POSSIBILITIES OF PRESENCE OF SCHLÖGL QUASICHEMICAL REACTIONS IN AN ATMOSPHERE OF OWN SILICON DEFECTS

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The important case of evolution of an atmosphere of own dot defects of silicon is considered. It is shown, that own interstitial atoms of silicon (I) and to concentration C_V of vacancies (V) in an atmosphere of own defects of silicon presence bystable states is probably inherent in concentration C_I , transition between which can be described Schlögl quasichemical reactions.

The consideration of evolution of properties of materials of nuclear and electronic technics lead by work on an example of silicon on the basis of simple models Schlögl, confirms the statement that properties nanomaterials and usual materials cannot be considered on cleanly mechanical basis. They should be considered as a part of the general problematics of the nonlinear dynamic systems working far from balance (I.R.Prigogine's postulate). Special value get in this connection experimental researches synergetic effects at synthesis and operation of these nanomaterials the most various physical and chemical methods. It will probably allow to establish, what of scripts synergetic models at the certain set parameters environments are realized during evolution of an atmosphere of own defects nanomaterials, for example, silicon.

Let's consider the most probable quasichemical reactions in an atmosphere of dot defects in silicon, being guided on researches Schlögl and Schöll [1,2] nonequilibrium generation-recombination- (GR) processes in semiconductors (mean GR – processes of electron-hole pairs). In system also course quasichemical reactions of Brusselator, Oregonator, Lottky-Volterr type [1-4] and by many other things of the reactions known and unknown now, certainly, is not excluded. Here we are limited to a case of Schlögl quasichemical reactions [1], as the most simple and consequently, apparently, the most probable in system of own dot defects. Researches of these reactions [5] have allowed to choose the most probable reactionary scheme from many possible interactions I and V among themselves and with divacancies V_2 in an atmosphere of own defects.

$$I + V \xleftrightarrow{k_{f1},k_{f2}} O, \qquad (1)$$

$$O + I \xleftrightarrow{k_{I1},k_{I2}} 2I + V, \qquad (2)$$

$$O + I \xleftrightarrow{k_{V1},k_{V2}} 2V + I, \quad (3)$$

$$I + V_2 \xrightarrow{k_{l1}} V, \quad (4)$$

$$V + V \xrightarrow{k_{l2}} V_2, \quad (5)$$

Where O - the symbol of unit of an ideal lattice of silicon, direct reaction (1) represents reaction of recombination I and V, and return to it – reaction of generation I and V under action of a stream of energy. Direct reactions (2), (3) represent reactions of shock generation I and V, and the return it reactions are reactions recombination I and V, k_{f1} - a constant of recombination speed I and V, k_{f2} - generation I and V, k_{I1}, k_{I2} - shock generation I and V, k_{V1}, k_{V2} - recombination of I and V, and k_{l1}, k_{l2} -constants of speeds of capture I and V, linear on their concentration (i.e. capture I byvacancies and condensation V in V_2 with formation divacancies which does not break balance in system [6])

$$C_I \approx C_V \quad (6)$$

Speeds of qusichemical reactions on C_I in view of (5) according to schemes (1) - (5) look like reactions

$$r_1 = -k_{f1} C_I^2 + k_{f2}, \quad (7)$$

$$r_2 = -k_{I1} C_I - k_{I2} C_I^3, \quad (8)$$

$$r_3 = -k_{V1} C_I - k_{V2} C_I^3, \quad (9)$$

$$r_4 = -k_{l1} C_I, \quad (10)$$

$$r_5 = -k_{l2} C_I. \quad (11)$$

According to standard approaches [1-4]

$$\dot{C}_I = dC_I / dt =$$
$$= r_1 + r_2 + r_3 + r_4 + r_5 = k_{f2} +$$
$$+ [(k_{I1} + k_{V1}) - k_{l1}]C_I -$$
$$- (k_{f1} + k_{l2})C_I^2 - (k_{I2} + k_{V2})C_I^3 \quad (12)$$

It is obvious, that change of concentration C_V in due course is given by the expression similar (12).

It is easy to see, that at $k_{f2} > 0$ the equation (12) has always the unique stationary decision $C_I > 0$. At $k_{f2} = 0$ ("low" temperatures and the termination of an irradiation when practically there are no processes of generation I) V as follows from (12), there is an possibility of nonequilibrium Schlögl transition of concentration of own dot defects of silicon C_I .

Really, in case of a stationary state $\dot{C}_I = 0$ at $k_{f2} = 0$ the equation (12) gives

$$- (k_{I2} + k_{V2})C_I^2 - (k_{f1} + k_{l2})C_I +$$
$$+ [(k_{I1} + k_{V1}) - k_{l1}] = 0 \quad (13)$$

From the equation (13) follows, that steady stationary decisions will be (see, for example, [3,4])

$$C_I == \begin{cases} 0, if\,(k_{I1} + k_{V1}) \le k_{f1} \\ \\ C_S, if\,(k_{I1} + k_{V1}) \ge k_{f1} \end{cases}, \quad (14)$$

$$C_S = \frac{(k_{f1} + k_{l2})}{2(k_{I2} + k_{V2})} \cdot \begin{Bmatrix} [1 + 4(k_{I2} + k_{V2})((k_{I1} + k_{V1}) - \\ - k_{f1})/(k_{f1} + k_{l2})]^{1/2} - 1 \end{Bmatrix} \quad (15\}$$

From here we see, that the equation (14) shows an possibility of transition C_I from value $C_I = C_S \neq 0$ to some value $C_I = 0$ in case the parameter of generation own interstitial atoms of silicon becomes equal to parameter of their losses, i.e $[(k_{I1} + k_{V1}) = k_{l1}$. Speed of such transition changes in steps and is very great.

We shall note, that if to neglect in the reactionary scheme (1) - (5) processes of recombination ($k_{I2} = 0, k_{V2} = 0$) the threshold of such transition will not change

$$C_I = \begin{cases} 0, if\,(k_{I1}+k_{V1}) \le k_{f1} \\ \{((k_{I1}+k_{V1}) - k_{l1})/(k_{f1}+k_{l2})\}, \\ if\,(k_{I1}+k_{V1}) \ge k_{f1} \end{cases} \quad (16)$$

Orders of sizes of effective constants k_{ij}, entering in (16), can be estimated on the basis of the given thermodynamic calculations in system $I - V - O$ [7,8]: $k_{f1} = 4\pi r_{IV}(D_I + D_V)$, $k_{f2} = k_{f1}C_{IO}C_{VO}$, $k_{I2} = 4\pi r_{IV}(D_I + D_V)/C_{VO}$, $k_{I1} = k_{I2}C_{IO}C_{VO}$, $k_{V2} = 4\pi r_{IV}(D_I + D_V)/C_{IO}$, $k_{V1} = k_{V2}C_{IO}C_{VO}$, $k_{l1} \approx 4\pi r_{IV_2}D_I C_{bV}$, $k_{l2} \approx 4\pi r_{VV}D_V$.Здесь D_j and C_{jO} - factors of diffusion and concentration I, V and divacancies in a condition of thermal balance (bV -a symbol divacancy), and $r_{IV} \cong r_{IV_2} \cong r_{VV} \cong 2{,}35\cdot 10^{-8}$ sm, as well as in works [6-8].

Shall calculate on these values k_{ij} to estimate a condition of supervision of nonequilibrium transitions of type (15). At 1100^0 C according to [6-8] $D_I = 3{,}6\cdot 10^{-8}$ sm^2/s, $D_V = D_I/5, C_{VO} = 8\cdot 10^{15}$ sm^{-3}, $C_{IO} = 1{,}6\cdot 10^{14}$ sm$^{-3.}$ With these values $k_{f1} = 1{,}06\cdot 10^{-14}$ sm^3/s, $k_{f2} = 1{,}36\cdot 10^{16}$ sm^{-3}/s, $k_{I1} = 1{,}7$ s^{-1}, $k_{I2} = 2{,}125\cdot 10^{-30}$ sm^6/s, $k_{V1} = 84{,}922$ c^{-1}, $k_{V2} = 6{,}64\cdot 10^{-29}$ sm^6/s, $k_{l1} \approx 1{,}06\cdot 10^{-14}C_{bV}$ s^{-1}, $k_{l2} \approx 2{,}12\cdot 10^{-15}$ sm^3/s.

These results allow to give some estimations of critical sizes of values of concentration divacancies C_{bV}^{kp} and constant values C_I, a definiendum (16). According to (16) it is had

$$C_{bV}^{kp} = \frac{k_{I1}+k_{V1}}{4\pi r_{IV}D_I} \qquad (16)$$

Substituting values of the sizes entering in (16), we have found critical value of concentration divacancies $C_{bV}^{kp} = 8{,}2\cdot 10^{15}$ sm^{-3}. Thus, at $C_{bV} > C_{bV}^{kp}$ size $C_I = 0$, and at $C_{bV} < C_{bV}^{kp}$ size $C_I = [(k_{I1}+k_{V1}) - k_{l1}]/(k_{f1}+k_{l2})$. For example, at $C_{bV} = 10^{15}$ sm^{-3} size $C_I = 6\cdot 10^{15}$ sm^{-3}, and at $C_{bV} = 5\cdot 10^{15}$ sm^{-3}: $C_I = 2{,}4\cdot 10^{15}$ sm^{-3}.

On the basis of the lead calculations it is possible to draw practically important conclusions. In the samples of silicon containing greater concentration C_I of own interstitial of atoms of silicon, at heat treatments and presence of the certain sort of traps (in our case divacancies) C_{bV} the size C_I can undergo nonequilibrium transition of Schlögl : $C_I = 0$ at $C_{bV} \ge C_{bV}^{kp}$ and $C_I = C_I$ (final value) at $C_{bV} \le C_{bV}^{kp}$. Speed of such transition changes in the spasmodic image and is possibly very great. Presence such distable states enables under certain conditions (for example, creation divacancies during an irradiation) to supervise presence own interstitial atoms in silicon. We shall note, that quasichemical Schlögl approach can be applied with success and by consideration of behaviour in silicon of alloying impurity Ш and V groups. The received results have the certain scientific and practical interest in general for understanding of essence of various power influences on materials of electronic technics during their reception and operation.

Conclusion. On the basis of Schlögl quasichemical reaction model the important case of evolution in an atmosphere of own silicon dot defects is considered. It is shown, that concentration own interstitial silicon atoms C_I and vacancy concentration C_V of vacancies in an atmosphere of own defects of silicon presence bistable states is probably inherent in concentration C_I, transition between which can be described Schlögl quasichemical reactions. On the basis of the lead calculations quasichemical Schlögl reactions in an atmosphere of own defects of silicon it is possible to draw practically important conclusions. In the samples of silicon containing greater concentration C_I own interstitial of atoms of silicon, at heat treatments and presence of the certain sort of traps (in our case divacancies) C_{bV} the size C_I can undergo nonequilibrium Schlögl transition: $C_I = 0$ at $C_{bV} \geq C_{bV}^{kp}$ and $C_I = C_I$ (final value) at $C_{bV} \leq C_{bV}^{kp}$. Speed of such transition changes in the spasmodic image and is possibly very great. Presence such of bistable states enables under certain conditions (for example, creation divacancies during an irradiation) to supervise presence own interstitial atoms in silicon, that finally can improve their performance data considerably. The received results have the certain scientific and practical interest in general for understanding of essence of various power influences on materials of electronic technics during their reception and operation.

These calculations allow to draw practically important conclusions. In the samples of silicon containing greater concentration C_I own interstitial of silicon atoms , at heat treatments and presence of the certain sort of traps (in our case bivacansies) C_{bV} size C_I can undergo Schlögl nonequilibrium transition: C_I =0 at $C_{bV} \geq C_{bV}$(critical value) and C_I = C_I (final value) at $C_{bV} \leq C_{bV}$ (critical value). Speed of such transition changes in the spasmodic image and is possibly very great. Presence such bistable states enables under certain conditions presence of traps of own defects (for example, creation bivacancies during an irradiation) to supervise presence own interstitial atoms in silicon that can improve their performance data considerably. The received results have the certain scientific and practical interest for understanding of essence of various power influences on materials of electronic technics during their reception and operation and can explain high operational characteristics of nanomaterials on the basis of silicon (for example, layers of nanometer sizes of flexible silicon). Here as traps of interstitial own atoms can serve the surface of a silicon film. In nanomaterial volumes as traps own interstitial atoms and vacancies can be interfaces, porouses, emptiness, vacancies, etc. of the nanometer sizes, as causes in many respects their high performance data.

This example confirms the general concept of school of Prigogine [3] transitions in the systems of the various nature which are being far from thermodynamic balance that leads to higher degree of self-organizing in ensembles of defects of silicon. It enables basically to choose optimum conditions of reception and operation SOI-structures, MOS – devices, MEMS and various devices.

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