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Influence of Interface Roughness on Spatial Distribution of Magnetization at Substitutional Adsorption of the Ultrathin Iron Film

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In this work, we use the variational spin-density functional method for theoretical description conditions of the formation of stable films and calculation of interface energy and spatial distribution of relative magnetization at activated adsorption of Fe film on the W and Au substrates with taking into consideration the interface roughness. We include into consideration the thermal effects of transition metal atoms intermixing inside film and their substitution with atoms of substrate surficial layer.

Keywords: adsorption, ultrathin magnetic films, spin-density functional theory.
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Introduction

Studies of thin magnetic films led to the discovery of a number of remarkable phenomena, including GMR and TMR effects, which enabled such systems to be utilized in microelectronics and computer components industry [1, 2]. So investigations focused on determination of the conditions for realizing practically useful properties of magnetic films, which determine their application, are of great importance.

In this work, we investigated for Fe/W(110) and Fe/Au(111) systems the behaviour of full interface energy by spin density functional theory (SDFT) with taking into account temperature effects and inhomogeneous spatial distribution of relative magnetization in surficial region. Influence of interface roughness and effects of intermixing between adatoms and substrate atoms is also taken into consideration.

1. Model and approach description

Configuration of our system is presented in Fig. 1(a). In accordance with SDFT total interfacial energy of the system $\sigma(D)$ is functional of $n_{\pm}(z) = n(z)(1 \pm m(z))/2$. Spatial distribution

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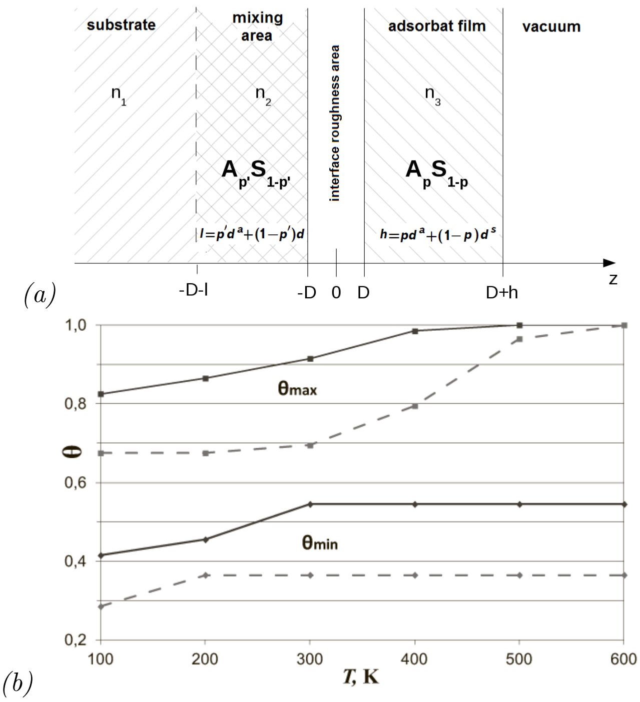

Fig. 1. (a) System configuration. Parameters p, p' are a relative fraction of the adsorbate atoms in film and in mixing area of the substrate respectively, d^a and d^s are distances between the most closely packed planes in crystals of the adsorbate and the substrate. (b) Coverage parameters $\theta_{\min}$ and $\theta_{\max}$ as a function of temperature. Solid line – Fe/W(110), dashed – Fe/Au(111)

of relative magnetization have the following form

$$m(z) = \begin{cases} 0.5m_2 e^{\beta(z+D)}\left[e^{\beta l-1}\right] + 0.5m_3 e^{\beta(z-D)}\left[1-e^{-\beta h}\right], & z < -D-l; \\ m_2\left[1-0.5e^{\beta(z+D)} - 0.5e^{-\beta(z+D+l)}\right] + 0.5m_3 e^{\beta(z-D)}\left[1-e^{-\beta h}\right], & -D-l < z < -D; \\ 0.5m_2 e^{-\beta(z+D)}\left[1-e^{-\beta l}\right] + 0.5m_3 e^{\beta(z-D)}\left[1-e^{-\beta h}\right], & -D < z < D; \\ 0.5m_2 e^{-\beta(z+D)}\left[1-e^{-\beta l}\right] + m_3\left[1-0.5e^{-\beta(z-D)} - 0.5e^{\beta(z-D-h)}\right], & D < z < D+h; \\ 0.5m_2 e^{-\beta(z+D)}\left[1-e^{-\beta l}\right] + 0.5m_3 e^{-\beta(z-D)}\left[e^{\beta h}-1\right], & z > D+h; \end{cases} \tag{1}$$

where $m_2 = m(T)p'(\Theta)$ and $m_3 = m(T)p(\Theta)$ are characteristic magnetizations in mixing area of substrate and in film respectively. The values of the variational parameters β,p, p' are obtained from the requirement of the minimum σ. For description of temperature dependence for the relative magnetization $m(T)$ we used the relation characteristic for the two-dimensional Ising model (for the Fe/W system):

$$m(T) = \left[1 - \sinh^{-4}\left(\frac{2T_c}{2.269T}\right)\right]^{1/8}, \tag{2}$$

and the relation characteristic for the 2D XY-model (for the Fe/Au system):

$$m(T) \simeq \left[\frac{T_c - T}{T_c}\right]^{0.231}, \tag{3}$$

where $T_c = T_c^{(s)}(\Theta) \cong \Theta T_c^{(b)} \frac{z_{surf}}{z_{bulk}}$ is film's Curie temperature, z_{surf} is the number of nearest neighbours in the film. For Fe $T_c^{(s)}(\Theta = 1) = 521.5$ K.

More detailed theoretical description is presented in [3].

2. Conditions of the formation of stable films

Analysis of the dependencies of the interface energy σ on D shows that there are two "bounding" coverage parameters: $\theta_{\min}(T)$ and $\theta_{\max}(T)$. When $\theta < \theta_{\min}$ interface energy does not have a minimum at $D > 0$, while at $\theta > \theta_{\max}$ minimum of interface energy has a negative value. This may apparently mean that when $\theta < \theta_{\min}$ interface roughness is negligible and, therefore, system has an ability to show a strong intermixing between substrate and adsorbate, while at $\theta > \theta_{\max}$ an opportunity for an island adsorption emerges, and, therefore, the stable films are realized at $\theta_{\min}(T) < \theta < \theta_{\max}(T)$ only.

Calculated values of $\theta_{\min}$ and $\theta_{\max}$ are presented in Fig. 1(b). It can be seen that for both systems decreasing of the temperature shifts mentioned intervals toward lower coverage values. For $T \leqslant 400$ K, the Fe/Au(111) system has a wider interval of stable films compared to the Fe/W(110) system, and conversely for $T > 400$ K.

3. Equilibrium interface roughness parameter

Further, we present our results of calculating equilibrium interface roughness parameter D_0, at which interface energy σ reaches its minimum. In cases where the minimum was not detected, $D_0 = 0$ was assumed. Dependence of D_0 on coverage θ is presented in Fig. 2.

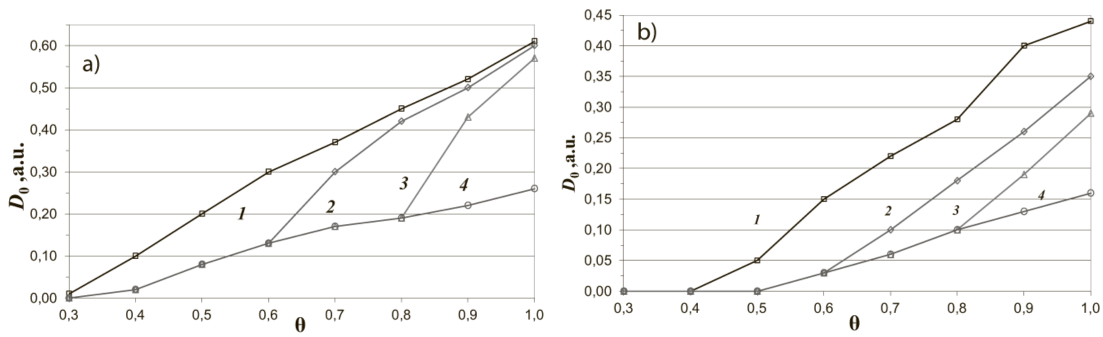

Fig. 2. The dependence of the equilibrium interface roughness parameter D_0 on the coverage θ for *a*) Fe/W(110) and *b*) Fe/Au(111) systems. Temperatures: *1.* $T = 100$ K, *2.* $T = 350$ K, *3.* $T = 450$ K, *4.* $T = 550$ K

It is seen, that for Fe/W(110) system values of D_0 are in the interval $[0, 0.61]$ a.u., and that this quantity decreases with the increase of temperature and grows with the coverage. The Fe/Au(111) system is generally characterized by lower values of interface roughness compared to the first system: values of D_0 are laid in the interval $[0, 0.44]$ a.u.

4. The spatial distribution of magnetization

In Fig. 3 we present our results of calculation the spatial distribution of magnetization for $T = 100,\ 300$ K, $\theta = 0.6,\ 1.0$.

For Fe/W(110) system it can be seen that in some cases taking interface roughness into consideration increases the maximum value of magnetization in film, thus improving its magnetic properties. In other cases changes in the maximum value of the magnetization in connection with

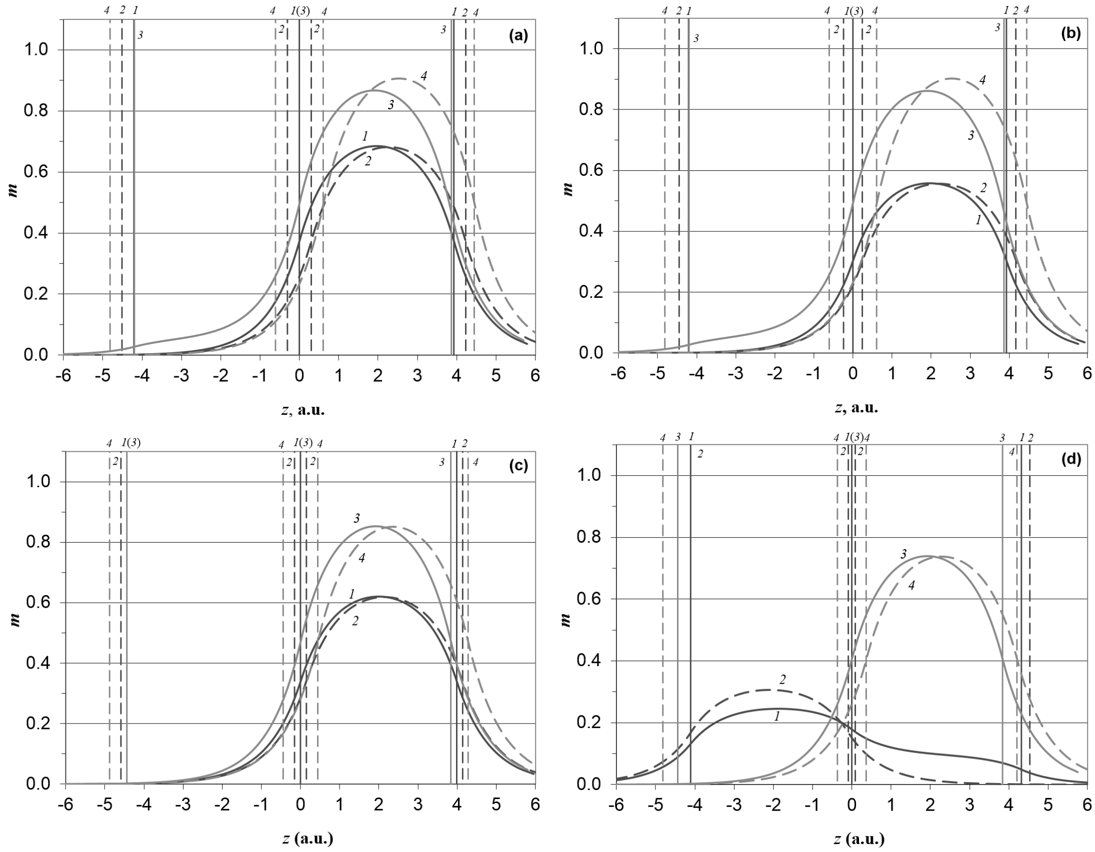

Fig. 3. The spatial distribution of magnetization for (*a*), (*b*) Fe/W(110) and (*c*), (*d*) Fe/Au(111) systems. Temperatures: (*a*), (*c*) $T = 100$ K and (*b*), (*d*) $T = 300$ K. Coverages: *1,2*. $\theta = 0.6$ and *3,4*. $\theta = 1.0$. Accounting of the interface roughness: Solid line – No ($D = 0$), dashed – Yes ($D = D_0$). Vertical lines denote the boundaries of the areas.

the account of the interface roughness do not occur. Unlike the first system, taking interface roughness into consideration for Fe/Au(111) system led to a minor decrease of maximum value of magnetization, and only in the case $T = 300$ K, $\theta = 0.6$, when maximum value of magnetization was shifted to surficial area of substrate, it has been increased.

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Влияние межфазной шероховатости на пространственное распределение намагниченности при заместительной адсорбции в ультратонких пленках железа

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В данной работе в рамках вариационного метода функционала спиновой плотности представлено теоретическое описание условий форирования стабильных пленок и результаты расчетов межфазной энергии и распределения относительной намагниченности пленок Fe на подложках W и Au с учетом межфазной шероховатости. Рассмотрено влияние температурных эффектов перемешивания атомов субстрата и адсорбата в приповерхностной области.

Ключевые слова: адсорбция, ультратонкие магнитные пленки, метод функционала спиновой плотности.