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P. Żukowski[1], J. Partyka[1], P. Węgierek[1], T. Kołtunowicz[1],
M. Kowalski[1], Yu. Sidorenko[2]

Generation-Recombination Mechanism of Hopping Recharging Between Deep Amphoteric Defects in Strongly Defected Semiconductors

[1]Lublin University of Technology, Lublin, Poland
[2]Belarusian State University, Minsk, Belarus

The paper presents a model of hopping recharging between amphoteric defects (impurities) of a basic charge state that is neutral. It has been -proved that an increase of defect concentration brings about a decrease of the life period, which consequently leads to a transition from the band conductivity to the hopping conductivity. The transition criterion is when the life period and relaxation time values approach each other.

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One of the best-known effects of hopping recharging is hopping conductivity between shallow donors in semiconductors compensated with shallow acceptors [1]. However, hopping recharging involves a wider spectrum of phenomena part of which has not been sufficiently examined yet. It is well known that processes of hopping recharging occur between defects in amorphous Si and Ge as well as in some strongly defected semiconductors. Those processes can determine paramagnetic and structural properties of strongly defected (amorphous) silicon [2], intrinsic restoration of implanted silicon layer structures [3], and thermally activated increase of permittivity in silicon irradiated with big doses of neutrons [4] and ions [5]. There can be two types of hopping recharging mechanisms. The first one is typical for impurities (defects) of two charge state types - neutral and positive - and concerns the case when an electron jump occurs from a neutral-state impurity to a positively charged one. Such a process brings about hopping conductivity in electric field [1]. The other type of hopping recharging is characteristic for the case of amphoteric defects that can be of neutral, positive and negative charge states of. An electron jump from one neutral defect to another leads to the formation of an electric dipole and consequently to additional polarization of strongly defected semiconductors, for instance of silicon irradiated with neutrons [4] and implanted [5] or compensated compounds of A^2B^2 and triple compounds A^2B^6 with transition metals [6]. Phenomenological model of such hopping recharging has been presented in [5,6]. A microscopic model of the process of electron exchange between amphoteric defects of a neutral charge state is presented below.

Defects that form in intrinsic silicon during its irradiation with big doses of neutrons or other high-energy particles for the most part are of a neutral charge state of. Most of defect types are amphoteric which means that apart from a neutral charge state they can also occur in the positive and negative states. For example, divacancies can be of «+», «0», «-», and «2-» states while interstitial defects - of «+», «0» and «-» states [7,8]. Moreover, those defects simultaneously make recombination centers and in their neutral charge state they are of a cross-section for recombination of ca 10^{-14} cm^{-2}.

Concentration of carriers in intrinsic semiconductors is a statistical quantity that can be found based on the Fermi level location [10].

$$n = 2\left(\frac{2\pi m_n kT}{(2\pi\hbar)^2}\right)^{3/2} \exp\frac{F - E_c}{kT} \qquad (1)$$

As in intrinsic semiconductors the Fermi level is located near the energy gap center then:

$$n \cong 2\left(\frac{2\pi m_n kT}{(2\pi\hbar)^2}\right)^{3/2} \exp\left(-\frac{E_g}{2kT}\right) \qquad (2)$$

On the other hand, electron concentration in the conduction band is determined by processes of their thermal generation from levels in the energy gap or from the valency band and by recombination processes that run in the reverse direction [11]. It means that an electron does not dwell in the conduction band constantly as it is in metals but only for a time determined by recombination processes. Over that time an electron participates in thermal motion and in the presence of electrical field it also participates in conduction current. When its life period is over the electron returns, for instance to the valency band, and a new electron is generated in its place. For pure intrinsic silicon the life period is of ca 10^{-3}s, which means that an electron from the moment of its generation to the recombination is a subject to 10^{10} scattering acts. Such an electron can be fully considered as a free one. Conduction processes in strongly defected silicon run another way. For instance, for a concentration of neutral divacancies of $N_w=10^{20}$cm^{-3}, which is a characteristic quantity for disorder areas in silicon, an assessment of the life period at the room temperature determined based on a cross-section of capture by neutral divacancies $W_w(0)=10^{-14}$cm^{-2} given in [9] amounts to:

$$\tau_w = \frac{1}{N_w S_w(0)v} \cong 10^{-13}\,\text{c} \qquad (3)$$

where: v - electron velocity.

In such a material, between the moments of the generation and recombination an electron practically does undergo any scattering, as its life period τ_w is comparable to the pulse relaxation time and is considerably shorter than the energy relaxation time [12]. In that case an electron that is excited from a neutral defect to the conduction band gets captured by a neutral defect practically without undergoing any scattering. That way in strongly defected crystals a transition from the band- to the hopping conductivity occurs. Fig. 1 illustrates the electron exchange between two neutral defects. As can be seen in the figure according to the discussed generation-recombination mechanism the presence of neutral defects of three charge states - «0», «+» and «-» - makes a necessary condition for hopping recharging. It can also be seen in the figure why in strongly defected semiconductors high energies (Δ≥0,1eV) of the hopping conductivity activation can be observed. Apart from the above the figure also illustrates one more important effect of the considered model i.e. a formation of field-oriented dipoles, whose presence can bring about an additional polarization [4,6]. As can be seen in Fig.1, charged defects on account of the energy states of their levels should have properties of one-time trapping levels. In that case trapping times τ_p,τ_n will be considerably longer that the life period ($\tau_n,\tau_p \gg \tau_w$) and the semiconductor will be a strongly compensated one.

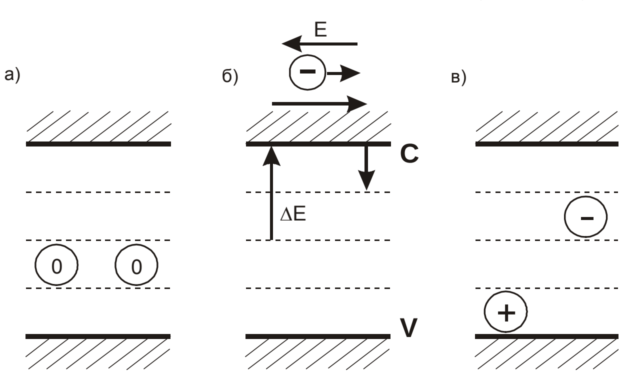

Fig. 1. Electron exchange between two neutral divacancies in an external electrical field a) initial state, b) electron jump - hopping recharging, c) final state - dipole

The compensation rate at its first approximation can be assessed from the following expression:

$$C \approx 1 - \frac{\tau_w}{\min(\tau_n, \tau_p)} \qquad (4)$$

In that case concentration of charged defects will be many times greater than the electron concentration.

$$N^+ \approx N^- \approx n\frac{\min(\tau_n, \tau_p)}{\tau_w} \qquad (5)$$

For example, for the trapping time of ca 10^{-6}s and the room temperature in silicon of $N_w=10^{20}$cm^{-3} the concentration of positively and negatively charged defects (dipoles) should be of the 10^{17}cm^{-3} order. At the temperature of 400K the dipole concentration grows up to 10^{19}cm^{-3}, which means that for example 20% of the defects will occur in charged states.

Compensation degree in semiconductors of high amphoteric defect concentrations has been more elaborately discussed by the Authors in [13].

It follows from the generation-recombination mechanism that a mean jump length is:

$$\overline{R} \cong \frac{3}{2S_e(0)N} \qquad (6)$$

A mean distance between defects is $R_{śr}=N^{-1/3}$. At the defect concentration of $N_k=[3/2S_e(0)]^{3/2}$ the mean jump length $\overline{R} = R_{śr} = N_k^{-1/3}$ equals a mean distance between defects. For neutral divacancies $N_k=3.5 \times 10^{20}$cm^{-3}. In the case of the generation-recombination mechanism probability of hopping recharging per time unit can be described as follows:

$$P(T,R) = S_e(0)v_e N_c e^{-\frac{\Delta E}{kT}} \qquad (7)$$

where: v_e - electron velocity, N_c - density of states.

Values of the above given parameters v_e and N_c should differ from the ones accepted in the classical theory of recombination. As an electron does not undergo scattering acts its velocity v_e can differ from the thermal velocity. As in strongly defected crystals «tails» that penetrate into the energy gap show up, density of states N_c differs from the quantity that is characteristic for non-defected semiconductors and is included in the expressions (1) and (2). Hence, N_c is a function of defect concentration and the rate of electron location on them.

Likewise, activation energy ΔE does not describe the location depth of a defect-related level as first - at big concentrations of defects a band of deep levels forms and secondly - a distance from that band to the conduction band gets reduced when the density-of-states «tails» show up. Density of states in the conduction band tails has been analyzed by many authors and its dependence on the concentration of charged defects can be considered by using, for example, results of [14]. Dependence of the deep-level band width on the defect concentration and temperature has been presented in [13].

Thus, in the case of amphoteric defect concentration increase, for instance at increasing an irradiation dose for a semiconductor, which results in the life period decrease, it naturally passes from the inter-band conductivity to the hopping conductivity. The transition criterion is when the life period and relaxation time values approach each other At the irradiation with particles (neutrons, ions etc.) that involve the formation of defect concentration areas hopping recharging can occur in separate areas at microscopic defect concentrations - much smaller than those described by the expression (3). One of the outcomes of the generation-recombination mechanism of hopping recharging is a possibility of an additional polarization of strongly defected materials.

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П. Жуковскі[1], Й. Партика[1], П. Вуйчек[1], Т. Кольтуновіч[1],
М. Ковальскі[1], Ю. Сідоренко[2]

Рекомбінаційно-генераційний механізм стрибковоподібної провідності в сильно дефектних напівпровідниках з глибоко амфотерними дефектами

[1]Люблінський технічний університет, Люблін, Польща
[2]Білоруський державний університет, Мінськ, Білорусія

Стаття представляє модель стрибковоподібної провідності в сильно дефектних напівпровідниках з амфотерними дефектами. Показано, що збільшення концентрації дефектів викликає зменшення періоду життя носіїв струму, що призводить до переходу зони провідності до стрибковоподібної провідності. Перехідний критерій – це, коли період життя і значення часу релаксації прямують один до одного.