Energy Parameters of Interfacial Layers in Composite Systems: Graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) and Semiconductor (Si,Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb)

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On the basis of the non-equilibrium thermodynamics relations and the surface physics phenomena we calculate adhesion and energy parameters to characterize the interfacial interactions in graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) and semiconductor (Si, Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb) systems. We analyze trends of the interfacial energy, interfacial tension, work of adhesion and the energy of adhesive bonds on the contacting element's atomic number in the periodic table and on the electronegativity difference of interacting elements. Thus, this work provides theoretical basis for the development of new composite materials.

Keywords: Adhesion, Surface, Tension, Interfacial.

1. INTRODUCTION

According to the specialists' forecasts graphene is the most promising material in nanoelectronics [1] and spintronics [2]. One of the most important directions is considered to be the development of the structures on the basis of the graphene that have low dimensional electron gas. These new materials have the opportunity to create optoelectronic devices with tunable parameters [3]. Furthermore, besides having a unique mechanical [4, 5] and electronic properties [6], graphene has broad prospects for practical application in specific structural and functional materials. As for semiconductors (silicon and germanium), the creation of new types of structures with predictable properties is one of the priority directions in the development of modern semiconductor micro-and nano-electronics.

It should be noted that the modern progress in nanoscale physics and low-dimensional structures is greatly due to the development of theoretical and applied research in the field of interfacial phenomena. Hence, the creation of the new graphene-based structures and composite materials with the unique properties that are capable of working in extreme conditions, requires the knowledge of the surface properties at different interfacial boundaries. For example, the technology of catalytic growth of graphene on metal and semiconductor surfaces is one of the most effective methods of obtaining graphene. These circumstances stimulate the study of interfacial layers of the formed structures, particularly, their energy parameters: interfacial energy - γ_m, the interfacial tension - σ_m, work of adhesion - A_{ad} and the energy of adhesive bonds - γ_{ad}.

This paper is based on the approach developed in [7, 8], in particular, the relations of non-equilibrium thermodynamics and physics of the surface phenomena, to calculate the energy parameters - γ_m, σ_m, A_{ad} and γ_{ad} of the interfacial layers for systems: graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) and semiconductor (silicon, germanium) – (Fe, Co, Cu, Al, Au, Cr, W, Pb). Method of using the eq. (6) - (8) to determine ξ, k, β, h is implemented for the first time in this study.

2. METHODS OF CALCULATION OF INTERFACIAL ENERGY, INTERFACIAL TENSION, THE WORK OF ADHESION AND THE ENERGY OF ADHESIVE BONDS

For the system "metal - semiconductor (or dielectric)" we use a macroscopic approach, which corresponds to the ratio of non-equilibrium thermodynamics and physics of solid surfaces. Let's consider the system of equations and boundary conditions for describing the change of energy parameters (σ_n, γ), which characterize the thermodynamic state of the system of contacting bodies [8, 9].

Relations for the thermodynamic model of the surface layer of metal ($x > 0$) (quasistatic situation) can be represented in Cartesian coordinates x, y, z (where x is perpendicular to the interface) in the form [8, 9]:

$$Div\,\hat{\sigma} + \rho \cdot \omega \cdot \vec{E} = 0, \quad \Delta\phi = \rho \cdot C_\phi \cdot \phi / \varepsilon_0, \quad (1)$$

$$\phi = -\Phi_0; \quad \phi + \psi = const; \quad \sigma_x = -\frac{\varepsilon_0}{2}\cdot\left(\frac{\partial\Psi}{\partial x}\right)^2 \text{ if } x = 0, \quad (2)$$

$$\sigma_{ij} = \left(\left(K - \frac{2}{3}G\right)e - \alpha_t K \cdot \Delta T - K(\beta\phi + \beta_c c)\right)\delta_{ij} + 2Ge_{ij}, \quad (3)$$

$$\omega_V = \rho\omega = \rho C_\phi(\phi - \gamma_t \cdot \Delta T) + \beta Ke - \rho\eta_c c, \quad (4)$$

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$$\mu_c = d_c c + d_t \cdot \Delta T + \beta_c K \frac{e}{\rho} - \eta_c \phi, \quad \Delta T = T - T_0, \tag{5}$$

$$\sigma_h = \int_0^h \sigma_y dx, \quad \sigma_y = \sigma_z, \quad \gamma = \gamma_e + \xi\gamma_d, \tag{6}$$

$$\frac{\partial \gamma}{\partial k} = \frac{\partial(\gamma_e + \xi\gamma_d)}{\partial k} = 0, \quad k = \sqrt{\frac{\rho \cdot C_\phi}{\varepsilon_0}}, \tag{7}$$

$$\sigma_y + p = 0 \ (\text{for } x = h), \tag{8}$$

Here γ, σ_h - surface energy (SE) and the surface tension in the case of contact of the metal with inert gas atmosphere (air) with the pressure $p = 100$ kPa; $\gamma_e = \int_0^h w_e dx$ - electric component of γ, $w_e = \frac{\varepsilon_0}{2}\left(\frac{\partial\Psi}{\partial x}\right)^2$ and $w_d = \frac{\sigma_x(\sigma_x - 4\nu\sigma_y)}{2E} + \frac{(1-\nu)\sigma_y^2}{E}$ – densities of the electrical and mechanical components of the SE; $\gamma_d = \int_0^h w_d dx$ - mechanical component of SE; h – effective thickness of the surface layer; σ_{ij}, e_{ij} – tensors of mechanical stress and strain ($i, j = 1,2,3$); $\sigma_{11} = \sigma_{xx} \equiv \sigma_x$; $\sigma_{22} = \sigma_{yy} \equiv \sigma_y$; μ_c, c – chemical potential and the concentration of impurities; δ_{ij} – Kronecker symbols; e – the first invariant of the strain tensor; ρ – density of the material; ω_v, ω – volumetric and mass charge density, respectively; $\varphi = \Phi - \Phi_0$ – deviation of the modified chemical potential Φ of the electrical charges from its equilibrium value Φ_0 in the volume of the body at a distance $x > 30$ nm from the surface ($\Phi = M_e/z_e$, M_e – chemical potential of the conduction electron of the metal; z_e – electric charge per unit mass of the conduction electrons ($[M_e] = J / kg$, $[z_e] = C / kg$, $[\Phi] = C$)); Ψ – the potential of the electric field ($[\Psi] = V$); $\psi = \Psi - \Psi_0$ – deviation of the potential Ψ from its equilibrium value Ψ_0; $\vec{E} = \nabla\Psi = grad\Psi$ - the amplitude of the electrical field; $\varepsilon_0 = 8,85\cdot10^{-12}$ F / m - electric constant; $\Delta T = T - T_0$ – temperature change; K, G – the bulk modulus and shear modulus; E, ν – Young's modulus and Poisson's ratio; C_φ – capacitance; k – the inverse value of the distance, at which the volume charge in the surface layer varies by a factor e; β - electrostrictive coefficient of thermal expansion; ξ - coefficient (dimensionless) that characterizes the change in γ when changing the mechanical component γ_d, for condition when the electric component γ_e remains unchanged $\left(\frac{\partial\gamma}{\partial\gamma_d}|_{\gamma_e=const} = \xi\right)$; α_t, β_c, γ_t, η_c, d_c, d_t - physical characteristics of the material (metal) which are included in the equation of state (4), (5) and (6) [9].

For more adequate fit of the model given by eq. (1)-(8) to the modern physical notions, it is necessary to take into account the offset Z_b of the electron double layer with respect to the boundary of the solid (metal). For this purpose we use a well-known formula [10]:

$$Z_b = \frac{3}{4k_F}\left(\frac{\pi}{2} + \left(\frac{5E_V}{3E_F} - 1\right)\arcsin\sqrt{\frac{3E_F}{3E_F + 5E_V}} - \sqrt{\frac{5E_V}{3E_F}}\right), \tag{9}$$

where E_F – Fermi energy, E_V – the work function of the conduction electron and k_F – Fermi wave vector.

By setting the values of γ and σ_h (SE and tension) in eq. (6)-(8) (taking into account eq. (1)-(5), (9)), we obtain a system of 4 equations. In this case we can determine the values of ξ, k, β and geometrical characteristics h of the surface layer for the metal, which is in contact with an inert gas atmosphere (air) at a pressure $p = 100$ kPa. Using the value of k, we can find C_φ and Φ_0 with the help of the eq. (7) and (9), [10]:

$$C_\phi = \frac{\varepsilon_0 \cdot k^2}{\rho},$$
$$\Phi_0 = \frac{q_0 W_e}{2\varepsilon_0 k^2}\cdot\left(2 - \exp(-kZ_b)\right), \tag{10}$$

where W_e - the bulk density of the conduction electrons of the metal away from the surface (at a distance of more than 30 nm, $[W_e] = 1/m^3$).

For most of metals values of the surface tension σ_h are determined experimentally [11]. The surface energies γ of the metals are determined both experimentally and theoretically. Among the theoretical studies one should note partial results obtained for a number of metals using the method of density functional [12-14]. According to the authors, the empirical formula for γ in steel [15] has good consistency with the experimental data. Hence it has been applied for a number of other metals:

$$\gamma = a_R \cdot \frac{E_V}{R^2} - a_C, \tag{11}$$

where R - atomic radius, a_R, a_C - empirical constants ($a_R = 7128$; $a_C = 110$ J/m²).

In particular, for steel the result is $\gamma = 1947$ J/m² [15], which is about three orders of magnitude different from the known data [16]. Therefore, here we use data for other metals, namely, copper, iron, germanium and silicon for evaluating values of a_R and a_C [16 – 21]:

Fe: $\gamma = 2.42$ J/m²; $R = 0.11376$ nm; $E_V = 4.855$ eV;
Cu: $\gamma = 1.85$ J/m²; $R = 0,11391$ nm; $E_V = 4.7$ eV; (12)
Si: $\gamma = 1.623$ J/m²; $R = 0.1358$ nm; $E_V = 4.8$ eV;
Ge: $\gamma = 1.398$ J/m²; $R = 0.1415$ nm; $E_V = 4.76$ eV.
Substituting (12) into (11), we find:
metals – $a_R = 0.2755$ and $a_C = 14.11$ J/m² (13)
semiconductors – $a_R = -0.01334$ and
$a_C = -2.1778$ J/m²(14)

Surface tension σ_h and surface energy γ are connected by Hering's relation [22]:

$$\sigma_h = K_R\left(\gamma + \Xi\left(\frac{\partial\gamma}{\partial\Xi}\right)_T\right), \qquad (15)$$

where K_R - factor for matching dimensions ($[K_R] = \dfrac{N\cdot m^2}{m\cdot J}$), since $[\sigma_h] = \dfrac{N}{m}$; $[\gamma] = \dfrac{J}{m^2}$;

Ξ – surface area and $\left(\dfrac{\partial\gamma}{\partial\Xi}\right)_T$ represents the change of the surface energy during surface layer deformation at a constant temperature.

Based on the model, wherein the interfacial layer consists of two parts, the interfacial energy γ_m and interfacial tension σ_m at the interface between the substrate (semiconductor or insulator) – metal are defined by the following relations [8]:

$$\sigma_m = \int_{-H}^{H}\sigma_y dx, \quad \sigma_y = \sigma_z, \qquad (16)$$

$$\begin{aligned}\gamma_m = \gamma_e + \xi_m\gamma_d, \quad \gamma_e = \int_{-H}^{H}w_e dx,\\ \gamma_d = \int_{-H}^{H}w_d dx\end{aligned} \qquad (17)$$

Here ξ_m – physical characteristics of the interfacial layer (dimensionless) $\left(\partial\gamma_m/\partial\gamma_d|_{\gamma_e=const} = \xi_m\right)$; $2H$ – its effective thickness; γ_e, γ_d – electrical and mechanical components of the interfacial energy γ_m respectively, as in eq. (6).

Finally, by the analogy to the equilibrium condition of the surface layer [12, 13], we can write the equilibrium condition for the interfacial layer as in [8]:

$$\frac{\partial\gamma_m}{\partial k} = \frac{\partial(\gamma_e + \xi_m\gamma_d)}{\partial k} = 0. \qquad (18)$$

Boundary conditions. Let us formulate boundary conditions for metal – semiconductor (or insulator) interface (at $x = 0$) which corresponds to the electrical double layer. This interface is formed by conduction electrons from the side of metal and by bounded electrical charges from the side of semiconductor (or dielectric) [7, 8]:

$$\phi_+ = -\Phi_0; \quad z_- = -Z_e; \quad j_x^+ = j_{xe}^-; \quad \sigma_y^+ = \sigma_y^-; \quad \sigma_x^+ = \sigma_x^-;$$

$$\Psi^+ = \Psi^-; \quad \vec{u}^+ = \vec{u}^-; \quad E_\tau^+ = E_\tau^-; \quad D_x^+ - D_x^- = \Omega, \quad (19)$$

where $\sigma_x^\pm$, $\sigma_y^\pm = \sigma_z^\pm$ – mechanical stresses along directions which are perpendicular to the interface between two media respectively; $\vec{u}^\pm$ displacement; $E_\tau^\pm$ - tangential component of the electrical field; $D_x^\pm, P_x^\pm$ - components of the electrical field induction and polarization vectors respectively are directed along the normal (axis x) towards the plane of interface ($x = 0$); Ω – density of the surface (excess, uncompensated) charges (created by free electrons). If the metal surface is not charged from the outside, then $\Omega = 0$.

The work of adhesion A_{ad} and adhesive bonds energy γ_{ad} are defined based on the known relations [8]:

$$A_{ad} = \sigma_h + \sigma_{ph} - \sigma_m, \quad \gamma_{ad} = \gamma + \gamma_p - \gamma_m, \qquad (20)$$

where σ_{ph} and γ_p - surface tension and energy of a semiconductor (silicon, germanium) which contacts with an inert gas medium (air) in which the pressure is 100 kPa.

3. RESULTS OF CALCULATIONS AND DISCUSSION

As input parameters for numerical calculations of the energy parameters in the interfacial layer of the contact system, we make use of the physical constants of elements (Young's modulus E, Poisson's ratio ν, surface tension σ_h, surface energy γ, the concentration of free electrons in the metal or bounded charged particles q). These values are summarized below [11-14, 16-21,24-29]:

$E_- = 154$ GPa; $\nu_- = 0.34$; $q_- = 8.38\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 2.16$ N/m, $\gamma_- = 1.85$ J/m^2 (Cu);
$E_- = 200$ GPa; $\nu_- = 0.277$; $q_- = 8.49\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 2.48$ N/m, $\gamma_- = 2.42$ J/m^2 (Fe);
$E_- = 210$ GPa; $\nu_- = 0.32$; $q_- = 9.58\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 2.84$ N/m, $\gamma_- = 2.52$ J/m^2 (Co);
$E_- = 83$ GPa; $\nu_- = 0.41$; $q_- = 5.837\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 1.86$ N/m, $\gamma_- = 1.43$ J/m^2 (Au);
$E_- = 83$ GPa; $\nu_- = 0.37$; $q_- = 5.837\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 1.29$ N/m, $\gamma_- = 0.836$ J/m^2 (Ag);
$E_- = 70$ GPa; $\nu_- = 0.34$; $q_- = 5.797\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 1.39$ N/m, $\gamma_- = 1.276$ J/m^2 (Al);
$E_- = 447$ GPa; $\nu_- = 0.3$; $q_- = 7.418\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 3.486$ N/m, $\gamma_- = 3.0$ J/m^2 (Ru);
$E_- = 78$ GPa; $\nu_- = 0.37$; $q_- = 4.46\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 2.617$ N/m, $\gamma_- = 2.439$ J/m^2 (Hf);
$E_- = 16$ GPa; $\nu_- = 0.44$; $q_- = 3.3\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 0.624$ N/m, $\gamma_- = 0.576$ J/m^2 (Pb);
$E_- = 411$ GPa; $\nu_- = 0.28$; $q_- = 12.61\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 3.96$ N/m, $\gamma_- = 4.37$ J/m^2 (W);
$E_- = 279$ GPa; $\nu_- = 0.21$; $q_- = 8.327\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 2.787$ N/m, $\gamma_- = 2.47$ J/m^2 (Cr);
$E_- = 138$ GPa; $\nu_- = 0.27$; $q_- = 5.0\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 1.829$ N/m, $\gamma_- = 1.623$ J/m^2 (Si);
$E_- = 103$ GPa; $\nu_- = 0.26$; $q_- = 3.3\cdot10^{28}$ m^{-3}; $\sigma_{h-} = 1.576$ N/m, $\gamma_- = 1.398$ J/m^2 (Ge). $\qquad$ (21)

Similarly as in (21), we write the source data for graphene (C) [30-32]:

$E_+ = 1100$ GPa; $\nu_+ = 0.37$; $q_+ = 2{,}646\cdot10^{28}$ m^{-3}; $\sigma_{h+} = 0.0467$ N/m, $\gamma_+ = 0.0543$ J/m^2, $\qquad$ (22)

We consider a few graphene layers (conductor) on the solid surface in the "metal – graphene" or "semiconductor – graphene". Furthermore we assume an ideal solid contact between the graphene and a solid body, neglecting the presence of adsorbed foreign particles (impurities) such as hydrogen, oxygen, etc. which is relevant in the present nanofabrication facilities. The calculation results of the studied systems are presented in Table 1.

As shown in [8], the most sensitive parameter is the interfacial energy of the interphase. Fig. 1a shows the

dependence of the interfacial energy for graphene based systems on the contacting element atomic number in the periodic table. As it can be seen, the approximated dependence $\gamma_m(N)$ doesn't have the monotonic trend and is characterized by several maxima for elements with atomic numbers 27, 45, 73.

During the processes of metal condensation on a solid substrate, the initial stage of nanocondensate substrate can significantly influence the processes of self-organization, thus forming specific structural complexes. The degree of self-organization is determined by the difference in electronegativity ΔX of interacting elements [8]. According to Pauling [23], at $\Delta X < 0.4$ covalent type of bonding is dominant, whereas for $\Delta X > 0.4$ ionic bonding is stronger. Therefore, it is appropriate to study the dependence of interfacial energy on this parameter. Fig. 1b shows the dependence of the fitted $\gamma_m(\Delta X)$ for the elements under study. The characteristic features of the dependence are significant non-

monotonic changes of interfacial energy with increasing ΔX. In particular, in the ΔX range of 0.15-1.3 we observe two maxima: broad at $\Delta X = 0.4$ and narrow close to $\Delta X = 0.7$. Furthermore, there is a sharp γ_m increase when ΔX increases above $\Delta X = 0.8$. The maximum γ_m value observed at $\Delta X = 0.4$, apparently corresponds to the predominantly covalent bonding behavior. Subsequent γ_m behavior with increasing ΔX can be interpreted only from the standpoint of a more complex type of chemical bond with a significant contribution of the ionic component, implemented by chemical elements in the formation of interfacial layers in contact pairs.

Finally, we would like to propose to use dimensionless coefficients Z_2 and Z_4 as the energy characteristics of interfacial layers. These coefficients are invariants for each of the studied system (see table). Also interestingly coefficients Z_3 and Z_4 are equal in all three "copper" systems as well as for Si-Al, Ge-Al and Cg-Fe.

Table 1 – Energy parameters of interfacial layers in composite systems: graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) and semiconductor (Si, Ge) – (Fe ,Co, Cu, Al, Au, Cr, W, Pb). Comment(ΔX – electronegativity difference for the interacting elements; interfacial energy – γ_m, the interfacial tension – σ_m, work of adhesion – A_{ad} and the energy of adhesive bonds – γ_{ad}; $Z_3 = \sigma_m / \gamma_{ad}$, $Z_4 = \sigma_m / A_{ad}$ – dimensionless coefficients)

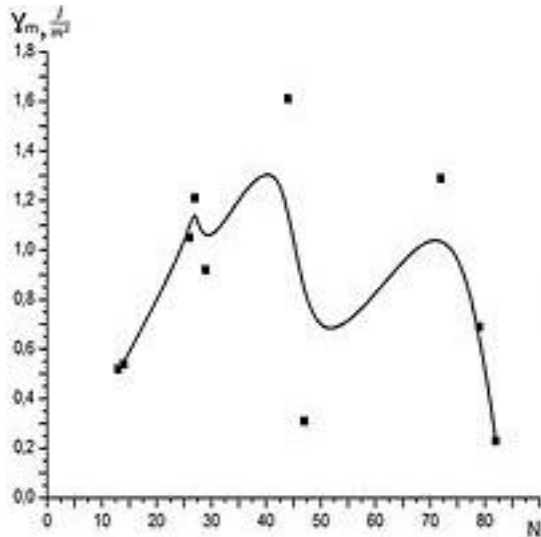| №	Systems	ΔX	$\gamma_m, \frac{J}{m^2}$	$\sigma_m, \frac{N}{m}$	$A_{ad}, \frac{N}{m}$	$\gamma_{ad}, \frac{J}{m^2}$	Z_3	Z_4
1	Cg-Si	0,65	0,54	0,73	0,66	0,69	1,06	1,11
	Cg-Cu	0,65	0,92	1,27	0,94	1,12	1,35	1,35
	Cg-Fe	0,72	1,05	1,38	1,15	1,21	1,14	1,14
	Cg-Co	0,67	1,21	1,69	1,21	1,36	1,24	1,40
	Cg-Au	0,15	0,69	0,98	0,93	0,79	1,24	1,05
	Cg-Ag	0,63	0,31	0,36	0,71	0,57	0,63	0,51
	Cg-Al	0,94	0,52	0,88	0,57	0,81	1,09	1,54
	Cg-Ru	0,35	1,61	1,79	1,76	1,43	1,25	1,02
	Cg-Hf	1,25	1,29	1,52	1,57	1,19	1,28	0,97
	Cg-Pb	0,75	0,23	0,41	0,52	0,9	0,46	0,79
2	Ge-Cr	0,45	0,71	1,29	2,25	2,06	0,63	0,57
	Ge-Cu	0,25	0,20	0,46	2,73	2,71	0,17	0,17
	GeAu	0,58	0,07	0,24	2,68	2,01	0,12	0,09
	Ge-Al	0,54	0,22	0,46	1,79	1,74	0,26	0,26
	Ge-W	0,31	3,23	2,71	3,22	4,97	0,65	0,84
	Ge-Si	0,11	0,64	0,66	1,77	2,94	0,33	0,37
	Ge-Co	0,13	1,50	2,10	1,84	2,42	0,62	1,14
	Ge-Fe	0,18	1,21	1,59	1,98	2,39	0,51	0,81
	Ge-Pb	0,21	0,43	0,52	1,21	1,6	0,28	0,43
3	Si-Cr	0,34	0,31	0,75	3,09	2,72	0,28	0,24
	Si-Cu	0,14	0,27	0,61	2,88	2,90	0,21	0,21
	Si-Au	0,38	0,12	0,37	2,84	2,24	0,17	0,13
	Si-Al	0,33	0,08	0,10	2,24	2,15	0,05	0,05
	Si-W	0,20	4,06	3,83	2,32	3,92	1,04	1,65
	Si-Hf	0,60	0,96	1,42	2,53	2,66	0,36	0,65
	Si-Sn	0,06	0,42	0,62	1,47	1,29	0,33	0,37
	SiGe	0,11	0,64	0,66	1,77	2,94	0,33	0,37
	Si-Fe	0,07	1,21	1,26	2,54	2,18	0,58	0,50
	Si-Co	0,02	1,43	1,44	2,72	2,28	0,63	0,53

Fig. 1a – Dependence of the interfacial energy in systems graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) on atomic number in the periodic table of the elements
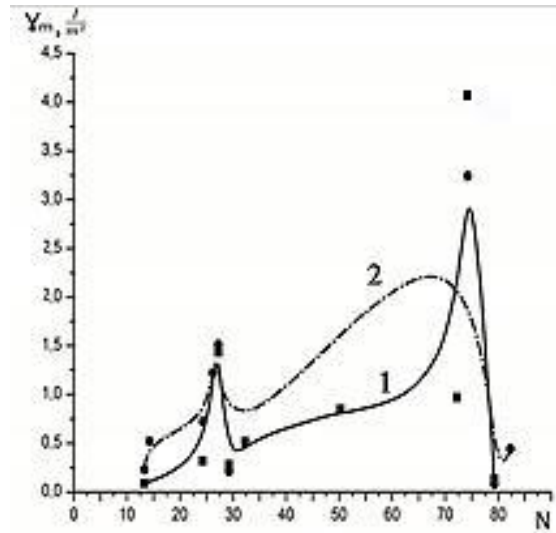

Fig 2a – Dependence of the interfacial energy in systems (Si, Ge) - (Fe, Co, Cu, Al, Au, Cr, W, Pb) on atomic number in the periodic table of elements
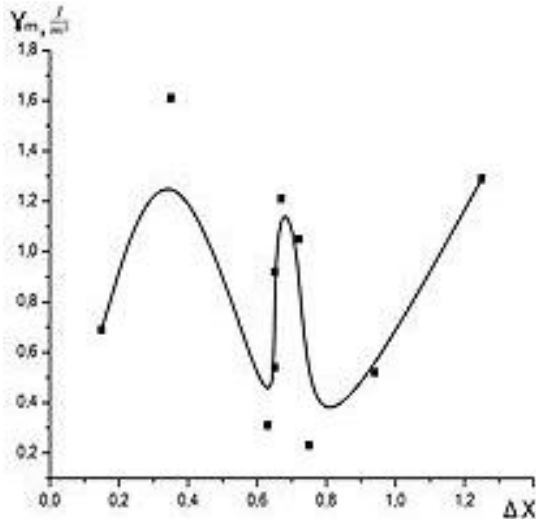

Fig. 1b – Dependence of the interfacial energy in systems graphene – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) on the elements electronegativity difference (points correspond to calculated values; solid line is an approximated dependency)
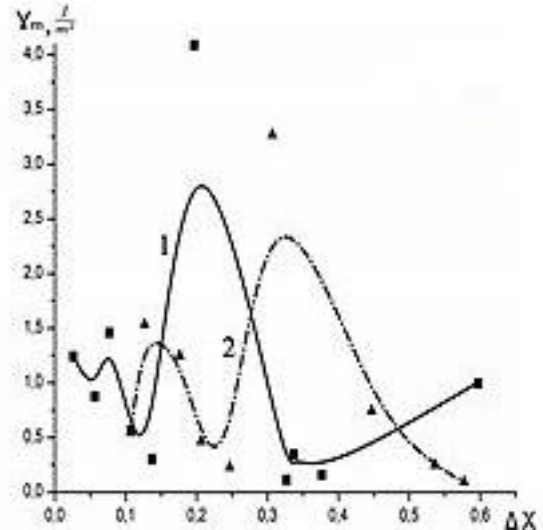

Fig. 2b – Dependence of the interfacial energy in systems (Si, Ge) - (Fe, Co, Cu, Al, Au, Cr, W, Pb) electronegativity difference (points correspond to calculated values; solid line is an approximated dependency)

Studied dependencies $\gamma_m(N)$ and $\gamma_m(\Delta X)$ have quite complex shapes also for structures in semiconductors Si and Ge. In particular, $\gamma_m(N)$ dependence for Si-system is characterized by two distinct peaks at $N = 26$ and 73, within which the interfacial energy reaches its maximum value(Fig. 2a). By increasing the sequence number from $N = 13$ to 73 we observe an increase in the interfacial energy, and its value at the second maximum is almost 2 times higher in comparison to the similar system based on graphene. For Ge-systems the dependence has a similar character. Interestingly there is a full match of the first maximum ($N = 26$) with Si-systems. The second maximum is bell-shaped with the maximum value of interfacial energy smaller by almost 1.5 times compared to Si-systems.

Despite Si and Ge are the closest analogs in several properties of the semiconductor, the interfacial energy for systems based on these semiconductors differs

substantially due to the difference values of electronegativity (1.9, 2.01). Nevertheless, $\gamma_m(\Delta X)$ dependencies are similar for two semiconductors (Fig. 2b). In particular, in both cases they have two distinct peaks. The first is a bland peak at $\Delta X = 0.07$ for Si-system and a sharper peak at $\Delta X = 0.11$-0.13 for Ge-systems. The second peak has higher maximum value and peaks at $\Delta X = 0.2$ for Si-system. For Ge-systems we observe a little bit smaller bell-shaped peak at $\Delta X = 0.31$. As follows from Fig. 2b, $\gamma_m(\Delta X)$ dependencies for both semiconductors are mutually shifted along ΔX axis due to the greater electronegativity of germanium. Other parameters presented in Table 1 (σ_m, A_{ad} and γ_{ad}) have similar dependencies and characteristic maximums on N and ΔX as for γ_m. This fact justifies our calculation approach as well as the generality of formation mechanisms in the analyzed surface pairs.

4. CONCLUSIONS

In this paper, based on the relations of non-equilibrium thermodynamics and physics of surface phenomena we calculated the values of the energy parameters for the interfacial interaction as well as it's dependencies on the atomic number in the periodic table and on the difference in electronegativity of interacting elements.

The analysis of the behavior of the energy and adhesion parameters opens new avenues for predicting the results of interfacial interaction in order to select the contact pairs, to create thermodynamically stable structures with specific values of the energy parameters of interfacial interaction and type of chemical bond, as well as the optimal level of stress [8].

Енергетичні параметри міжфазних шарів у системах графен – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) і напівпровідник (Si, Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb)

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На основі співвідношень нерівноважної термодинаміки та фізики поверхневих явищ розраховані енергетичні та адгезійні параметри міжфазних взаємодій в системах графен – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) і напівпровідник (Si,Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb). Аналізуються закономірності змін величин міжфазної енергії, міжфазного натягу, роботи адгезії, енергії адгезійних зв'язків за номером контактуючого елемента в таблиці Менделеєва та різниці електронегативностей взаємодіючих елементів.

Ключові слова: Адгезія, Поверхня, Напруження, Міжфазний.

Энергетические параметры межфазных слоев в системах графен – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) и полупроводник (Si, Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb).

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На основании соотношений неравновесной термодинамики и физики поверхностных явлений рассчитаны энергетические и адгезионные параметры межфазных взаимодействий в системах графен – (Si, Cu, Fe, Co, Au, Ag, Al, Ru, Hf, Pb) и полупроводник (Si, Ge) – (Fe, Co, Cu, Al, Au, Cr, W, Pb). Анализируются закономерности изменений величин межфазной энергии, межфазного натяжения, работы адгезии, энергии адгезионных связей по номеру контактирующего элемента в таблице Менделеева и разнице электроотрицательностей взаимодействующих элементов.

Ключевые слова: Адгезия, Поверхность, Напряжения, Межфазный.

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