SIMULATION OF INSULATOR CONDUCTIVITY IN ELECTRIC FIELD

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Due to the development of the elements of integrated curcuits on the basis of the metal-insulator-semiconductor structures lately considerable attention is paying to the physical investigation of the conductivity of thin films of amorphous insulators. One of the most complicated objects is the silicon nitride with deep trapping centres(energy ~ 1.5 eV) of free carriers in its volume which is used as the active medium in MNOS(metal-silicon nitride-silicon oxid-semiconductor) memory element. The element in record regime is schematically represented in Fig.1. At positive bias applied to the metal contact a tunnel injection of electrons from Si into Si_3N_4 through the barrier on the contacts $Si-SiO_2-Si_3N_4$ takes place. The injected carriers drift over the the insulator conductive band with the following trapping on the fixed traps, ionization from them and so on. As the result of the trapping centres high concentration($\sim 10^{19} sm^{-3}$) the electric field of the trapped electrons' becomes comparable to the external one, screens the injective contact and lately a steady-state situation is obtained

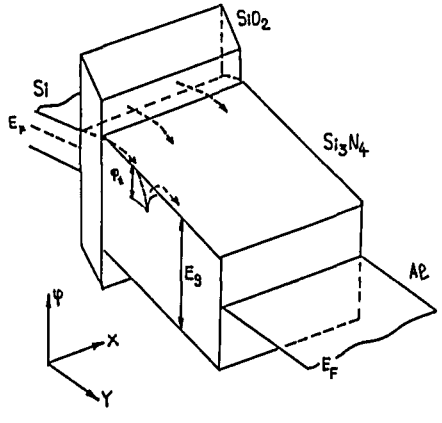

Fig. 1

Up to now the simulation of the conductivity of MNOS-structures was carried out with the help of the method suggested in [1,2]. It's

based on the solution of the equation system including the continuity equation for the charged carriers, equation for kinetics of filling of localization centres and Poisson equation [1-3]. But such a model ignores the peculiarities of the current flow process connected to the noncrystallinity of the medium, nonregularity of trapping centres.

The estimations show that the fluctuations of the electric field caused by a random distribution of the trapping centres of Coulomb type (donors and acceptors) may essentially influence the probability of the trap's ionization, the probability of the injection of minority carriers in the insulator volume [4] and further current relaxation. In Fig.2 one can see a two-dimensional potential relief formed by the randomly distributed donors and acceptors on the area 150Å×150Å at the external field $E = 2 \cdot 10^6$ v/sm. In the present paper we suggest a method of a direct dynamic simulation of the charge transport in insulators in the electric fields.

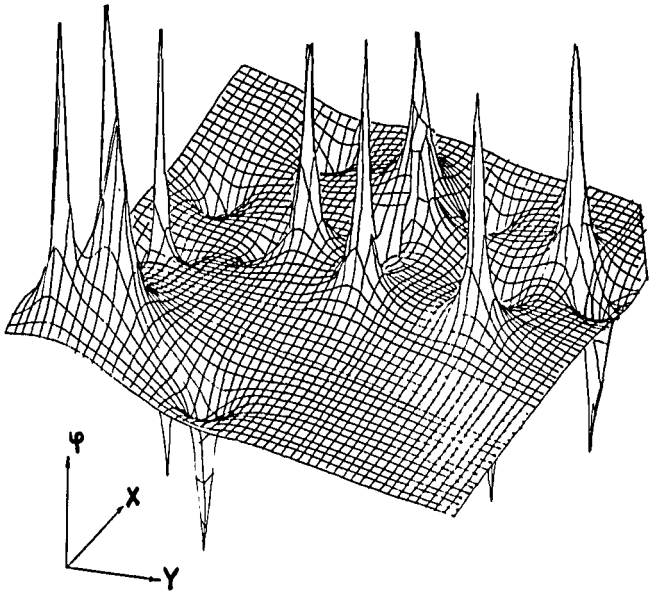

Fig. 2

1. Model

The experimental data obtained before show that Si_3N_4 is a compensated material that is the number of traps of the donor and acceptor types are equal and that's so an initial nonpolarized insulator is quasi-neutral. As possible variants in our calculations we used uncorrelated and correlated

distribution of the trapping centres.

The simulation of the charge transport was made in a two-dimensional approximation in the area d_x d_y = 500A 500A; the charge of the imagine on the contacts with Si and Me was taken into account, periodic boundary conditions choosen. In our case we used the two-dimensional Coulomb potential with the density of charge $\varkappa$:

$$\varphi(x,y) = -\varkappa \ln \frac{\sqrt{a^2+x^2+y^2} - a}{\sqrt{a^2+x^2+y^2} + a},$$

where 2a is the section length, $\varkappa \sim q \cdot N_{a,d}^{-1/3}$.

The probability of the injection of carriers through the contact was taken according to [5] in the form:

$$W_{inj} \sim AE_c^2 \cdot \exp\left(-\frac{4}{3\hbar}\sqrt{2m^*q}\,\frac{V^{3/2}}{E_c}\right),$$

where E_c is the electric field at the boundary SiO_2-Si_3N_4; q,m* - charge and effective electron mass respectively; $\hbar$ is the Plank constant; V is the energy of the barrier Si-SiO_2; A is the constant, characterizing the current through the contact Si-SiO_2.

The simulation of the trajectories of free carriers in a permissible band was carried out under the following assumptions:

a) the constant module of the momentum; this assumption is based on the fact that for insulator in electric field $\sim 10^6$ v/sm the drift velocity of carriers trends to saturation and obtains the value close to the thermal one (10^7 sm/s) due to the effective scattering on the LO-phonons.

b) the momentum vector coinsides with the electric field one because the scattering on the LO-phonons, giving the main contribution to the energy loss, does not change the angular distribution function [6].

c) the electron scattering on LA and TA-phonons that could change the character of current flowing through the volume of the insulator due to an isotropic angular distribution was not taken into account for it is small compared to LO-scattering at low energies of carriers [7]. Unlike [7] the high-energies electrons in silicon nitride were not experimentally observed and more over data [8] show that the heating of the carriers in Si_3N_4 does not occur. It should be noted that if the heating of electrons took place due to the localization of the electrons with low energy (~kT) at the trapp-

ing centres is the process limiting the level of current, the suggested model of the trajectory calculation would be sufficiently substantiated.

In the present paper one of the possible variants suggested that the electrons did not heat in the field; the act of the carrier's trapping was considered to be fulfilled if the distance among them was less then 2.5Å.

The possibility of the trap ionization was taken in the form:

$$W_{ion} = B \cdot \exp\left(- \frac{1}{kT}(\Phi_t - \Delta\Phi)\right),$$

where k,T are the Boltzmann constant and temperature; Φ_t is the energy of ground state of the trapping center; $\Delta\Phi$ is the change of the ionization barrier due to the external electric field and moreover owing to the presence of neighbouring centres; B is the frequency factor($\sim 10^{14} s^{-1}$).

It should be noted that the value $_t$ may change in case if the neighbouring centres(^{t}of any sign) are at the distance ~10Å between them caused by electrons' wave functions overlap. That's why in such a situation the value Φ_t has been recalculated like in the problem of the electron energy levels in the molecule H_2^+.

2. Algorithm.

Step 1. With the help of a random number generator the coordinates of the traps of both types were chosen then the calculation of the electric field at the contact and the probability of injection were carried out.

Step 2. The fields in the points of the traps' locations were calculated.

Step 3. The probabilities of the ionization of the traps were calculated taking into account the possibility of the ionization of the electron from the center in 8 different directions and one of them was chosen.

Step 4. The choise of process (injection or ionization).

Step 5. The choise of the time-odered step and process coordinates (electron injection point or location of the ionized trap).

Step 6. Free particle trajectory calculation Both trapping to the center or free escape to the metal are possible.

Step 7. The calculation of the fields at the boundary and at the trap locations, probability of the injection. Then steps were repeated from Step 3.

One should note that within the framework of the described procedure the possibility of injection the trajectory and the probability of delocalization of one electron are calculated simultaneously. This is caused by the fact that the characteristic times of injection and ionization of the carriers from the traps are much more than the characteristic time of the drift through the sample.

To accelerate the process of finding the nearest neighbours to a given point in some radius, which is used to calculate the trajectories and probabilities of ionization the linked lists method [9] was applied. To simulate the polarization of the structure for one variant of the donors and acceptors distribution one needs about 10 min CPU of BESM-6.

3. Results.

The calculation results made according the model given above showed that in an overwhelming majority of cases for used variant of uncorrelated traps the conductivity of a channel type is realized. A typical current pattern is represented in Fig.3, where trajectories of electrons passed through the insulator layer are plotted. In our opinion such an inhomogeneity of the current is caused by a strong fluctuation of the values of electric field at the boundary SiO_2-Si_3N_4, which is set by a random location of the centres N_d and N_a in the silicon nitride volume This result is in a good conformity with the data [4] and is also shown in some strain of the initial C-V characteristics(Fig.4a). Besides it is seen (Fig.4b) that in the process of the structure relaxation the field fluctuations are

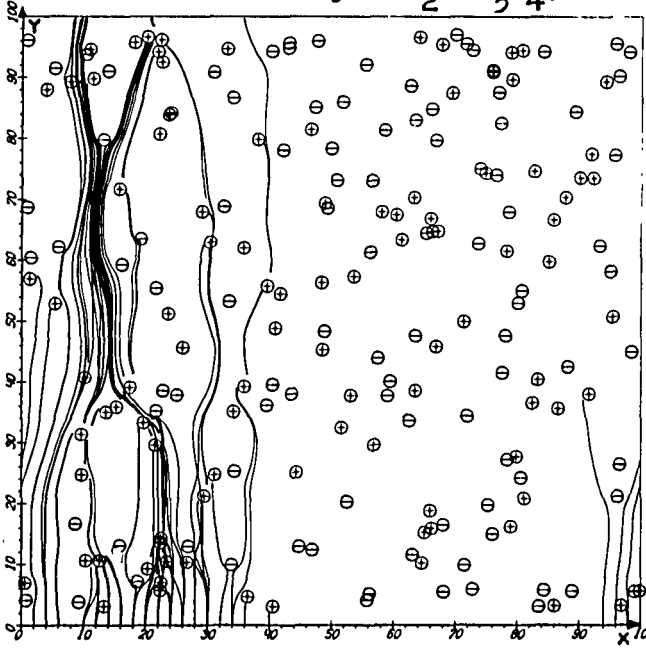

Fig.3

smoothed due to the injected charge and as it was pointed out in [4] in the first place - large-scale ones.

The introduction of the correlation in the distribution of donors and acceptors leads to the transfer from the channel to more homogeneous in structure current flow(Fig.5). As the calculations have shown the introduction of the scattering of electrons on acoustic phonons does not lead to a strong distortion of the trajectory in field $\sim 3 \cdot 10^6$ v/sm(Fig.6), that is also confirmed by the result [7]. In Fig.7a the current vs voltage characteristics of the MNOS-structure with parameters: a layer's thickness SiO_2=20Å, d_y= 500Å, Φ_{st}=1.3 eV, N_d= N_a= $6 \cdot 10^{18}$ sm^{-3}; the averaging was carried out on 25 realizations of trap distributions.

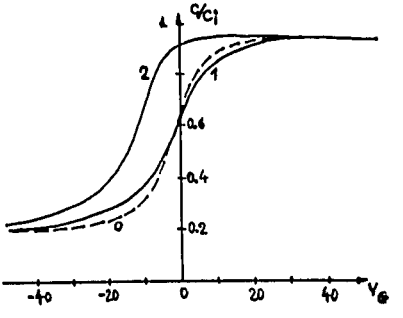

Fig.4a C-V characteristics:"o"-ideal structure,"1"-initial,"2"- at the time $t=10^{-3}$ s. C_i is the insulator capacity. Distribution of the centers is uncorrelated. V_G=25v.

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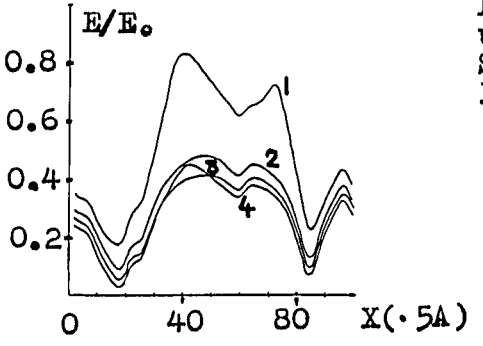

Fig. 4b Electric field strength at the boundary SiO_2-Si_3N_4 for different time moments: 1-t=0, 2-$t=10^{-8}$s, 3-$t=10^{-5}$ s, 4-$t=10^{-3}$ s; $E_o=8 \cdot 10^6$ v/sm, the rest parameters are the same Fig.4a.

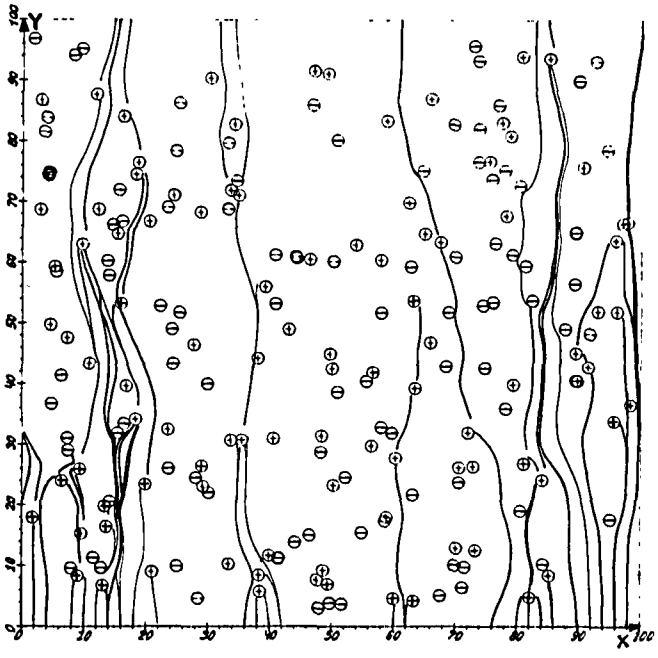

Fig. 5 Electrons trajectories. Distribution of the donors and acceptors is correlated.

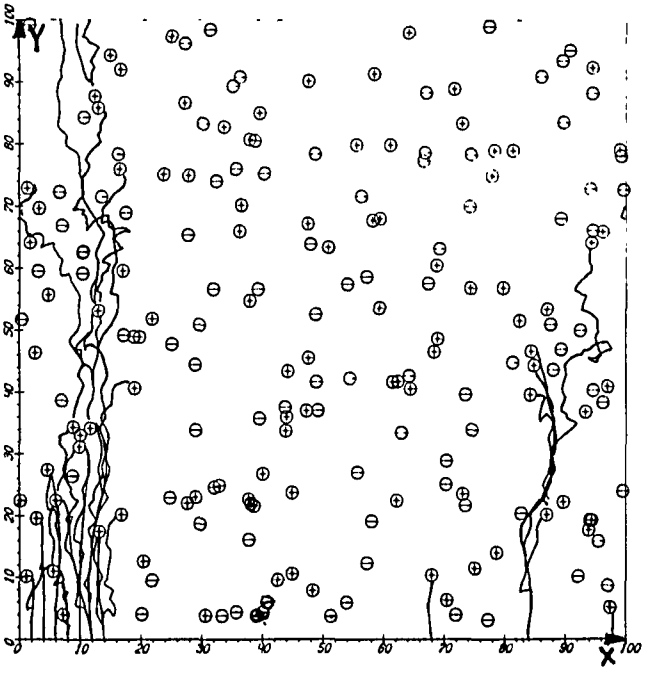

Fig. 6 Electrons trajectories calculated with the introduction of the electron-phonon scattering. Distribution of the centres is uncorrelated

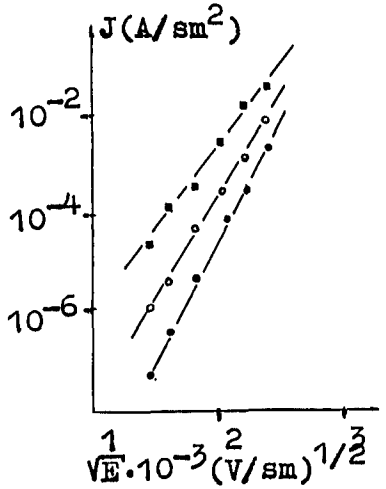

Fig. 7a
■ - T=500 K, o - T= 400 K, ● - T= 300 K.

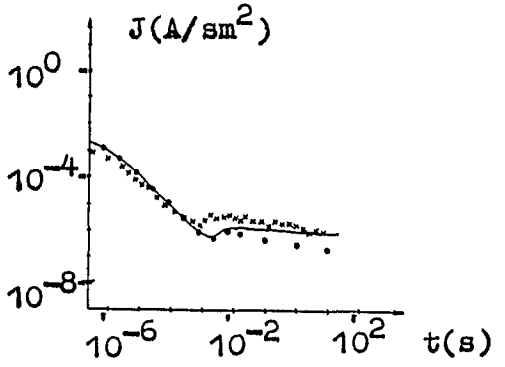

Fig. 7b Current through the structure vs time. T=300 K, the rest parameters are the same as in Fig.7a. •••• - experimental data [8], —— - simulation results for diffusion-drift model [8], × - our calculation.

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