cm^{-1}. The Raman spectra were specially processed in order to be able to compare the intensity ratios between the samples. Before normalizing the spectra at the peak at 522 cm^{-1}, which corresponded to the most intense peak in the spectral region 4265-50 cm^{-1}, we subtracted the baseline for each spectrum [11].

Mathematical data preprocessing included offset and cosmic ray removal, baseline correction, and intensity normalization. The intensity of the one-phonon silicon line "523 cm^{-1}" was chosen as a condition for normalization, and the value equal to 1 was chosen. Preliminary processing was carried out using the OPUS 8.5 program (Senterra II, Bruker, Germany). The measured spectra for materials with high κ were compared with the data obtained for n-Si and p-Si.

Samples: n-Si, p-Si and lutetium-doped silicon, n-Si<Lu>, p-Si<Lu> were characterized by Raman spectroscopy.



a) **b)**

Figure 1. Raman spectrum measured for n-Si and p-Si samples, excitation wavelength 532 nm
a) n-Si spectrum; b) p-Si spectrum

Figure 1 shows the data collected for n-Si and p-Si samples. In the studied spectra are present as signals modeling a single-phonon silicon line. The following bands can be recognized in the spectrum (except for the Si "523 cm^{-1}" line):

(I) faint band peaking around 230 cm^{-1};

(II) relatively strong propagation of the band from 300 cm^{-1} to the one-phonon Si line (~550 cm^{-1});

(III) band with one maximum at about 623 cm^{-1};

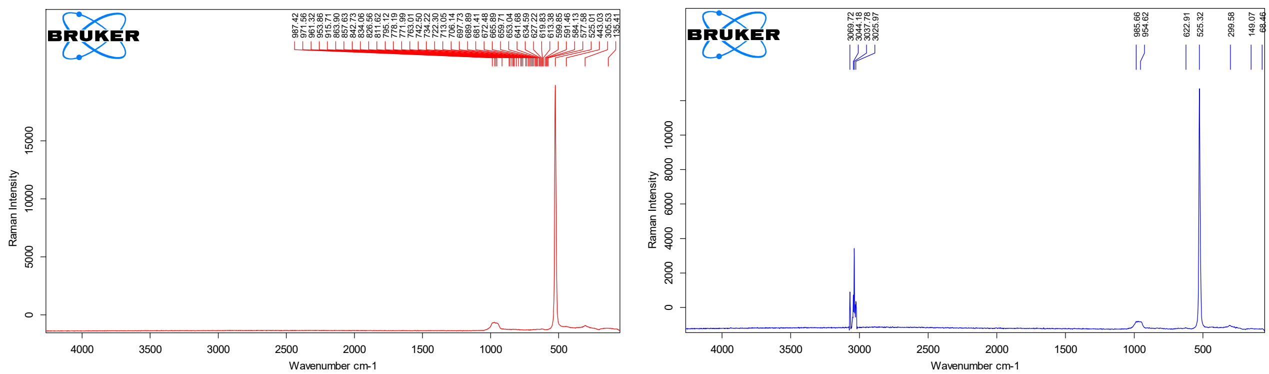
(IV) a broad band with a maximum at about 810 cm^{-1};

(V) relatively average band spread from 930 cm^{-1} to 1030 cm^{-1};

The Raman spectra measured for silicon wafers doped with Lu (n-Si<Lu> and p-Si<Lu>) are shown in Fig. 2. The two most important similarities observed for both semiconductor materials can be distinguished without detailed analysis:

(I) the absence of the so-called bosonic band;

(II) the presence of a band between 930 cm^{-1} and 1030 cm^{-1} in the literature is attributed to multiphonon scattering generated in a silicon substrate [12].



a) Spectrum of p-Si<Lu> b) Spectrum of p-Si<Lu>

Figure 2. Raman spectrum measured for n-Si<Lu> and p-Si<Lu> samples, excitation wavelength 532 nm

Analysis of the Raman spectrum taken for reference samples of n-Si and p-Si (Fig. 1). The band located between 930 cm^{-1} and 1030 cm^{-1} refers to multiphonon scattering generated in the silicon substrate [12]. The first feature that appears in the spectra recorded for silicon wafers doped with Lu (n-Si<Lu> and p-Si<Lu>) (Fig. 2) is a significant signal below 300 cm^{-1}. This corresponds to the boson band recorded for excitation with visible Raman scattering [15]. The absence of a relatively strong band in the Raman shift range between 930 cm^{-1} and 1030 cm^{-1} is attributed to second-order scattering in doped silicon also observed for both impurity layers (n-Si<Lu> and p-Si<Lu>). The spectra obtained for n-Si<Lu> and p-Si<Lu> contain not only broad bands, but also narrow lines; the full width at half-height of these lines is about 1 cm^{-1}. This suggests fluctuations in crystal structures as the origin of these lines. Amorphous structures generate bands with a half-width on the order of 10 cm^{-1}. The appearance of the first line in the scattering observed for both semiconductors has a maximum of about 300 cm^{-1}. The broad band merged with the one-phonon Si line begins between 305 cm^{-1} and 440 cm^{-1} and is much narrower than the main band. This is followed by a lower growth in the range of 420 cm^{-1}÷500 cm^{-1}. In the Raman shift range of 500 cm^{-1} and 540 cm^{-1}, the single-phonon Si line dominates in the Raman spectrum. One narrow line peaking at 395 cm^{-1} and a slightly wider band peaking at 452 cm^{-1} appear in the spectrum of the obtained composites. The next two bands appearing in the Raman spectra have maxima at 622 cm^{-1} and 680 cm^{-1}. A maximum of 622 cm^{-1} corresponds to an unconsolidated structure, and 680 cm^{-1} corresponds to a densified structure. The next band present in the Raman spectra, registered for composites, has a maximum at about 780 cm^{-1}. The intensity of the band related to the intensity of the one-phonon Si line in the case of composites is approximately two times greater than that for silicon. The following features can be distinguished in the range of the Raman shift from 930 cm^{-1}÷1030 cm^{-1}.

The Raman spectra recorded for n-Si<Lu> and p-Si<Lu> show a broad oval background that ranges from 623 cm^{-1} ÷ 1400 cm^{-1}. The bands described earlier appear against this background. In this case, the Raman scattering signals do not have the typical shape of the observed band for the Si layer and are assigned to multiphonon scattering from the silicon substrate [12]. It is possible that the band assigned to multiphonon scattering is modified and partially masked by the broad background. The last two bands that can be recognized in the spectra measured for the obtained composites have maxima around 1070 cm^{-1} and 1200 cm^{-1}. The band with the maximum at 1070 cm^{-1} has a symmetrical shape. The group with a maximum at 1200 cm^{-1} seems asymmetric. The tail of this band reaches 1400 cm^{-1}. The maxima of these bands reported in the literature are approximately 1075 cm^{-1} and 1200 cm^{-1}, respectively.

CONCLUSIONS

In this work, samples of n-Si, p-Si were studied, as well as samples doped with lutetium, n-Si<Lu>, p-Si<Lu>, according to the data obtained, were characterized using Raman spectroscopy. Raman spectra of doped n-Si<Lu> and p-Si<Lu> samples were compared with silicon. It was found that the intensity of Raman scattering of doped samples is 2-3 times higher than the scattering from silicon. The comparison was made for intensities related to the intensity of the single-phonon line of the silicon substrate.

The last thing to sum up is the behavior of the Raman spectra in the range 930 cm^{-1}÷1030 cm^{-1}. The band appearing in this range is similar to the reduction of data for multiphonon scattering on silicon.

For the obtained n-Si<Lu> and p-Si<Lu> samples, the bands in this range of Raman scattering are shifted with a broad and oval background in the range from 623 cm^{-1}÷1400 cm^{-1}. This background can change the shape of the observed bands.

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ВИЗНАЧЕННЯ СТРУКТУРИ ТА АНАЛІЗ ДЕФЕКТІВ n-Si<Lu>, p-Si<Lu> ЗА ДОПОМОГОЮ РАМАНІВСЬКОЇ СПЕКТРОСКОПІЇ

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У даній роботі методом комбінаційного розсіяння досліджено леговані лютецієм зразки кремнію. Проведено реєстрацію та ідентифікацію компонентів як кристалічної, так і аморфної фаз у зразках. Спостерігається деяке порушення в спектрах комбінаційного розсіювання світла зразків кремнію, легованого лютецієм, порівняно з вихідним зразком. Встановлено, що інтенсивність комбінаційного розсіювання легованих зразків у 2-3 рази перевищує розсіювання кремнію. Порівняння проведено для інтенсивностей, пов'язаних з інтенсивностями однофононної лінії кремнієвої підкладки. Цей ефект спектрів комбінаційного розсіювання в діапазоні 930 $см^{-1}$ – 1030 $см^{-1}$, що з'являється в цьому діапазоні, подібний до зменшення даних для розповсюдження мультифононів на кремнії. Для отриманих зображень (n-Si<Lu> і p-Si<Lu>) смуги в атомному діапазоні комбінаторного розсіяння мають змішаний широкий і овальний фон в діапазоні від 623 $см^{-1}$ до 1400 $см^{-1}$. Цей фон може змінювати форму спостережуваних смуг.
Ключові слова: *кремній; лютецій; раманівська спектроскопія; дифузія; легування; температура*