WIDENING OF Si UNDER THE IMPACT OF ILLUMINATION

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Based on the experimental data, the article demonstrates the increase of the interatomic distances in a monocrystalline Si under the stationary illumination with white light. The appropriate estimation has been carried out in the harmonic approximation within the athermal mechanism of widening of semiconductors. The theoretical results are in good agreement with the experimental data.

As known [1], electrons taking part in the generation of chemical bonds in solid bodies may be in two states: in a bonding state where they strengthen interatomic chemical bonds and in an antibonding one where they weaken them. Semiconductors in bonding states correspond to the valence band, while anti-bonding ones correspond to the conduction band [1]. Hence, electrons in the conduction band and a hole in the valence band (antibonding quasiparticles — AQP) weaken the chemical bonds between atoms, in the vicinity of which they will be situated during their chaotic movement. Judging from the above-said, the transfer of an electron in a semiconductor from the valence band into the conduction one results in a decrease of the energy of chemical bonds. The more the concentration of free carriers, the more is the decrease [2]. It is known that a decrease of the energy of chemical bonds increases the length of chemical bonds and decreases its force constants [3], which should lead to the widening of a semiconductor.

The changes in the size of a crystalline Ge under the influence of impulse light were reported in [4]. The quantitative interpetation of the obtained results was complicated by the fact that, in Ge, a change of the lattice parameter occurred in the same direction as under the influence of heat. However, several arguments support the share of the optical nature in the observed phenomenon. In [5], the deformation of a crystalline Si under the impulse laser influence has been studied. The mark of these effects is the same as the mark of the coefficient of a change in the forbidden zone under pressure, and, therefore, the obtained experimental data are a better reflection of the deformation of a crystalline Si under the impact of a shock wave generated by means of mighty laser radiation, than the change of an interatomic distance as a result of the excitement of unequal carriers, whenever the outer deformation does not influence a crystal.

Below presented are the preliminary results of the investigation of a change of the dimension of the lattice of Si under the action of the illumination with white light and the corresponding theoretical calculation in the harmonic approximation.

The object of the investigation was a non-dislocational monocrystalline Si of the n-type with the specific resistance 200 $\Omega\times$cm and with the surface orientation (100). The disorientation did not exceed 0.3°. We applied the radio-diffraction method of the precession measurement of the dimension of a lattice by means of the standard allowing to carry out the estimation to within 10^{-6}—10^{-7} Å [6]. The Cu$K_{\alpha 1}$ monochromatic radiation was applied. The lighting was carried out by means of two incandescent tungsten lamps. The photo-Hall effect was measured, and, in the process of lighting, the concentration of charged carriers excited by the light on the surface of the sample was 4×10^{14} cm^{-3}. To decrease the thermal influences upon crystals, the system was being cooled by a flow of air. Temperature was measured relatively to the temperature of ice by means of a thermocouple adhered on samples with heat-conductive glue. By means of the experiment, we determined $\Delta\theta$ — a change of the angular distance between the peaks (from the standard and the sample in darkness), having occurred as a result of the lighting of the sample. Based on Bragg's differential formula, we evaluated the relative change of the interatomic distance $\frac{\Delta a}{a} = \Delta\theta\,\mathrm{ctg}\theta_{\mathrm{B}}$, where θ_{B} is Bragg's angle for the standard.

The control experiments were carried out in order to measure the dimensions of the lattice in darkness at the same temperature, introduced as an addition (29°) by

means of the illumination. The bond's method for the determination of a lattice dimension [7] was applied.

Subtracting the relative increment caused by the temperature without lighting (8.1×10^{-5}) from the common (light + temperature) relative increment of the interatomic distance (9.6×10^{-5}), we get the relative increment caused by the pure optical impact of light: (1.5×10^{-5}) (see the table).

While the electron transfers from the bonding state into the antibonding one, the force constants of chemical bonds have been weakened at the permanent temperature, which should result in an increase of the interatomic distance even in the harmonic approximation. We will try to assess this increase in the interatomic distance by means of elementary calculations.

For simplicity, we will discuss a linear chain in the light of the fact that the energy of the bond between atoms, while AQPs are present near them, falls down (the weakening impacts of an antibonding electron and a hole have been considered identical). Assume that, at a certain moment of time t_1, an AQP appears at an atom, by remaining with the given atom for the period of time Δt. $\Delta t = t_2 - t_1$, where t_2 is the moment of the AQP's departure. Within the harmonic approximation, we can write the system of differential equations for the oscillation of the given atom under these conditions as

$$\begin{cases} x_1'' + \omega^2 x_1 = 0 & 0, \le t \le t_1, \\ x_2'' + \omega_1^2 x_2 = 0, & t_1 \le t \le t_2, \\ x_3'' + \omega^2 x_3 = 0, & t_2 \le t \le \tau, \end{cases} \tag{1}$$

where ω and ω_1 are the cyclic frequencies of non-excited and excited atoms, respectively. It is clear that $\omega > \omega_1$. The contiguous and initial conditions for the system of equation (1) look as

$$x_1(0) = 0, \quad x_1(t_1) = x_2(t_1),$$

$$x_1'(t_1) = x_2'(t_1), \quad x_1'(0) = V,$$

$$x_2(t_2) = x_3(t_2), \quad x_2'(t_2) = x_3'(t_2),$$

$$x_3'(\tau) = 0, \tag{2}$$

where V is the maximum velocity of an atom.

Conditions of the experiment	$\Delta d/d$	
Illumination+temperature	9.6×10^{-5}	
Temperature	8.1×10^{-5}	
Illumination	Experiment	Calculated
	1.4×10^{-5}	1×10^{-5}

The contiguous conditions include the continuity of coordinates and the velocity. By means of the latter condition, the period of oscillation can be established.

The solution of the system of equations (1) under the contiguous conditions (2), in view of $\omega \sim 10^{13}\text{s}^{-1}$, $\Delta t \sim 10^{-15}$ s (i.e. $\omega\,\Delta t \ll 1$), is as follows:

$$x(t) = \frac{V}{\omega}[\sin\omega(t-\Delta t) + \omega\,\Delta t\cos\omega(t-\Delta t)]. \tag{3}$$

From (3), in view of (2), we get

$$\tau = \tau_0\left[1 + \frac{2(\omega\,\Delta t)^3}{3\pi}\right], \tag{4}$$

where τ_0 is the period of oscillations of the non-excited atom, while$\tau$is the period of oscillations under excitation.

By averaging (3) over the period of oscillations τ, we obtain

$$\overline{x} = (1/\tau)\int_0^{\tau_0} x(t)dt = \frac{V}{\omega}\,\frac{(\omega\,\Delta t)^2}{2\pi}. \tag{5}$$

The latter formula shows that, as far as $\overline{x} > 0$, the chain becomes wider due to an increase of the inter-atom distance, which may depend, in its turn, on the concentration of AQPs.

Let us estimate the relative increase of a linear chain. For the period of a single oscillation, each AQP runs the number of atoms in the chain $\alpha = n' v_{e,h}\tau/d$, where $n' = \sqrt[3]{n}$, $v_{e,h} = \sqrt{kT/m^*_{e,h}}$ is the thermal velocity of an AQP, and d is the interatomic distance in the chain.

We suppose that $m^*_{e,h} \sim 10^{-27}$g. Then, the average growth of the chain will be $\overline{x}\,\alpha = \Delta l$, while the average increase in the interatomic distance in the chain is $\Delta d = \frac{\Delta l}{N'}$, where $N' = \sqrt[3]{N_A}$, N_A is the concentration of atoms in Si.

Therefore, the relative increase in the interatomic distance has the form

$$\frac{\Delta d}{d} \sim \quad \sqrt[3]{\frac{n}{N_a}}\sqrt{\frac{m^*_{e,h}}{M}},$$

where M is the mass of a Si atom.

As a result, we get $\frac{\Delta d}{d} \sim 1\times10^{-5}$, which is in a satisfactory accordance with the experimental data.

Thus, the simple calculations in the harmonic approximation have demonstrated that the growth of the concentration of AQPs results in the increase in the interatomic distance. The theoretical value well agrees with the experimental data.

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РОЗШИРЕННЯ КРЕМНІЮ ПІД ВПЛИВОМ СВІТЛА

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Р е з ю м е

Експериментально показано збільшення міжатомної відстані у монокристалічному кремнії у стаціонарному режимі освітлення білим світлом. Проведено відповідний розрахунок у гармонічному наближенні на основі атермічного механізму розширення напівпровідників і отримано задовільне узгодження між експериментальними і теоретичними даними.