RAMAN SPECTRA IN HETEROSTRUCTURES Ge/$Ge_{1-X}Si_X$

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The structure studied in this work has been obtained by the method MLE on Ge substrates. The parameters of the samples were determined by method of x-ray structure analysis. The method of combined light scattering spectroscopy was used for the regulation of the content.

At modern stage of scientific and technological revolution special emphasis is placed on the advancement of those fields of science the achievements of which define the wide prospect of technological development. These fields of science include semiconductor physics, one of the main tasks is search, study and modification of crystal properties with high values of applied-physics characteristics in order to develop new materials promising different technological applications.

Solid solutions of Ge and Si are of great interest from scientific and technological aspect. This interest is conditioned by multiple unique properties: complete solubility, continuity of electrical properties' change, resistance against thermal actions, large energy gap width, high fusion temperature, mechanical strength, resistance against the effect of high-energy particle bombardment and others.

At present it was experimentally showed that Ge and Si really form solutions not only in liquid state but also in solid state and the quantity of lattice parameter of $Ge_{1-X}Si_X$ solid solutions change almost linearly with the change of solution and alloy composition.

The interest to the study of defectless films of $Ge_{1-x}Si_x$ solid solutions at substrates of Ge is connected with practical significance of such structures for developing of transistors with high charge carrier mobility in channel. In such devices the channel has thin (10 nm) stressed layer of Si and Ge grown in buffer layer from solid solution. At the result of significant mechanical stress stretching for Ge (constriction for Si) leading to splitting of valley, charge carrier mobility can increase for several times the value of unstressed material [1]. As vibration spectrum of lattice depends substantially on atomic composition of films and amount of mechanical deformation in them and are considered relevant for Raman spectroscopy (RS) to evaluate these parameters.

Raman spectroscopy is a rapid, informative and nondestructive technique. The first analysis of the composition and mechanical stress in $Ge_{1-x}Si_x$ solid solutions were carried out in the 60s of the last century, the technique improved and developed [1-3] but there still remain methodical difficulties bringing to ambiguity in interpreting of obtained results.

So the purpose of the work is formulation of refined parameter description of the dependence of intensity and position of Raman scattering peaks on the composition and permanent and mechanical deformation in the films of $Ge_{1-x}Si_x$ solid solutions on the substrates of Ge with orientation (100).

Experimental samples were developed with application of molecular beam epitaxy (MBE) on the substrates of Ge with orientation (100). After standard procedure of chemical cleaning the substrate of Ge charged into growing vessel MBE. Disposal of protective and chemically applied germanium was conducted at the temperature 650-700°C in low flow of Ge (0.02nm/s). The next stage was growing of buffer layer of Ge the thickness of which was 50 nm with the purpose of obtaining of maximum pure surface of Ge (100) and this had superstructure transformation such as 2x1. After observing such surface transformation film growth of $Ge_{1-X}Si_X$ solid solutions was realized with the help of DBE, for the obtaining of which the method of low-temperature MBE had been used [4,5]. Growth rate of $Ge_{1-X}Si_X$ solid solutions was about 0.1nm/s. The thickness of the films varied between 250 and 500 nm. The composition and residual mechanical stress in obtained structures were checked by the method of X-ray diffraction. Analysis of rocking curves of X-ray diffraction taken in several allowed reflections for Ge (for example, (113) and (004)) was used for this purpose.

Peculiarity series were detected during thermal treatment of deposited $Ge_{0.85}Si_{0.15}$. Films of solid solutions $Ge_{0.85}Si_{0.15}$ are extremely resistant against thermal annealing. Condensates obtained at the temperature T_n=490K carried quasi- amorphous character. At the temperature range 350-450K they carry semiconductor character of conductivity with thermal activation energy which equals to 0.052eV. This value was determined according to inclination of graphics $lg\ \sigma=f(1/T)$ constructed for experimental values, at the temperature regions 450-550K, 550-680K semiconductor character of conductivity remains unchanged but activation energy slightly increases and reaches to 0.096eV. At these temperature regions three sections are observed with more abrupt change of electrical conduction (350-420K, 510-540K, 590-620K) which are responsible for crystallizing process realized in condensates.

Crystallization kinetics and thermal stability were studied by heating amorphous films directly in electron microscope column UEMV-100K using adapters PRON-2 (fig.1). At the same time thermal stability of amorphous state was determined with the appearance of diffuse maximums of amorphous phase on the background which are more

intensive than diffraction reflections of crystalline phase. Films formed at the substrates in the process of deposition at the room temperature and at the temperature 490K.

For example, in Fig. 1 sequential stages of structural transformations in amorphous films were given. Amorphous films $Ge_{0.85}Si_{0.15}$ don't be in equilibrium in initial state but they relax to metastable state. At that with the increase of temperature annealing of defects, change of free volume and short-range topological order occur too, but composite order remains unchanged.

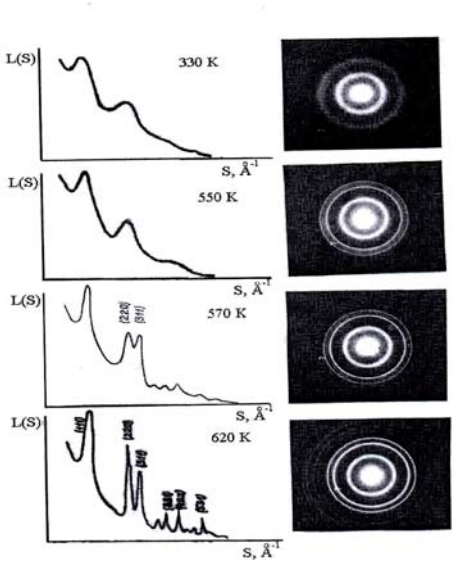

Fig. 1. Crystallization kinetics of films of solid solutions $Ge_{1-x}Si_x$ (x-0.15).

In order to study thin films $Ge_{1-x}Si_x$ by the method of Raman scattering it would be better to use wave-lengths of laser radiation of blue-green range in consequence of light absorption's shallow depth (less than 10nm). But Raman spectra have data only on upper layer.

Raman spectra were registered at room temperature with the help of automatic plant on the basis of spectrometer DFS-52 using lines of Ag-laser 514.5 nm.

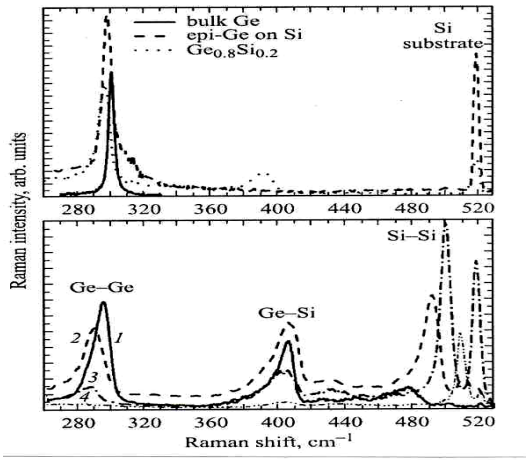

Fig. 2. Raman spectra of relaxed germanium films (dashed line) and solid solutions $Ge_{1-x}Si_x$ (dots) are shown above. For comparison spectrum of bulk germanium (full line) are shown too. Raman spectra of the films of solid solutions $Ge_{1-X}Si_X$ are given below.

In fig.2 Raman spectra of pure germanium films and germanium- silicon solid solutions were shown at frequency ranges of optical oscillations Ge-Ge (about 300 cm^{-1}), Ge-Si (about 400 cm^{-1}) and Si-Si (about 500 cm^{-1}).

It is seen that peaks of Raman scattering on oscillations Ge-Ge –coupling films of silicon grown on germanium substrate shift to the side of low frequency (approximately for 2cm^{-1}) and broadened. For silicon and germanium tensile stress shifts phonons' frequency to the side of low frequency. Tensile stress in the films of silicon and germanium may occur at cooling of heterostructures due to different coefficients of thermal expansion of germanium and silicon. If structural stress was relaxed in growth process at epitaxial temperature, then tensile stress may occur in the film at cooling of the sample. Observed high-frequency arm may be conditioned by the presence of local mechanical compression stress near dislocations. On spectrum of $Ge_{1-x}Si_x$ films you can see peaks from scattering to coupling vibration Ge-Si (~395cm^{-1}).

In some works authors tried to determine the composition of films according to the state of Raman scattering peaks [4-6]. The basic difficulty of this technical approach is that state of peaks depends on mechanical stress (shift may reach 17cm^{-1} for the peak of Ge-Ge and 35cm^{-1} for the peak of Si-Si). Another difficulty is that if the composition of silicon is small in heterostructures, Raman scattering peaks can't be seen in coupled vibrations of Si-Si and its state can't be determined.

Numerous simulations of Raman spectra were conducted to determine the dependence of peaks' state. Due to cyclic and boundary conditions natural frequency and eigenvectors of oscillation were calculated in Ge-Si solid solutions basing on Bohr model, then according to the obtained data Raman spectra were calculated basing on Wolkenstein's additive bond polarizability model [6]. Coupling constants of hardness for germanium in Bohr model were determined by approximation of computational phonon dispersion in bulk material to experimental data obtained according to the one on neutron scattering [7]. As phonon dispersion both for germanium and silicon are very identical, mass substitution method was used to construct Ge-Si heterostructure. Solid solution was simulated on the basis of random filling of unit cell by germanium and silicon atoms with necessary relationship *x*. In order to avoid the influence of periodical boundary conditions quite big unit cell containing 432 atoms was chosen for calculations.

Relation of derived coupling polarizability for germanium and silicon was defined on normalized relationships of Raman scattering intensity to scattering volume for germanium and silicon. More detailed calculations were given in the works [8-10].

According to literary data state of Raman scattering peaks on optical phonon for bulk germanium are 300-302cm^{-1}. As for the germanium GES-40 studied by us, the state of the given peak was 300.3 cm^{-1}. Dispersion of optical phonons has such character that localization effects make their frequencies decrease. Phonons having frequencies peculiar to optical coupling oscillations Ge-Ge scatter and damp by more light atoms and become local ones.

It was established that electrical conduction of the films of $Ge_{0.85}Si_{0.15}$ solid solutions at high temperature (300-500K) carries band-to-band conductivity character.

At the result by determination of parameters and by the method itself it was shown that the composition and mechanical stress in heterostructures $Gt/Ge_{1-x}Si_x$ can be defined on the basis of Raman scattering data.

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Ge/$Ge_{1-x}Si_x$ GETEROSTRUKTURLARINDA KOMBİNASİON SƏPİLMƏ SPEKTRLƏRİ

$Ge_{1-x}Si_x$ əsasında Ge altlıq üzərində molekulyar dəstədən səpilmə yolu ilə alınmış hetorokeçidin parametrləri rentgenstruktur analiz və rekombinasiya olunmuş işığın səpilmə metodu ilə təyin olunmuşdur.

Qüsursuz Ge/$Ge_{1-x}Si_x$ nazik təbəqənin alınması yüksək yürüklüyə malik tranzistorun hazırlanmasında böyük əhəmiyyət kəsb edir.

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СПЕКТРЫ КОМБИНАЦИОННОГО РАССЕЯНИЯ В ГЕТЕРОСТРУКТУРАХ Ge/$Ge_{1-X}Si_X$

Структуры, исследованные в настоящей работе, получены методом МЛЭ на Ge подложках. Параметры образцов определены методом рентгеноструктурного анализа. Метод спектроскопии комбинационного рассеяния света использовался для контроля состава.

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