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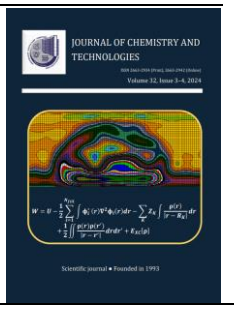

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QUANTUM-MECHANICAL METHODOLOGY FOR DETERMINING THE TEMPERATURE DEPENDENCE OF CONTACT ANGLE IN MELT–SOLID METAL SYSTEMS

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Abstract

Aim. In order to determine the composite materials' manufacturing process parameters, it is necessary to evaluate the stability of their structural components and determine the contact angle of wetting of the filler with the molten binder at the infiltration temperature. The development of a theoretical method for determining the dependence of the contact angle of wetting on temperature in melt – solid metal systems makes it possible to reduce the volume of experimental studies. Methods. The paper presents a quantum mechanical methodology for calculating the binding energy of interacting substances, as well as an experimental study of the dependence of the contact angle on temperature for tin – steel systems. The methodology is based on the calculation of the binding energy between atoms of interacting substances using density functional theory. Results. The calculations show an anomalous behavior of contact angle values for the tin–steel system with increasing temperatures. It means that, when the temperature increases, the values of the contact angle initially become lower, and later, in the temperature range of 450-510 °C, an increase in the contact angle is observed. The obtained theoretical and experimental data correlate well with each other. Conclusions. The appearance of extreme regions in the experimental and theoretical temperature dependences is associated with the thermal expansion of interatomic distances in the crystal lattice. The obtained theoretical and experimental data correlate well with each other and base on the thermal expansion of interatomic distances in the crystal lattice.

Keywords: contact angle; temperature; density functional theory; binding energy; liquid tin drop; steel substrate.

КВАНТОВО-МЕХАНІЧНА МЕТОДОЛОГІЯ ВИЗНАЧЕННЯ ЗАЛЕЖНОСТІ КОНТАКТНОГО КУТА ЗМОЧУВАННЯ ВІД ТЕМПЕРАТУРИ В СИСТЕМАХ РОЗПЛАВ–ТВЕРДИЙ МЕТАЛ

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Анотація

Ціль. Для визначення технологічних параметрів виготовлення композиційних матеріалів необхідно оцінити стабільність їх структурних компонентів та контактний кут змочування наповнювача розплавленою зв'язкою за температури просочення. Розробка теоретичного методу визначення залежності крайового кута змочування від температури в системах розплав – твердий метал може скоротити обсяг експериментальних досліджень. Методи. У роботі представлено квантово-механічну методологію розрахунку енергії зв'язку взаємодіючих речовин, а також експериментальне дослідження залежності контактного кута від температури для системи олово – сталь. Методологія заснована на розрахунку енергії зв'язку між атомами взаємодіючих речовин з використанням теорії функціонала густини. Результати. Розрахунки показують аномальну поведінку значень контактного кута для системи олово–сталь під час підвищення температури. Це означає, що за підвищення температури значення контактного кута спочатку зменшуються, а згодом, в інтервалі температур 450–510 °C, спостерігається збільшення контактного кута. Отримані теоретичні та експериментальні дані добре корелюють між собою. Висновки. Поява екстремальних ділянок на експериментальних і теоретичних температурних залежностях пов'язана з тепловим розширенням міжатомних відстаней у кристалічній ґратці.

Ключові слова: кут змочування; температура; теорія функціоналу густини; енергія зв'язку; крапля рідкого олова; сталева підкладка.

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Introduction

The development of materials with specified properties, as well as appropriate production technologies, are important issues of modern materials science. In particular, powder metallurgy of composite materials offers unique opportunities in terms of efficiency, productivity, and reliability. The resulting materials can have complex shapes and a wide range of mechanical properties. Composites are widely used in automotive, aerospace, power and medical engineering [1; 2]. The uniform distribution of reinforcing particles in a composite with a metal matrix is one of the most important advantages of powder metallurgy compared to casting methods [3].

Sintering is one of the methods used in powder metallurgy [4; 5]. Sintering process is affected by many factors, such as pressure, temperature, time, sintering atmosphere (argon or nitrogen), and sintering method [6; 7]. Size and shape of reinforced particles, as well as volume fraction and composition of the reinforcing material in the matrix, have a significant impact on the microstructure and mechanical properties of composites based on sintered metal matrix [8]. In addition, the wetting of the reinforcing particles by the matrix material, namely the contact angle, is an important factor affecting sintering.

The production of composite materials requires strict control of the contact interaction processes occurring at the interfaces between reinforcing particles and matrix material. These processes should, on the one hand, ensure the required strength of the interfaces and, on the other hand, avoid the appearance of undesirable phases in the structure [9]. Therefore, the determination of the value of the adhesion work between the structural components of composite materials and the chatacter of wetting of the filler by the molten binder is of paramount importance in the fabrication of composite materials [10; 11]. The work of adhesion is inseparably linked to the contact angle; the better the wetting of the solid phase by the liquid one and the smaller the contact angle, the greater the work of adhesion is [12].

It is known that the value of the contact angle depends heavily on the temperature. In some cases, when heated above a threshold temperature, the contact angle sharply decreases, i. e. a wetting threshold is detected [13; 14]. In the sintering process, in order to achieve the highest adhesion between the reinforcing material and the matrix material, it is necessary to know the temperature dependence of the contact angle values. Currently there is no theory that could describe this dependence. Therefore, to determine sintering process variables, it is necessary to find the temperature dependence of the contact angles and to detect the wetting threshold experimentally [13; 14].

Consequently, finding an algorithm to determine the dependence of the contact angle value on temperature is highly relevant and promising both from theoretical and practical points of view.

This paper presents the results of the study of the behavior of the contactangle as a function of temperature for the tin–steel system, which were calculated using quantum mechanics methods, and their experimental validation.

Methodology for calculating contact angle behavior as a function of temperature

Surface wetting processes are affected by a number of factors such as temperature, surface cleanliness, surface structure and chemical composition, etc. [17]. There are several approaches to theoretically calculate the contact angle and investigate its dependence on temperature [16–20]. For example, the calculations of the authors of [16] are based on the change in the geometry of the drop during the transition from a convex to a concave surface.

Attempts to find approximate solutions for the contact angle values were made in [17–19] using perturbation methods, based on the Young-Laplace equation for capillary pressure. The most successful results obtained in [19] were based on the drop parameters: radius of the apex curvature, surface tension, mass, contact radius and height. However, in practice this equation is of little use, since measurement of the radius of apex curvature for a small drop is associated with uncertainty.

The contact angle value is directly related to the wetting phenomenon, which depends on the energy of interaction between the particles of the drop and the substrate. Therefore, we consider promising the calculations of the values of the contact angle through various types of energy. The paper [20] provides an overview and direct comparison of the most widely used methods, their advantages and disadvantages.

Our proposed method does not allow us to determine the exact values of the contact angle, but, as mentioned above, for the sintering process it is most important to obtain the dependence of the contact angle values on temperature and to determine the wetting threshold The method is

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based on the calculation of binding energy between atoms of the substrate (matrix) (E_m), atoms of the drop (reinforcing material of the composite) (E_c) and between atoms of the substrate and atoms of the drop at different temperatures (E_{mc}).

To calculate the binding energy, we have chosen the density functional theory (DFT) method, which is widely used in the calculations of the electronic structure of atoms, molecules, clusters, solids and so on [21].

Total energy (W) in the density functional theory is defined as follows [22]:

$$W = U - \frac{1}{2}\sum_{i=1}^{N_{fill.}} \int \phi_i^*(r)\nabla^2\phi_i(r)dr - \sum_K Z_K \int \frac{\rho(r)}{|r-R_K|}dr + \frac{1}{2}\iint \frac{\rho(r)\rho(r')}{|r-r'|}drdr' + E_{XC}[\rho], \quad (1)$$

where Z_K and R_K – charge and spatial coordinates of the stationary nucleus with number K, respectively, and electron density $\rho(r) = \sum_{i=1}^{N_{fill.}}|\varphi_i(r)|^2$, where $\varphi_i(r)$ – one-electron Kohn-Sham (molecular) orbital.

In a compressed form, expression (1) looks like:

$$W = U + T_S\{\phi_i(r)\}_{i=1}^{N_{fill.}} + V_{ne}[\rho] + J[\rho] + E_{XC}[\rho]. \quad (2)$$

On the right side of equation (2) the first term U is the potential energy of interaction of the nuclei; the second term T_s, describes the electron kinetic energy; the third term V_{ne} is the attraction of electrons to the nuclei; the fourth term J is the classical contribution to the interelectron repulsion energy, and the last contribution E_{xc} is the exchange-correlation functional including the static electron correlation.

Numerous studies of the characteristics of molecules and clusters using the DFT method [23] have shown good results when the exchange-correlation functional is chosen correctl. As referred to in [24; 25], three-parameter hybrid functional B3LYP is the most relevant for the calculations of the structural and thermochemical characteristics of metal complexes.

To perform the calculations of the energies of structural complexes in the condensed state [26–28], including those for the composite materials [29; 30], we used the GAUSSIAN 09 software package [31].

The calculations were carried out using the 6-31g(d) basis set, which allowed us not only to describe the electron density distribution between completed and virtual orbitals, but also to calculate the thermodynamic parameters.

Binding energy was calculated as a difference between the total energy of the crystal (W_{total}) and the sum of energies of its constituent parts (W_o) [26]:

$$\Delta E = |W_{total} - W_0|. \quad (3)$$

Table 1

Total energy of substrate atoms (W_m), atoms of the drop (W_c), sum of the energies of tin atoms (W_s), energy of the interaction of atoms of the drop with substrate atoms (W_{mc}), difference between the binding energy of atoms of the drop with substrate atoms (E_{mc}), binding energy of pure tin (E_c), difference between the binding energy of atoms of the drop with substrate atoms and binding energy of the tin drop (ΔE) to the dependence of temperature (T)

T, °C	W_m, eV	W_c, eV	W_s, *5eV	W_{mc}, eV	E_{mc}, eV	E_c, eV	ΔE
330	–15090.89644	–29996.31018	–5999.172612	–45087.20098	–0.0091046	0.0894242	0.0905514
360	–15090.96784	–29996.30972	–5999.172612	–45087.20504	–0.0017438	0.0893312	0.1038346
390	–15090.97317	–29996.30925	–5999.172612	–45087.21464	–0.0072726	0.0892376	0.1027934
420	–15091.06166	–29996.30878	–5999.172612	–45087.21668	–0.0011272	0.0891432	0.1198938
450	–15090.98976	–29996.3083	–5999.172612	–45087.21597	–0.0145034	0.0890482	0.1054656
480	–15091.03278	–29996.30782	–5999.172612	–45087.13784	–0.0135558	0.0889524	0.1295054
510	–15091.03783	–29996.30734	–5999.172612	–45087.11475	–0.0307506	0.088856	0.1349402
540	–15091.04078	–29996.30686	–5999.172612	–45087.18404	–0.0164174	0.088759	0.1214784

We used tin alloys with a purity of 99.9995 wt. % and steel AISI 201 for the calculations and experimental validation. In the process of calculations, we modeled a crystalline structure consisting of atoms of iron, carbon and chromium. A drop of liquid tin was modeled taking into account the short-range order only. Inour calculations, the temperature was set in the range from 330° to 540 °C in increments of 30 °C. Furthermore, the change in the interatomic distance at different temperatures was taken into account as well. The atoms within three coordination spheres were considered in the calculations.

In order to explore the behavior of the wetting process and, accordingly, the contact angle, we calculated the total energy of particles in the composition of the substrate (W_m), atoms of the drop (W_c) and the drop-substrate complex (W_{mc}). After that the difference between the binding energy of atoms of the drop with substrate atoms $E_{mc} = W_{mc} - (W_m + W_c)$ was found. The binding

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energy of pure tin is $E_c = W_c - W_s$,where W_s is the sum of energies of individual tin atoms. The data are shown in the table 1. Fig.1 shows the graphs of the temperature dependence of the binding energy of atoms of the drop with substrate atoms (E_{mc}), binding energy of the tin drop (E_c), and the difference between these two binding energies (ΔE).

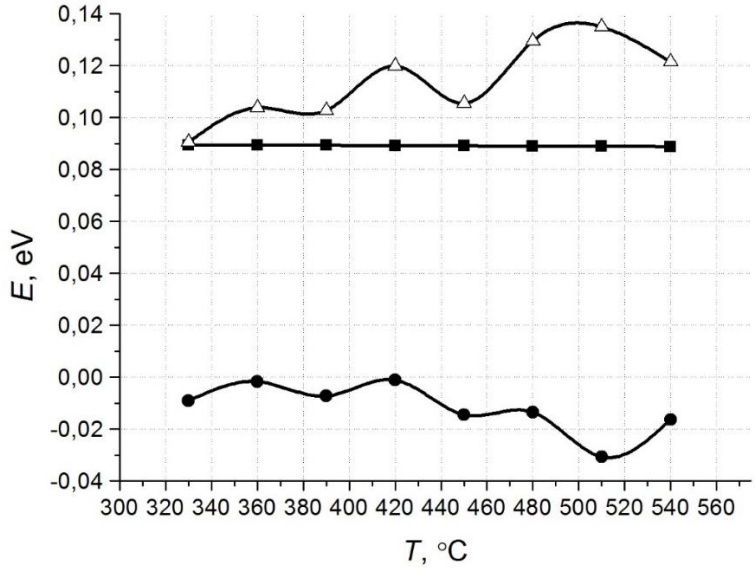

Fig.1. Temperature dependencies: • – binding energy of atoms of the drop with substrate atoms (E_{mc}), ■ – binding energy of atoms of the tin drop (E_c), Δ – difference between the binding energy of atoms of the drop with substrate atoms and binding energy of the tin drop (ΔE)

Experimental determination of contact angle

The optical method [32] was used to determine the contact angle of AISI 201 solid steel substrate by liquid tin. In order to ensure that the temperatures of components in the system are equal at the moment of the contact angle formation, i.e., that tin is in a molten state with a temperature equal to the substrate temperature, a high-temperature unit with high temperature stabilization was created (Fig. 2). To prevent the formation of undesirable compounds, heating was carried out in the nitrogen atmosphere, since no compounds are produced at the direct interaction of nitrogen and tin [33]. For maintaining a stationary pressure equal to the atmospheric pressure, working chamber 1 was equipped with the outlet and inlet valve 4, combined with a pump 7 injecting inert nitrogen from a tank 8. A drop of tin under study was applied to the substrate located on the object stage of the working chamber through a piston 6. Quartz tube 3 had a sufficient height (40 cm) to avoid heating of its upper part with the piston allowing to squeeze out the dosed amount of a tin drop 5 onto the substrate. The weight and, accordingly, the size of a tin drop was determined by the diameter of the narrowed end of the quartz tube forming the weight of a drop before its detachment. In our case, the weight of the drop was 80 mg. The distance between the end of the tube and the substrate was equal to 8 mm, actually excluding the impact of the kinetic energy of a falling tin drop on the formation of its shape on the substrate. At the preset temperature, the tin drop was kept on the substrate for 12 minutes. Then the furnace was cooled, the drop was removed, the furnace was heated again to a higher temperature, and the next drop of liquid tin of the same type was fed through the piston. Measurements were made in the temperature interval of 250 – 525 °C. The outline of the drop was photographed using a digital camera 9 through a quartz glass 2. The resulting image was scanned and processed using the TLC-manager software [34]. When scanning the image, the software program generated matrices of light absorption coefficients corresponding to each pixel. Therefore, after scanning a corresponding image was formed (Fig. 3) with the clearly outlined drop and the coordinate grid. To find out the factors that could influence the results of the experiment, we studied the chemical composition of the substrate and solidified tin drop using ion-selective method and atomic absorption method before and after the experiment. Besides, studies using the X-ray fluorescence method were carried out to detect iron atoms in the tin drop.

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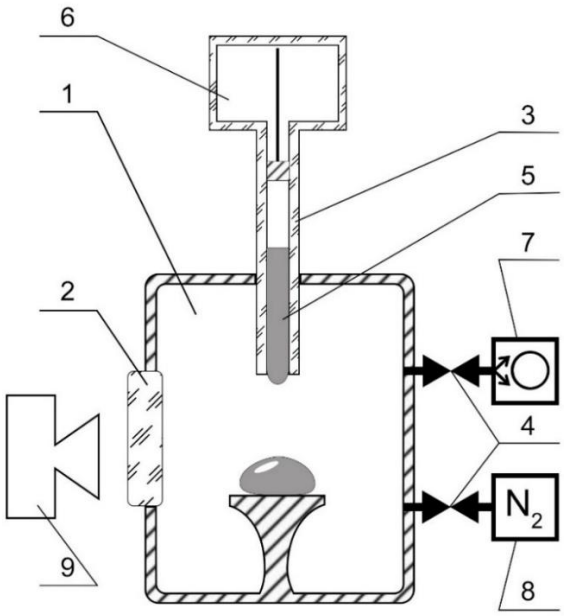

Fig. 2. Schematic diagram of the experiment: 1 – working chamber with the temperature control, 2 – quartz glass, 3 – quartz tube, 4 – outlet and inlet valve, 5 – molten tin in the quartz tube, 6 – piston allowing to squeeze out a dosed drop of molten tin, 7 – pump, 8 – nitrogen tank, 9 – chamber

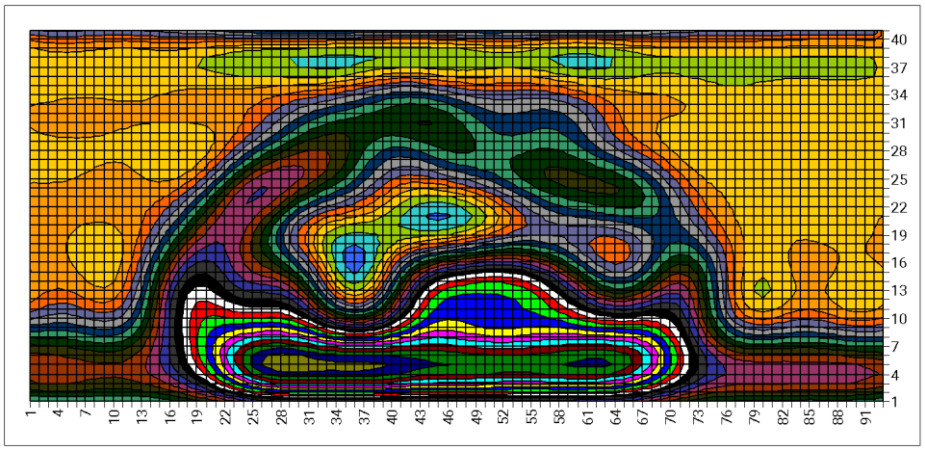

Fig. 3. Scanned image of the liquid tin drop on AISI 201 steel substrate

Results and discussion

Calculations of the difference in the binding energy between the atoms of the drop and the substrate and the binding energy between the atoms of the drop at different temperatures (Fig. 1) showed the extreme nature of this dependence. An experiment to determine the contact angle of the steel substrate with liquid tin as a function of temperature revealed a similar dependence. Fig. 4 shows photographs of the drop for three specific temperatures, which confirm a decrease and then an increase in the contact angle.

a b c

Fig. 4. Photographs of the drop of liquid tin on AISI 201 steel substrate at the temperatures: a – 300 °C; b – 425 °C; c – 500 °C

Fig. 5 shows the contact angle values obtained experimentally, depending on temperature.

This dependence bears the extreme nature as well. The contact angle values become lower with increasing temperature, which agrees well with the current theories of wetting [35]. Subsequently, in the temperature interval of 425–500 °C, an increase in the contact angle is observed. Similar dependence is also found in theoretical calculations of binding energy. As shown in Fig. 1, the binding energy of the atoms of the drop with the substrate atoms (E_{mc}) decreases in the temperature range of 450–510 °C, while the tin drop binding energy (E_c) remains almost unchanged. The characteristic extreme in the temperature dependence of the binding energy is observed only when the thermal expansion of interatomic distances in the crystal lattice of the studied structures is taken into account in the calculations. A slight shift in the extrema of the theoretical and experimental dependences is caused by the fact that a multicomponent steel substrate was experimentally studied.

Cases of the contact angle increase with rising temperature are considered anomalies [36]. The authors of [37] suggest that the increase in contact angles is due to the formation of new chemical compounds at the drop-substrate interface. To verify this, we carried out the chemical analysis of the surface of the substrate and the drop after the experiment using atomic absorption and ion-selective methods. These studies did not reveal any newly formed iron compounds. A small amount of nitrogen oxides was detected, but it could not significantly affect the results of the experiment. According to X-ray fluorescence analysis, no iron content was detected in the tin drop as well.

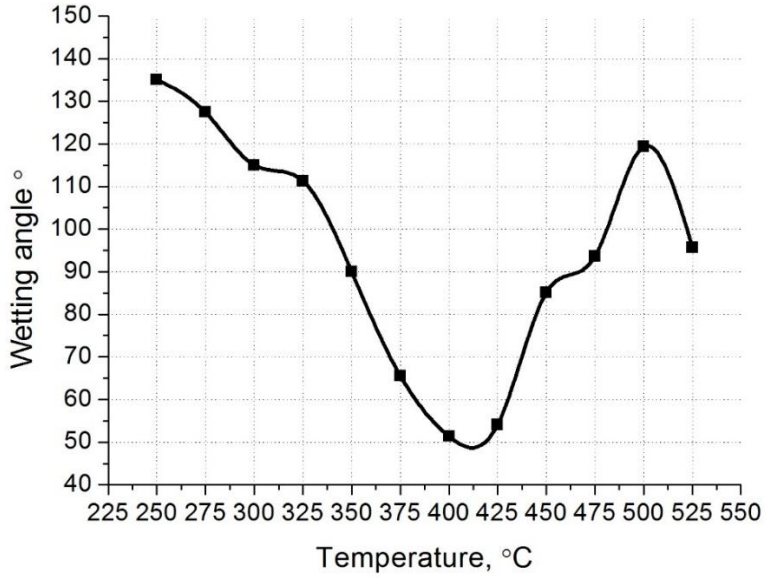

Fig. 5. Temperature dependence of the contact angle of AISI 201 steel substrate by molten tin, obtained by experiment

Studies of the temperature dependence of the contact angle in the tin–steel and tin–iron systems were previously carried out in [38; 39]. However, an anomalous increase in the contact angle with increasing temperature was not detected, since for the heated system being in equilibrium the temperature rise cannot result in the contact angle increase [35]. The system in [38; 39] was heated continuously, i.e., the same system was heated to high temperatures. Here the contact angle decreased with the increase in temperature and did not increase with the further temperature growth. In our study, in order to plot the contact angle versus temperature, a new tin drop was supplied and examined. Therefore, the contact angle at higher temperatures was formed anew, which did not exclude its higher values compared to its previous values at lower temperatures.

By comparing the dynamics of changes in the temperature dependences of the contact angle and the binding energy, it is possible to determine the correlation between calculated and experimental data. To establish a correlation relationship between the theoretical data of the binding energy and the experimental data of the contact angle, we used the factor of similarity of profiles of the temperature dependence curves for these indicators on the most significant area. This area was determined by the presence of an extremum (minimum) on the temperature dependence curves of the contact angle in the range of 350–550 °C and 420–540 °C of the binding energy.

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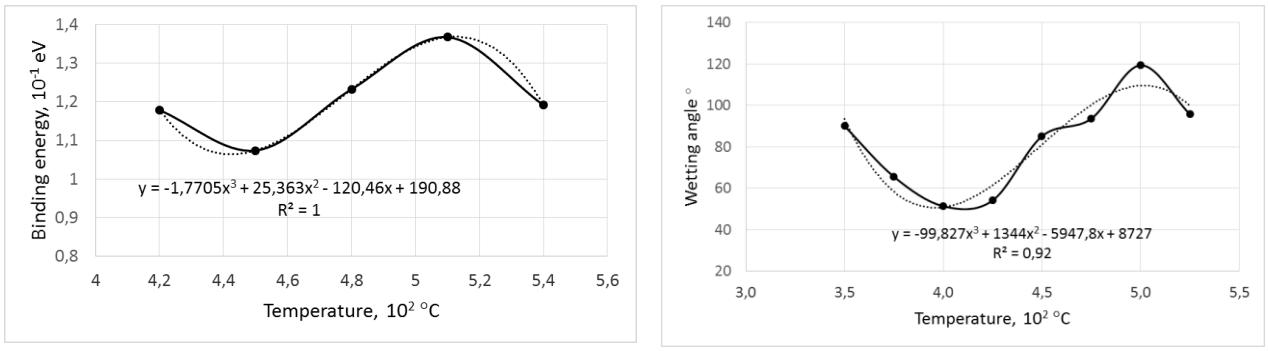
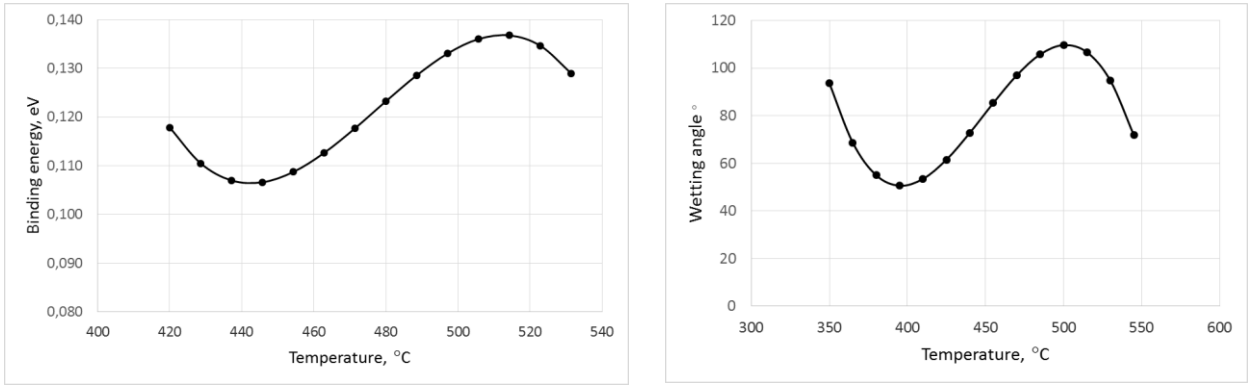
Initially, with the use of the third-degree polynomials, the regression equations of the indicators under study were derived (Fig. 6). In order to avoid large degrees in the regression equations, which can distort the regression coefficients, we used only significant parts of the variables, when setting up these equations. Further, using the regression equations, we compressed the data obtained for the indicators under study using the calculated values in the specified temperature interval (Fig. 7). Because of the differences between the initial temperature intervals, the calculated values were linked together by the number of subinterval of each interval, the quantity of which was the same and amounted to 14. This procedure allowed the curve profiles to be superimposed on one another, eliminating their deformation and distortion.



a **b**

Fig. 6. Regression equation for the temperature dependence of: a – binding energy; b – contact angle



a **b**

Fig. 7. Values calculated with the use of regression equations depending on the temperature: a – binding energy values; b – contact angle values

At the final stage, a graphic layout was formed using the calculated numerical series: X-axis – binding energy values, Y-axis – contact angle values (Fig. 8). The graphic layout allowed us to find the linear regressional dependence with the significance coefficient of R^2 = 0.81, which is identical to the correlation coefficient between the theoretical and experimental data.

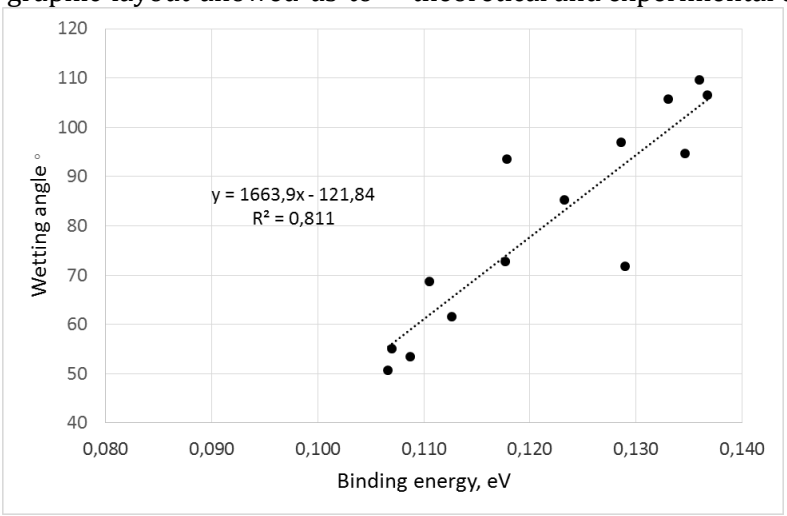


Fig. 8. Correlation relationship between the values of binding energy and contact angle

The comparison of the experimental data with the calculated data based on the determination of binding energy indicates that the proposed model can be used to theoretically determine the dependence of the contact angle at different temperatures. The anomalous phenomenon of an increase in the contact angle with further temperature growth can be explained by the change in binding energy due to the thermal expansion of the crystal lattice.

The slight difference between the theoretical and experimental data can be explained by the fact that we used the multicomponent steel substrate in the experiment, while pure iron was taken into account in the calculations. Consideration of the multicomponent systems will be the subject of our further research. This methodology can be used for nonequilibrium metallic systems, and studying of its application for nonmetallic systems is promising as well. The use of this methodology makes it possible to predict processes in nonequilibrium systems by calculation without experiments, which can be useful in the development of composite materials, soldering processes and other applied problems.

Conclusion

To determine the character of wetting by the density functional theory method, calculations of the binding energy between the atoms of the substrate and the atoms of the melt of tin–steel system in the temperature interval of 330 – 540 °C were performed It is found that along with the decrease of the contact angle in the temperature interval of 330 – 360 °C at further temperature increase there should be deterioration in wetting and increase of the contact angle.

The temperature dependence of the contact angle of the tin–steel system was constructed by experiment. To construct each point of dependence, a new drop of tin was applied to the steel substrate and examined. Thus, at each preset temperature, new similar system was studied and the contact angle was formed anew, which did not exclude its higher values compared to the previous ones. Experimental dependence of the contact angle on the temperature also bears an extreme nature. A decrease in the contact angle was found at the temperature interval of 300–400 °C, while further increase of the contact angle was determined at 425–500 °C. The data obtained by calculation and experiment have a certain correlation. The anomalous effect of increase in the contact angle of the tin–steel system with further temperature increase occurs as a result of change in the binding energy of atoms of the contacting substances due to the thermal expansion of the crystal lattice.

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