DETERMINING THE ENERGY FOR THE ELECTRON TRANSMISSION BETWEEN TWO NEUTRAL ISLANDS IN A DISCONTINUOUS LAYER

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The common properties of discontinuous metal films deposited on insulating substrates are discussed. An attempt has been made to determine the energy necessary to transpose an electron from one neutral island to a neighbouring neutral island, using the Thomas–Fermi method. From the analysis it follows that the value of this energy will depend significantly on the kind of metal, dimensions of the islands, and distance between them.

1. Introduction

The properties of discontinuous metal layers associated with insulating substrates and the conditions for an electron transition from one neutral island to another, i. e. generation conditions of pairs of islands (electron-hole) with different (positive and negative) charges are the subjects of this paper. A problem, similar to the electron transition one discussed here, was solved by Neugebauer–Webb [1], Hill [2], Abeles and others [3]. Their solutions were based on electrostatics.

In the present paper an attempt has been made to determine the energy necessary for an electron to translate from one neutral island to a neighbouring neutral island, using the Thomas–Fermi method. The above method, unlike the former ones, allowed one to take into account the effect of the metal used for the construction of the island on the generation energy of the electron-hole pair. The determination of the generation energy of the pair contributes to the understading of the nature of the activation energy of electric conductivity in discontinuous metal layers.

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2. Generation of a pair of islands having different charges

We determine the energy necessary to transfer an electron from one neutral island to a neighbouring neutral island. The electron leaving the island charges it positively (it moves in the field of a positively charged island), whereas entering the island it charges it negatively (it moves in the field of a neutral island).

Let us assume that each hemispherical island consist on N atoms distributed regularly, and that each atom can be described by the Thomas-Fermi potential (φ). The potential of an electron at point A (Fig. 1) has the form:

$$V_A = \sum_{\substack{n=1 \\ n\neq k}}^{N} \varphi_0(|\bar{r}_1-\bar{a}_{1n}|)+\varphi_+(|\bar{r}_1-\bar{a}_{1k}|)+\sum_{n=1}^{N}\varphi_0(|\bar{r}_1-\bar{P}-\bar{a}_{2n}|)+\Delta_1, \tag{1}$$

where the first term of the sum denotes the total potential produced by neutral atoms of island 1; the second term denotes the potential produced by a singly ionized atom of island 1; the third term denotes the total potential of the deformation of the system of electrons produced by neutral atoms of island 2; Δ_1 — global potential associated with the deformation of the system of electrons caused by the electron leaving the island.

$$\bar{a}_{1n} = \bar{a}_{1x}i+\bar{a}_{1y}j+\bar{a}_{1z}k$$

i, j, k — integral numbers $\bar{a}_{1x}$, $\bar{a}_{1y}$, $\bar{a}_{1z}$ — vectors of the lattice basis.

At point B the electron possesses the potential

$$V_B = \sum_{n=1}^{N}\varphi_0(|\bar{r}_2-\bar{a}_{2n}|)+\sum_{\substack{n=1 \\ n\neq k}}^{N}\varphi_0(|\bar{r}_2+\bar{P}-\bar{a}_{1n}|)+\varphi_+(|\bar{r}_2+\bar{P}-\bar{a}_{1k}|)+\Delta_2, \tag{2}$$

where the first term of the sum denotes the global potential produced by the neutral atoms of island 2; the second term denotes the global potential produced by the neutral atoms of island 1; the third term denotes the potential produced by singly ionized atoms of island 1; Δ_2 — global potential associated with the deformation of the system of electrons caused by the electrons entering the island.

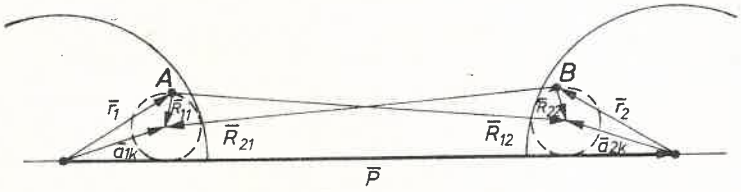

Fig 1. System of two neighbouring islands. $\bar{R}_{11} = \bar{r}_1-\bar{a}_{1k}$; $\bar{R}_{12} = \bar{r}_1-\bar{P}-\bar{a}_{2k}$; $\bar{R}_{21} = \bar{r}_2+\bar{P}-\bar{a}_{1k}$; $\bar{R}_{22} = \bar{r}_2-\bar{a}_{2k}$

From geometrical considerations (Fig. 1) it follows that

$$|\bar{r}_1-\bar{a}_{1n}| = |\bar{r}_2-\bar{a}_{2n}| \tag{3}$$

and

$$|\bar{r}_1-\bar{P}-\bar{a}_{2n}| = |\bar{r}_2+\bar{P}-\bar{a}_{1n}|. \tag{4}$$

Inserting (3) and (4) into (2) we get

$$V_B = \sum_{n=1}^{N} \varphi_0(|\bar{r}_1 - \bar{a}_{1n}|) + \sum_{\substack{n=1 \\ n \neq k}}^{N} \varphi_0(|\bar{r}_1 - \bar{P} - \bar{a}_{2n}|) + \varphi_+(|\bar{r}_1 - \bar{P} - \bar{a}_{2k}|) + \Delta_2. \tag{5}$$

We determine the difference between the potentials at points A and B using the relations (1) and (5).

$$\Delta V = V_A - V_B = \Delta\varphi(|\bar{r}_1 - \bar{a}_{1k}|) - \Delta\varphi(|\bar{r}_1 - \bar{P} - \bar{a}_{2k}|) + \Delta_1 - \Delta_2. \tag{6}$$

Further on we determine $\Delta\varphi$ with the help of the Thomas–Fermi method.

3. Thomas-Fermi method [4]

The statistical Thomas–Fermi method is, among others, used to determine the atomic potential taking into account the effect of all the electrons. In this method the following differential equation is solved numerically

$$\frac{d^2\Phi}{dx^2} = \frac{\Phi^{3/2}}{\sqrt{x}}. \tag{7}$$

With the following boundary conditions

$$\Phi(0) = 1, \quad \Phi(x_0) = 0, \quad x_0\Phi'(x_0) = -\frac{Z-M}{Z},$$

where $\Phi(x)$ is a normalized potential, x — normalized distance from the nucleus, Z —atomic number, x_0 — normalized radius of the atom, M — number of electrons.

The relations between normalized and real quantities are given by the following equalities

$$\varphi = A + \Phi\frac{eZ}{4\pi\varepsilon_0 r} \tag{8}$$

$$r = 4.685 \cdot 10^{-9}\, xZ^{-1/3}\ [\mathrm{cm}] \tag{9}$$

$$A = \varphi(x_0) = \frac{e(Z-M)}{4\pi\varepsilon_0 R}, \tag{10}$$

where R is the atomic radius ($R = r(x_0)$), ε_0 — dielectric constant.

It follows also from the Thomas–Fermi method that for $x > x_0$ i. e. for $r > R$, $\varphi(x)$ takes the form of the Coulomb equation

$$\varphi(r) = \frac{e(Z-M)}{4\pi\varepsilon_0 r}. \tag{11}$$

In Fig. 2 the outline of the solutions of (7) is given, whereas in Table I the values of x_0 are given for different values Z of atoms singly positively ionized. The potential difference between neutral and ionized atoms can be calculated from the relations (8) and (10).

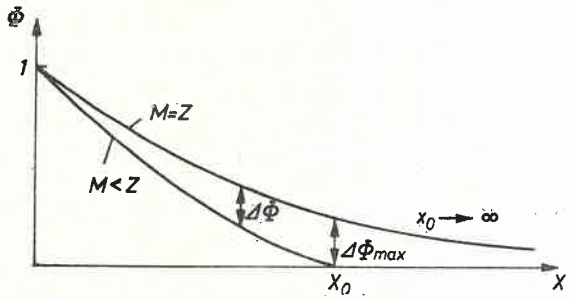

Fig. 2. Function $\Phi(x)$ in outline

TABLE I

Values of x_0 for different Z of atoms singly positively ionized after Brudner [5]

Element	Z	x_0 (TF Brudner)	x_0 (TFA Kobyashi)
Li^+	3	4.589060	—
Na^+	11	11.60870	11.604
K^+	19	15.68552	15.678
Rb^+	37	21.87429	21.857
Ca^+	55	26.31931	—

TABLE II

Some values of $\Phi(x)$ for a neutral atom after Bush [6]

x	10	15.01	20	20.87	21.82	26.67	30	34.29
$\Phi(x)$	0.0244	0.0109	0.0058	0.0053	0.0048	0.0030	0.0022	0.0016

In view of the data given in Tables I and II we get

$$\Delta\varphi \simeq \begin{cases} -\dfrac{e}{4\pi\varepsilon_0 r} \to r \geqslant R \\ -\dfrac{e}{4\pi\varepsilon_0 R} \to \dfrac{R}{2} < r < R. \end{cases} \tag{12}$$

Then we can write (6)

$$\Delta V = \Delta\varphi' + \Delta\varphi'',$$

where

$$\Delta\varphi' = -\frac{e}{4\pi\varepsilon_0|\bar{r}_1-\bar{a}_{1k}|} \tag{13}$$

$$\Delta\varphi'' = -\frac{e}{4\pi\varepsilon_0\varepsilon_r R_{12}} + \Delta_1 - \Delta_2 \tag{14}$$

ε_r is a relative dielectric permittivity of the medium separating the islands.

$$R_{12} = |\bar{r}_1 - \bar{P} - \bar{a}_{2k}|.$$

4. Determining the change in electron energy corresponding to the change in the potential

According to the first order of disturbance calculus we can write that

$$E_l = E_{0l} - \langle\psi_{0l}|\Delta\varphi|\psi_{0l}\rangle = E_{0l} - e\int_v |\psi_{0l}|^2\Delta\varphi dv \tag{15}$$

where E_l is an electron energy at a disturbed state, E_{0l} — electron energy at an undisturbed state, ψ_{0l} — wave function of an undisturbed state, v — volume.

Hence,

$$\Delta E = E_l - E_{0l} = e\int_v |\psi_{0l}|^2\Delta\varphi dv. \tag{16}$$

It may be written that

$$\int_v |\psi_{0l}|^2 dv = 1. \tag{17}$$

A fragment of the island in the neighbourhood of the k-th (ionized) atom is presented in Fig. 3. Because of the low probability that a conduction electron is within the ion of the lattice.

$$|\psi_{0l}|^2 \simeq 0 \quad \text{for } r < r_j,$$

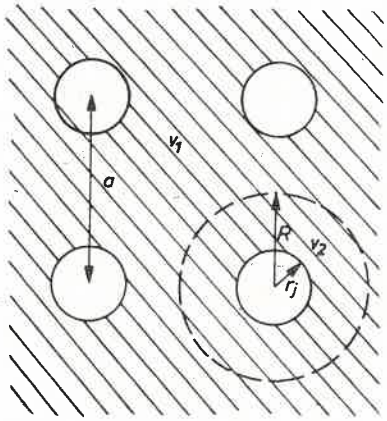

Fig. 3. Fragment of the crystal lattice of an island in the neighbourhood of an ionized atom. r_j — radius of a lattice ion; R — atomic radius resulting from the Thomas–Fermi method

where r_j is the ion radius, i. e. $|\psi_{0l}|^2 \neq 0$ only within the volume v_1 (Fig. 3). Therefore, formula (16) can be written in the form

$$\Delta E = e \int_{v_1} |\psi_{0l}|^2 \Delta\varphi dv = |\overline{\psi}_{0l}|'^2 e \int_{v_1} \Delta\varphi dv. \tag{18}$$

Similary

$$\int_{v} |\psi_{0l}|^2 dv = \int_{v_1} |\psi_{0l}|^2 dv = |\overline{\psi}_{0l}|^2 \int_{v_1} dv = 1. \tag{19}$$

Assuming that $|\overline{\psi}_{0l}|'^2 \simeq |\overline{\psi}_{0l}|^2$ and inserting (19) to (18) we get

$$\Delta E = \Delta E' + \Delta E'', \tag{20}$$

where

$$\Delta E' = \frac{e}{v_1} \int_{v_1} \Delta\varphi' dv \tag{21}$$

$$\Delta E'' = \frac{e}{v_1} \int_{v_1} \Delta\varphi'' dv. \tag{22}$$

On the grounds of Fig. 3. equality (21) can be written in the form

$$\Delta E' = \frac{e}{v_1} \int_{v_2} \Delta\varphi' dv + \frac{e}{v_1} \int_{v_1 - v_2} \Delta\varphi' dv \tag{23}$$

from (12) we see that within the volume v_2

$$\Delta\varphi = -\frac{e}{4\pi\varepsilon_0 R}$$

hence

$$\Delta E_1' = \frac{e}{v_1} \int_{v_2} \Delta\varphi' dv = -\frac{e^2}{4\pi\varepsilon_0 R} \frac{v_2}{v_1} \tag{24}$$

$\Delta\varphi'$ for $r > R$ due to charge screening in the electron gas can be described by the formula resulting from application of the Thomas–Fermi method to the electron gas

$$\Delta\varphi' = B \exp\left(-\frac{r}{\lambda}\right) r^{-1}, \tag{25}$$

where

$$\lambda = \left(\frac{n_0 e^2}{2\varepsilon_0 E_F}\right)^{-1/2}$$

(for example $\lambda = 0.7$ Å for Au — see [7] Fig. 8.8).

Since

$$\Delta\varphi' = -\frac{e^2}{4\pi\varepsilon_0 R} \quad \text{for } r = R \text{ then}$$

$$B = -\frac{e^2}{4\pi\varepsilon_0}\exp\left(\frac{R}{\lambda}\right). \tag{26}$$

Thus

$$\Delta E_2' = \frac{e}{v_1}\int\limits_{v_1-v_2}\Delta\varphi' dv = \frac{B}{v_1}\int\limits_{v_1-v_2} r^{-1}\exp\left(-\frac{r}{\lambda}\right)dv \tag{27}$$

To evaluate the integral (27) let us notice that the integrating function is strongly decreasing, and for this reason the essential contribution to this integral is given by the nearest neighbourhood of volume v_2. Thus, neglecting lattice ions surrounding volume v_2 we can write

$$\Delta E_2' = \frac{B}{v_1}\int\limits_0^{2\pi} d\xi \int\limits_0^{\pi}\sin\theta d\theta \int\limits_R^{+\infty} re^{-\frac{r}{\lambda}}dr = -\frac{e^2}{\varepsilon_0 v_1}\lambda R\left(1+\frac{\lambda}{R}\right). \tag{28}$$

We can also write that

$$v_1 = v_i - \tfrac{4}{3}\pi r_j^3 N = \tfrac{4}{3}\pi N\left(\frac{3}{4\pi n_a} - r_j^3\right), \tag{29}$$

where v_i is a volume of island, n_a — atomic density in the island, and

$$v_2 = \tfrac{4}{3}\pi(R^3 - r_j^3). \tag{30}$$

According to (29) and (30) we can rewrite (24) as follows

$$\Delta E_1' = -\frac{e^2}{4\pi\varepsilon_0 R}\,\frac{R^3 - r_j^3}{N\left(\frac{3}{4\pi n_a} - r_j^3\right)}. \tag{31}$$

Similary

$$\Delta E_2' = -\frac{e^2}{4\pi\varepsilon_0}\lambda R\left(1+\frac{\lambda}{R}\right)\left[\frac{N}{3}\left(\frac{3}{4\pi n_a} - r_j^3\right)\right]^{-1}. \tag{32}$$

Thus, finally

$$\Delta E' = \Delta E_1' + \Delta E_2' = -\frac{e^2}{4\pi\varepsilon_0 N R_{ef}}, \tag{33}$$

where

$$R_{\mathrm{ef}} = \frac{\left(\frac{3}{4\pi n_a} - r_j^3\right) R}{(R+\lambda)^3 - (r_j^3+\lambda^3)}. \tag{34}$$

Let us now estimate the quantity $\Delta E''$. To estimate the difference $\Delta_1 - \Delta_2$ occuring in (6) we shall use the mirror reflection method. The system metal ball-charge is replaced by the system of 3 point charges [8].
Then

$$\Delta\varphi'' = \sum_{m=1}^{3} \frac{q_m}{4\pi\varepsilon_0 R_m}, \tag{35}$$

where R_m is the distance from the charge $q_m (m = 1, 2, 3)$. By assuming that the electric field penetrates only into a thin surface layer of the ball (the thickness of the layer is C) we get

$$\Delta E'' = \frac{e}{4\pi\varepsilon_0\varepsilon_r v_1} \int_0^{2\pi} d\xi \int_{R_i - C}^{R_i} r^2 dr \int_0^{\pi} \sin\theta \left(\sum_{m=1}^{3} \frac{q_m}{\sqrt{r^2 + L_m^2 - 2rL_m\cos\theta}} \right) d\theta, \tag{36}$$

where L_m is the distance of the charge q_m from the centre of the ball ($m = 1, 2, 3$), R_i — ball radius. Hence we can write

$$\Delta E'' = \frac{e^2 R_i^2 C}{\varepsilon_0\varepsilon_r L_1 v_1}, \tag{37}$$

where $L_1 = (|\overline{P}| - R_i)$. Because for connected islands ($|\overline{P}| = 2R_i$) is $\Delta E' = \Delta E''$, finally we get

$$\Delta E = -\frac{e^2}{4\pi\varepsilon_0 N R_{\mathrm{ef}}} \left(1 - \frac{R_i}{\varepsilon_{\mathrm{ef}}(|\overline{P}| - R_i)}\right), \tag{38}$$

where

$$\varepsilon_{\mathrm{ef}} = \begin{cases} 1 \to L_1 = R_i \\ \varepsilon_r \to L_1 - R_i > C. \end{cases} \tag{39}$$

5. *Final remarks*

Calculation of the energy ΔE of electron transition from one neutral island to a neighbouring neutral island has been based on the Thomas–Fermi method. From the analysis of formula (38) it follows that the value of the energy will depend significantly on the kind of metal, geometry of the system and kind of medium. In the theories so far considered the kind of metal of which the discontinuous layer was made has not been considered.

TABLE III

Material	Radius of island (Å)	Island spacing (Å)	Experimental data [2] (eV)	Theoretical data [2] (eV)	From Eq. (38) for $\varepsilon_{ef} = 1$	From Eq. (38) for $\varepsilon_{ef} = 3.5$
Gold on soda glass	R_i(Å)	P-$2R_i$	δE	δE_0	ΔE (eV)	ΔE (eV)
	25	40	0.087	0.062	0.056	0.081
	30	40	0.038	0.050	0.037	0.058

Table III compares values of ΔE obtained from equation (38) with theoretical and experimental data obtained by Hill [2]. The present paper is an analysis of a system consisting of two identical islands. It should be considered additionally that we are dealing with a multi island system, that the islands have different dimensions and the distances between them are different, and that there exists an interaction between islands and surroundings. (This has been partly considered in formula (39)).

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