MODEL CALCULATION OF IONIZED CLUSTER BEAM INDUCED BIAS DEPENDENT INTERFACE CHARGE*

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Abstract: Within the framework of the simple one dimensional tight binding model of two coupled semiinfinite linear chains of atoms it is argued that the intrinsic interface charge induced at the interface between the two chains in principle depends on the applied bias. Approximate expressions in the limits of small and large applied bias are explicitly given and the necessity of self-consistent treatment of the induced interface charges is being discussed. In spite of the simplicity of the model, chosen as a first step towards investigation of the microscopic aspects of the interface physical properties, the findings seem to be in general agreement with our recent measurements of the reverse excess capacitance of the ionized cluster beam deposited Ag/p-Si(100) Schottky diode. Consequently, the findings might be relevant also to the theory of the disorder induced gap states, as the derived results imply that even at the given, lattice matched and undoped interface between the two (even identical) semiconductors, a strong, approximately bell shaped, bias dependent electric field is expected in general to appear, of which the consequence on the Fermi level pinning is presently unclear.

Modelski izračun odvisnosti induciranega naboja na vmesni plasti od zunanje napetosti v polprevodniških strukturah narejenih z metodo curka ioniziranih skupkov atomov

Ključne besede: vmesniki izolator-polprevodnik, vmesniki kovina-polprevodnik, DIGS stanja energijska nereda v reži energijski, DIGS modeli, SCHOTTKY strukture, ICB nanašanje s curkom skupkov ioniziranih, naboji električni vmesnika, povezave tesne, GREEN funkcije

Izvleček: V okviru enostavnega enodimenzionalnega modela stika med dvema linearnima verigama atomov je raziskana odvisnost induciranega naboja na stiku od zunanje napetosti. Podani so aproksimativni izrazi za odvisnost induciranega naboja pri velikih in majhnih vrednostih zunanje napetosti ter vpliv samousklajenosti pri računanju naboja na stiku. Čeprav izredno preprost, predstavlja podani model prvi korak k razumevanju mikroskopskih mehanizmov nastanka naboja na stiku odvisnega od zunanje napetosti in kaže, da so grobi rezultati v skladu z našimi ugotovitvami, ki temeljijo na izmerjenih karakteristikah kapacitete stikov Ag/p-Si(100) narejenih z metodo curka ioniziranih skupkov atomov. Predstavljeni rezultati lahko prav tako pomagajo osvetliti problem vpetja Fermijevega nivoja in z neredom induciranih stanj na stiku med različnimi materiali v okviru teorije DIGS.

1. Introduction

The unified model of disorder induced gap states (DIGS) for insulator-semiconductor and metal-semiconductor interfaces as proposed by Hasegawa /1/ seems to be able to explain the salient features of the metal-semiconductor interface formed either on the bare or oxide covered semiconductor /2/.According to DIGS model a deposition of either an insulator or a metal (or even semiconductor) on a given semiconductor effectively produces a thin disordered semiconductor interlayer, characterized by fluctuations of bond length and bond angles. The DIGS theory provides a formal understanding of the weak Fermi level pinning mechanism at semiconductor-metal junctions in terms of the microscopic morphology of the interface and is also, for a given metal-semiconductor junction, able to give a clue as to how and why seems to be possible to tailor Schottky barrier height /2/ over large interval, for which the manifestation of the induced interface dipoles might be most likely responsible /3/.

The problem of controlled variation of Schottky barrier height throughout its entire range, ranks as one among the important fundamental questions of semiconductor device physics remaining to be solved, notwithstanding also from the technological point of view. Although an old one /4/, it seems to be best amenable to the experimental investigation by utilizing the method of ionized cluster beam deposition ICB /5, 6/, the results of which seem to be strongly correlated to the basic assumption of DIGS theory of ref. /1, 2/. In particular, it has been found recently /7/ that the reverse excess capacitance of suitable ICB deposited Ag and Pb/Si(100) Schottky junctions could be understood in terms of the specific (modeled) biased voltage dependent excess interface charge density. Figure 1 shows the measured capacitance spectra of ICB deposited Ag/p-Si(100) Schottky structure (dots) and the calculated capacitance within the model incorporating the bias dependent interface charge density (full line). The details of the model and explicit expression for the interface charge are given elsewhere /7/. Although it is for the first time that such

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an explicit bias voltage dependent excess interface charge density has been introduced for the successful description of the measured low-frequency C-V data, its implicit existence seems to be introduced and in different context investigated by Darling /8/ and Gomila /9/.

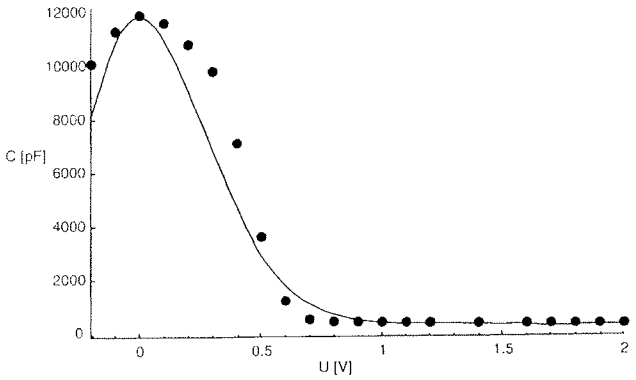

Fig. 1: Experimentaly determined low frequency capacitance of the ICB deposited Ag/p-Si(100) Schottky junction (dots) and calculated capacitance of the structure using the bias dependent interface charge model described in detail in /7/. As shown in /7/, the reasonable agreement with the measured spectra can only be achived by introducing bias dependent interface charge density.

Since the effect of the externally supplied bias voltage dependent interface charge density is expected strongly to correlate with the equilibrium as well as non-equilibrium transport properties of Schottky junctions it seems most appropriate to investigate its occurrence and its bias voltage functional dependence form the first principles, starting from the simple model of one dimensional chain of atoms.

In this paper we are tying to argue on the basis of a simple one dimensional model that the charge induced at the interface is in principle bias dependent (thus within certain interval of bias voltage always appearing at the junction, i.e. site of a broken periodicity of interatomic potential, even in cases of homojunctions, contrary to DIGS theory) and that special care should therefore be taken when modeling devices that incorporate the interface charge. We propose that the total interface charge in these models should be divided into intrinsic which is present even in most simplified and idealized models of homojunctions as shown below, and extrinsic which is a consequence of the possible disorder at the interface. In this note we are considering only the intrinsic interface charge. The study of both type of interface charges and possible effects of their interaction is the subject of the forthcoming paper.

2. One dimensional microscopic model of interface charge

Since we are interested in the charge localized near the ideal interface it is appropriate to consider the junction in the local description. We choose a very simple and highly idealized one dimensional model of the "device" in the tight binding approximation with N identical atoms on both sides with a single energy level E_0. We further postulate that the only effect of the explicit change of the applied bias ΔU in the "device" is a rigid shift of the atomic-state energies of N atoms on one side with respect to atomic-state energies of atoms E_0 on the other side of the interface. The problem is to determine the possible induced charge ΔZ on both sides of the interface when $\Delta U \neq 0$ and to study its dependence on the change of the applied bias. The calculation follows the approach used in obtaining heterojunction band offset /10, 11/.

The interface in our model is thought of as occurring on account of an infinitely thin, lattice matched, interface control layer /2/ imagined to be inserted at, say, at the middle of the linear chain of 2N identical atoms and consequently in the model it represents the region of the space where expected induced charge $\Delta Z \neq 0$. We start with the brief description of the "perfect" case when $\Delta U = 0$, when the solution is well known /12, 13/. The basis states are single localized atomic states centered at each site

$$|i> = c_i^+|0> \qquad \text{or} \qquad \Phi(x-x_i) = <x|c_i^+|0>$$

where c_i^+ is the creation operator. The tight binding Hamiltonian /13/ is:

$$H = \sum_i E_0 c_i^+ c_i + \sum_{i \neq j} W_{i,j} c_i^+ c_j \qquad (1)$$

and the solution of the Schrodinger equation is the linear combination of the basis states /14,13/:

$$\psi_k = \sum_i d_i(k)|i> \qquad (2)$$

which are assumed to form the complete orthonormal set. When only coupling $W_{i,j}=W$ between the nearest neighbors is considered the eigenvalues lie in the energy band of width $4W$ /14, 13/:

$$E(k) = E_0 + 2W \cos(ka) \qquad (3)$$

where $\vec{k}$ is the wave vector and a the distance between the neighboring atoms. As soon as the bias is applied to the "device" the periodicity of the problem is broken and the solution cannot be so easily found. One proceeds along the steps as for instance presented in /17, 18/.

The quantity of interest when calculating the induced charge at particular site m is the local density of states normalized to unity /17, 18/:

$$LDOS_m(E) = \sum d_m^*(k) d_m(k) \delta(E - E(k)) \qquad (4)$$

The perturbation induced by the applied bias changes the $LDOS_m(E)$ in the vicinity of the interface with respect to the unperturbed sites in the bulk. The occupied electron states localized at the interface are assumed to determine the induced interface charge ΔZ_m at the particular site m. Since the eigenvalues E of the localized energy states in one band model are found outside the band $|E-E_0|>2|W|$, we have to inspect the part of the perturbed local density of states which is extending over the band edges with respect to unperturbed ideal case. This is in accordance with /10/ where the interface charge in the vicinity of the heterojunction is defined as the difference between the local density of states in the neighborhood of the interface and the local density of states for an uniform (no interface) crystal summed over all occupied states. In our case in non-perturbed state ($\Delta U=0$) the local density of states is the same for every site and the sum over all band states serves as a reference value. Finally the sum of the induced charge ΔZ_m given with:

$$\Delta Z_m = \int_{|E-E_0|>2|W|} LDOS_m(E)dE \qquad (5)$$

at particular sites m, is performed. The number of atoms in the model N should be large enough to approximately ensure the bulk-like density of states sufficiently far from the interface on either side (m turns out ≈ 15). The approach we adopted here follows in some respect the model studied in /16/ where the charge transfer between two bands across the heterogap is considered in a perturbative manner. In contrast to /16/ we focus ourselves to a single (valence) band and specifically consider the diagonal heterocoupling of the states on opposite sides of the junction which was not investigated in /16/.

3. Numerical results and approximate solutions

In order to numerically obtain the bias induced interface charge in the described one dimensional model, we used exact diagonalization of the pertinent Hamiltonian matrix with N=40 and from orthonormal eigenstates calculate local density of states and induced charge at each site for different values of the applied bias. Since the in calculation of the induced interface charge involves only the coefficients $d_i(k)$ of the linear combination of the basis states (2) and the eigenvalues, the explicit set of basis states is not required. Because the change of all atomic-state energies by a constant value merely shifts the overall spectrum the only important parameter in the model is the hopping integral between the nearest neighbors W, which we take to be of the order of 1 eV as it is appropriate for semi-conducting materials /4/. Furthermore we assume that the change in the applied bias does not affect the coupling between nearest neighbors and that also the heterocoupling across the interface is of the same order as W /16/. In addition, we found from our computations that only the ratio of the applied bias and the hopping integral, or the "scaled" bias, determines the induced charge. Furthermore, since both sides of the interface are identical, apart for the rigid shift of atomic energies due to applied bias, the interface charge forms the induced interface dipole with equal amount of the total charge on both sides to comply to the overall charge neutrality of the problem as stated in /10/.

A further remark should be made considering the self-consistency of the calculated charges. In the first approximation the induced charge ΔZ_m at site m changes only the atomic-state energy of the atom by δV_m due to the intra-atomic or onsite interaction with energy J and inter-atomic coulomb interactions /19/:

$$\delta V_m = J\Delta Z_m + \frac{e^2}{4\pi\varepsilon_0}\sum_{n\neq m}\frac{\Delta Z_n}{b_{m,n}} \qquad (6)$$

where $b_{m,n}$ is the distance between the m-th and the n-th atomic site. On the other hand adding the δV_m to the atomic energies changes the Hamiltonian matrix, so the $LDOS_m(E)$ and consequently the induced charge are implicit function of the perturbation:

$$\Delta Z_m = \int LDOS_m(E,\delta V_m)dE \qquad (7)$$

In order to find the self-consistent charges the equations (6) and (7) ought to be simultaneously solved. The final self-consistent solution yields the applied potential as shown in fig. 2. The change of the potential near the interface extends only a few lattice sites far from the interface, suggesting the screening of the interface charge near the junction.

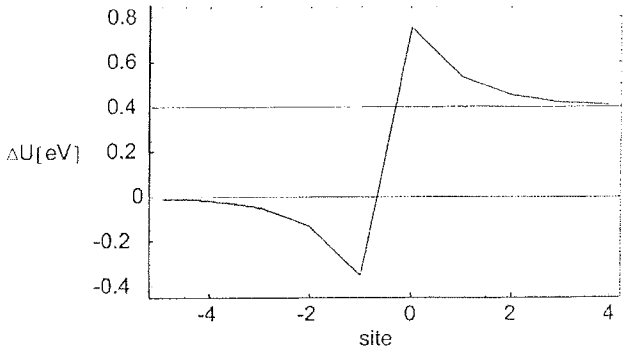

Fig. 2: Self-consistent applied potential in the vicinity of the interface for $\Delta U=0.4eV$. Sufficiently far from the interface ($m>5$) is the induced self-consistent potential difference practically equal to applied bias (dashed lines), suggesting that the the induced changes in the potential are effectively screened.

Total induced charge on one side of the junction, (at the junction m=0):

$$\Delta Z = \sum_{m=0}^{N}\Delta Z_m \qquad (8)$$

as a function of the change in the scaled applied bias $\Delta U/W$ is shown in fig. 3. It is evident that within this model the numerically obtained interface charge shows a distinct bias dependence with low values at low and high bias and a pronounced maximum between this two limits.

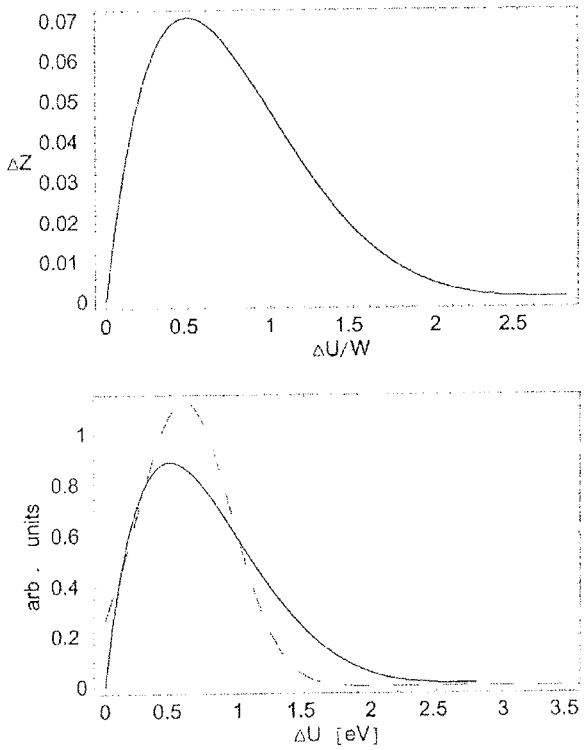

Fig. 3: Above - Total induced charge in one dimensional interface model on one side of the interface (at N=40) vs. "scaled bias" $\Delta U/W$. The interface is situated between N=40 identical atoms on each side and the bias is assumed to affect only the atomic-state energies. W is the hopping integral between nearest neighbors. Below - Total induced charge in one dimensional interface model (full line) and bias dependent interface charge function $\sigma(\Delta U)$ /7/ (dashed line) determined from measured excess capacitance in ICB deposited Ag/Si Schottky junctions, and given by $\sigma(\Delta U)=n_\sigma \exp(-(\Delta U/V_0 + K^2))$ /7/ (used in model for the capacitance shown in fig. 1), where n_σ, V_0, K are constants determined from fitting to the experimentally obtained capacitance spectrum. Both functions are for comparison normalized to 1.

The bias dependence in the very low and high bias regime can be qualitatively understood on the basis of the following arguments. In the limit of small bias $\Delta U/W<<1$ we assume that the perturbing constant potential at one side of the interface simply rigidly shifts the energy bands. The shift causes the part of the local density of states near the interface to extend over the non-perturbed band edges. The induced charge in this case can be approximated with the help of the expression for the local density of states in the infinite crystal /17, 18/:

$$\Delta Z_m = \int_{E_0-2W}^{E_0-2W+\Delta U} LDOS_m(E)dE \approx \frac{1}{\pi}\sqrt{\frac{\Delta U}{W}} \qquad (9)$$

The specific square root functional dependence of the induced charge on the bias is a consequence of the one dimensional model. In more detailed three dimensional models a linear dependence is expected /15/. The case $W/\Delta U<<1$ corresponds to the other limit of low values of induced charge and can be described in perturbative manner as shown /16/ for the case of two one dimensional bands, where now instead of the heterogap the applied bias is substituted in our model. In this limit the induced charge is given with the expression /16/:

$$\Delta Z = \left(\frac{W}{\Delta U}\right)^2 \qquad (10)$$

It is worth noting that the form (10) is equal to the expression one obtains in the one dimensional semi-infinite lattice when the atomic-state energy of the first atom is changed by $E_1=\Delta U$ with respect to others. It is well known (see for instance /17/) that if the difference is larger than the hopping integral between nearest neighbors $E_1>W$, the localized state outside the energy band exists with the energy $E_{loc} = E_1+W^2/E_1$. The weighting factor of this localized state $|d_j(E_{loc})|^2$ on the atoms at sites $j>1$ falls exponentially into the bulk /17/:

$$|d_j|^2 = \left(\frac{W}{E_1}\right)^{2(j-1)}\left(1-\frac{W^2}{E_1^2}\right) \qquad (11)$$

The sum over all atomic sites apart from the first is:

$$\sum_{j=2}^{\infty}|d_j|^2 = \sum_{j=1}^{\infty}|d_j|^2 - |d_1|^2 = 1-\left(1-\frac{W^2}{E_1^2}\right) = \left(\frac{W}{E_1}\right)^2 \qquad (12)$$

which is equal to (10).

4. Analytic expressions for the intrinsic induced interface charge in 1D model semiconductor junction

Our model semiconductor junction consists of two semi-infinite linear chains with identical atoms, which are held separately at different electrical potentials so that in each chain the thermal equilibrium is established. Let the two different potentials be $-\Delta U/2$ and $\Delta U/2$ respectively. The junction is formed when the beginnings of the two parts are brought into interatomic distance a so that the translational symmetry of the lattice is conserved. Let´s number the atoms in such a way that the $n \geq 1$ counts the atoms to the right and

$n \leq 0$ to the left of the interface. The one electron properties of the system are described in the tight binding approximation with the Hamiltonian given by (1). The most idealized conditions one can imagine occurs when all of the hopping integrals have the same value $W_{i,j}=W$ and when the formation of the system does not influence the atomic energies in the vicinity of the interface i.e. $E_n=-\Delta U/2$ for $n \geq 1$ and $E_n=\Delta U/2$ for $n \leq 0$. We have chosen $E_0=0$ for the origin from which all energies are measured.

The local density of states is found from the elements of the Green´s matrix or resolvent of the corresponding Hamiltonian (1):

$$G=\frac{I}{zI-H}\ , \tag{13}$$

where I is the identity matrix and $z=E+i\eta$. The diagonal element of the Green´s matrix is in this representation:

$$g(n,n)=\sum_k \frac{d_n^*(k)d_n(k)}{z-E(k)}\ , \tag{14}$$

where E(k) are the eigenvalues of the problem. Using the identity:

$$\lim_{\eta\to 0}\frac{1}{x+i\eta}=P\left(\frac{1}{x}\right)-i\pi\delta(x), \tag{15}$$

where P is the Cauchy principal value of the integral, it follows for the diagonal Green´s matrix element:

$$g(n,n)=P\left(\sum_k \frac{d_n^*(k)d_n(k)}{z-E(k)}\right)-i\pi\sum_k d_n^*(k)d_n(k)\delta(E-E(k)) \tag{16}$$

Knowing the definition of the local density of states at site n in the chain it follows immediately that the local density of states is given with the imaginary part of the diagonal element of the Green´s matrix. The explicit expression for the local density of states is therefore:

$$LDOS_n(E)=-\frac{1}{\pi}\mathrm{Im}\,g(n,n) \tag{17}$$

In writing the matrix element of the resolvent G as $g(m,n)=\langle m|G|n\rangle$ we always assume also the dependence upon the energy $E+i\eta$ and that the corresponding limit of $\eta\to 0$ is always understood.

In order to calculate the matrix elements of G we rewrite the equation for the resolvent as:

$$(H-zI)G=-I \tag{18}$$

First we calculate the bulk and surface Green´s functions for the one dimensional linear chain with no applied potential. Since the tight binding Hamiltonian in nearest neighbor approximation is a tridiagonal matrix, the following set of difference equations for the matrix elements g(m,n) is obtained /21, 22/:

$$-Eg(m,n)+W(g(m+1,n)+g(m-1,n))=-\delta_{m,n} \tag{19}$$

The general solution for the function g(m,n) can be written as:

$$g(m,n)=a_1p_1^{m-n}+a_2p_2^{m-n}\ . \tag{20}$$

The right-side Green´s function $g_>(m,n)$ for $m>n$ is matched to the left-side Green´s $g_<(m,n)$ for $m<n$ at $m=n$. p_1 and p_2 are the roots of the characteristic equation:

$$Wp^2-Ep+W=0 \tag{21}$$

and their explicit form is

$$p_{1,2}=\frac{E}{2W}\pm\sqrt{\left(\frac{E}{2W}\right)^2-1} \tag{22}$$

Characteristics roots obey the relation $p_1p_2=1$ so they can always be chosen such that $|p_1|<1$ and $|p_2|>1$.

Let´s consider the "bulk" matrix element far from both ends of the linear chain at some site n. Then g(m,n) should approach zero when m is near the end. Thus $g_>(m,n)=a_2p_2^{m-n}$ and $g_<(m,n)=a_1p_1^{m-n}$. Matching the solutions at $m=n$ yields:

$$g_>(m,n)=g(n,n)p_2^{m-n}\ \text{ and }\ g_<(m,n)=g(n,n)p_1^{m-n} \tag{23}$$

Substituting the above solutions into the equation for the diagonal matrix element:

$$-Eg(n,n)+W(g(n+1,n)+g(n-1,n))=-1 \tag{24}$$

yields the expression:

$$g(n,n)=\frac{1}{E-2Wp_2}\ . \tag{25}$$

With the site number $n=1$ the surface Green´s function is obtained:

$$-Eg(1,1)+Wg(2,1)=-1 \tag{26}$$

and

$$g(1,1)=\frac{1}{E-Wp_2} \tag{27}$$

To derive the interface Green´s function for the model semiconductor junction under applied bias we separate the total Hamiltonian H into two parts:

$$H = H_0 + V \tag{28}$$

H_0 describes the two linear chains separated at interatomic distance kept at different potentials (-ΔU/2, ΔU/2). V is the coupling between the two chains. When there is no applied potential i.e. ΔU=0, the perfect infinite linear chain is obtained and in this case the operator V is
$V = W(c_1^+c_0+c_0^+c_1) = W(|1><0|+|0><1$Times New Roman"Symbol"đ).
We consider the idealized case when in the presence of nonzero applied bias the coupling part of the Hamiltonian H (or more precisely the value of the hopping integral W) does not change. The perfect resolvent G_0 equals:

$$G_0 = \frac{1}{z - H_0} \tag{29}$$

and the total resolvent is

$$G = \frac{1}{z - H} = \frac{1}{z - H_0 - V} \tag{30}$$

From the above expression the Dyson´s equation is obtained connecting the two resolvents:

$$G = G_0 + G_0VG. \tag{31}$$

The interface Green´s function on the right-side of the connected linear chain is given by diagonal matrix element g(1,1) of G. Since G_0 represents the resolvent of the perfect semi-infinite linear chain it follows that its matrix elements $g_0(0,1)$ and $g_0(1,0)$ are zero by definition /23/ ($n \geq 1$ denotes the right-side of the coupled chain and $n \leq 0$ denotes the left-side). The matrix elements $g_0(1,1)$ and $g_0(0,1)$ are given by the equations:

$$g(1,1) = g_0(1,1) + Wg_0(1,1)g(0,1), \tag{32}$$

$$g(0,1) = Wg_0(0,0)g(1,1) \tag{33}$$

From the two equations the expression for the interface Green´s function follows:

$$g(1,1) = \frac{1}{g_0^{-1}(1,1) - W^2 g_0(0,0)} \tag{34}$$

Explicit expression suitable for practical calculations are obtained by inserting the appropriate surface Green´s functions (27) into the interface Green´s function. In the expressions for the surface Green´s function we now must transform E→E-ΔU/2 on the right-side and E→E+ΔU/2 on the left. Also let $p_{1,2}$ and $q_{1,2}$ denote the characteristics roots on the right and left respectively. Using this we derive the following expression for the interface Green´s function:

$$g(1,1) = \frac{1}{E - \Delta U/2 - W(p_2 + q_2)} \tag{35}$$

The interface density of states as a function of applied bias is:

$$LDOS_1(E, \Delta U/2) = IDOS(E, \Delta U/2) = -\frac{1}{\pi} \mathrm{Im} g(1,1). \tag{36}$$

The interface induced charge ΔZ is defined as the charge given by the localized electron states at the interface and is therefore given by the part of the local density of states extending over the corresponding "bulk" band edges. The important point one should notice is that depending on the value of the energy the characteristics roots are either real or complex. If the energy falls into the interval $E \in [-2W+\Delta U/2, 2W+\Delta U/2]$ the corresponding eigenstate is inside the "bulk" band and represents the extended Bloch state. The characteristic roots are in this case complex conjugated.

The interface density of states has two forms depending on the energy. If $\Delta U/2 \geq 2W$ then for $\forall E \in [-2W+\Delta U/2, 2W+\Delta U/2]$ the characteristic roots on the left side (p_2) are real and the interface density of states is:

$$IDOS(E,\Delta U/2) =$$

$$= \frac{1}{\pi} \frac{W\sqrt{1-\left(\frac{E-\Delta U/2}{2W}\right)^2}}{W^2\left(1-\left(\frac{E-\Delta U/2}{2W}\right)^2\right)^2 + \left(W\sqrt{\left(\frac{E+\Delta U/2}{2W}\right)^2 - 1} - \Delta U/2\right)^2} \tag{37}$$

If $\Delta U/2 < 2W$ then if for $\forall E \in [2W-\Delta U/2, 2W+\Delta U/2]$ the previous expression for the IDOS(E,ΔU/2) applies. If $E \in [-2W+\Delta U/2, 2W-\Delta U/2]$ then the correct expression for the interface density of states becomes:

$$IDOS(E, \Delta U/2) = \frac{1}{\pi} \frac{\varepsilon(E, \Delta U/2)}{(\Delta U/2)^2 + \varepsilon^2(E, \Delta U/2)}, \tag{38}$$

where

$$\varepsilon(E, \Delta U/2) = W\left(\sqrt{1-\left(\frac{E-\Delta U/2}{2W}\right)^2} + \sqrt{1-\left(\frac{E+\Delta U/2}{2W}\right)^2}\right)$$

In the limit ΔU→0 the interface density of states takes on the shape of the bulk density of states for the infinite one dimensional crystal:

$$IDOS(E, \Delta U/2 \to 0) = \frac{1}{\pi} \frac{1}{2W\sqrt{1-\left(\frac{E}{2W}\right)^2}} \tag{39}$$

When applied bias takes on large values $\Delta U/2>>W$ then the interface density of states has the form of the surface local density of states:

$$IDOS(E,\Delta U/2>>W)=\frac{1}{\pi W}\sqrt{1-\left(\frac{E}{2W}\right)^2} \tag{40}$$

The induced interface charge ΔZ given by the electron states with the energy lying outside the bulk band i.e. $|E-\Delta U/2|>2W$ is calculated as follows:

$$\Delta Z=1-\int_{-2W+\Delta U/2}^{2W+\Delta U/2} IDOS(E,\Delta U/2)dE \tag{41}$$

The calculated interface induced charge according to the previous expression is shown on figure 4.

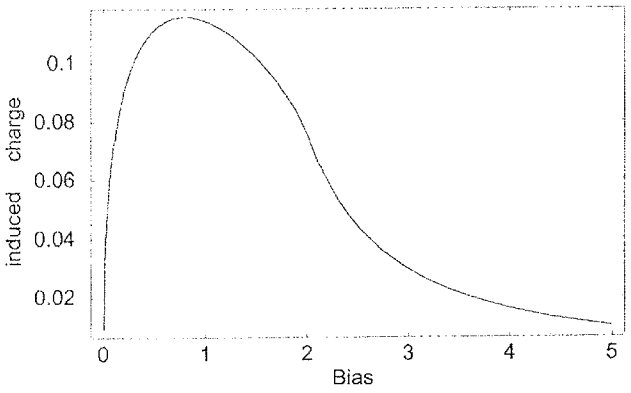

Fig. 4: Calculated induced interface charge from the analytic expression for the interface density of states.

As stated earlier, the complete interval of the applied bias should be divided into two parts depending on the ratio between the applied bias ($\Delta U/2$) and the hopping integral between nearest neighbors W. Let´s introduce non-dimensional variables $t=E/2W$ and $s=(\Delta U/2)/2W$. With these substitutions the integrals of the interface density of states i.e. $1-\Delta Z$) are cast into the following forms: for $s\geq 1$:

$$\frac{1}{2\pi s}\int_{-1+s}^{1+s} f_2(t,s)dt \tag{42}$$

and for $s<1$:

$$\frac{2}{\pi}\int_{-1+s}^{1-s} f_1(t,s)dt+\frac{1}{2\pi s}\int_{1-s}^{1+s} f_2(t,s)dt \quad . \tag{43}$$

Functions f_1 and f_2 are given with:

$$f_1(t,s)=\frac{\sqrt{1-(t-s)^2}+\sqrt{1-(t+s)^2}}{4s^2+\left(\sqrt{1-(t-s)^2}+\sqrt{1-(t+s)^2}\right)^2} \tag{44}$$

and

$$f_2(t,s)=\sqrt{1-(t-s)^2}(t+s)+\sqrt{\left((1+s)^2-t^2\right)\left(t^2-(1-s)^2\right)} \tag{45}$$

We are interested in the asymoptic behavior of the interface charge bias dependence for large values of applied bias, i.e. we seek the value of the above integral for $s>>1$. Since the induced interface charge monotically limits to zero for large values of applied bias, it is convenient to approximate the integrand with the power series up to the first non-vanishing order in $1/(\Delta U/2)$. Introducing the new variable $u=t-s$, the following expression needs to be evaluated for $s>>1$:

$$\Delta Z=\frac{2}{\pi}\int_{-\pi/2}^{\pi/2}\frac{\cos^2 u\ du}{\cos^2 u+\left(\sqrt{(\sin u+2s)^2-1}-2s\right)^2}. \tag{46}$$

The power series of the part of the integrand containing s is:

$$\sqrt{(\sin u+2s)^2-1}-2s=\sin u-k+2k^2\sin u \tag{47}$$

where $k=1/4s=W/\Delta U$. Expanding the whole integrand in power series to the second order in k and integrating the obtained series yields:

$$\frac{2u+\sin 2u}{2\pi}-\frac{3\cos u+\cos 3u}{3\pi}k-\frac{2u+\sin 2u}{2\pi}k^2 \tag{48}$$

Evaluation of the obtained asymptotic expression at the upper and lower integral boundary $[-\pi/2,\pi/2]$ yields:

$$\Delta Z=k^2=\left(\frac{W}{\Delta U}\right)^2. \tag{49}$$

For the very low values of applied bias, which equals the case when $s<<1$, the interface charge shows a square root dependence on the applied bias:

$$\Delta Z=\frac{4}{3\pi}\sqrt{s}=\frac{2}{3\pi}\sqrt{\frac{\Delta U}{W}}. \tag{50}$$

The asymptotic expressions for the bias dependence of the interface charge for small and large values of applied bias are in accordance with the ones previously presented in the numerical study of the induced interface charge. The forms (50) and (49) were previously obtained using simple yet plausible arguments of the rigid band shift in case of small bias, and considering the case of the seminfinite lattice with an adsorbed atom.

The origin of the maximum in the bias dependence of the interface charge reveals the structure of the expression (43) entering the calculation of the interface charge for $s<1$ which is a sum of a monotonically increasing and decreasing part. The sum of the two yields the curve exhibiting a maximum point in the interval $s\in[0,1]$. The situation is illustrated in fig. 5.

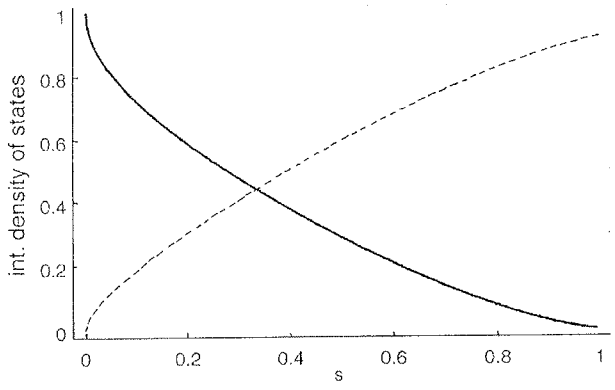

Fig. 5: Partial contributions to the total induced interface charge from the integrated density of states over the appropriate energy interval. The full curve shows the contribution of the states with the energy $E\in[-2W+\Delta U/2, 2W-\Delta U/2]$ whereas the dashed curve shows the integral over the states from the energy interval $E\in[2W-\Delta U/2, 2W+\Delta U/2]$.

5. Conclusions

Recently /7/ it has been realized that the measured capacitance spectra of the ICB deposited Ag/p-Si(100) can be suitable well described only if the charge model for the capacitance of the structure incorporated the bias dependent interface charge density. In this paper the first step towards the microscopic picture of the underlying physical processes is taken.

On the basis of the very simple model the bias dependence of the induced charge at the interface is calculated in tight binding approximation. The expressions for the limiting cases at small (9) and (50) and large (10) and (49) values of the applied bias are shown in the compact form. For the intermediate values between the limits the induced charge is expected to reach a maximum value. It is argued that the interface charge used in models of semiconductor devices should in general be divided into intrinsic, which is induced even in ideal heterojunctions and extrinsic, which is is a consequence of disorder present at the junction between dissimilar materials. In this study the effect of the disorder at the interface is not considered and only the applied bias dependent intrinsic induced interface charge is explored. As the preliminary investigations show, the presence of the disorder changes the bias dependence of the induced charge in accordance with the model of disorder and the details of the bonding so that the simple scaling of the bias does not apply, but still the pronounced maximum of the induced interface charge is to be expected. The detailed effects of the interface charges at the interface in the charge transport in semiconductor junctions is a subject of an ongoing research.

Note added in proof: Latest results show that the model function for the interface charge density of the form: $\sigma(\Delta U)=n_\sigma(a\Delta U+b)\exp(-(\Delta U/V_0+K)^2)$ included in the model for the capacitance /7/ gives a suitable description of the published measured capacitance data /23, 24, 25/ of the *ordinary* (i.e. *not* ICB deposited) Al/p-Si and Mo/p-Si Schottky structures. The parameters used to model the published data in *absolute scale* were:
for Al/p-Si: $n_\sigma=0.00710^{-5}$ As/cm^2, $V_0=0.19$V, $K=2.5$, $a=0.081V^{-1}$, $b=0.06$ and
for Mo/p-Si: $n_\sigma=0.000810^{-5}$ As/cm^2, $V_0=0.16$V, $K=1.6$, $a=0.01V^{-1}$, $b=0.51$. As it seems, the proposed model for the capacitance incorporating the bias dependent interface charge density could have a general validity for the metal/thin interlayer/semiconductor structures, and not only for the ICB samples. A detailed presentation of these findings is to be published.

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