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Numerical model for studying 3*D*-island films by Auger electron spectroscopy. The Sm–Si(111)

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A model for quantifying the peak intensity in Auger electron spectroscopy for thin-film structures formed by the Volmer–Weber, Stranski–Krastanov or similar mechanisms has been proposed. This model can be used to process experimental results and provides information on the density and shape of three-dimensional islands. It is tested for the reactive Sm–Si(111) system. It is found that in this system, a change in the structure of the wetting layer, i. e., the transition from the $\sqrt{3}$ to (5×1) reconstruction, is accompanied by an increase in the aspect ratio of samarium disilicide crystallites by more than seven times. A physical explanation for this transformation is proposed.

Keywords: thin films, Auger electron spectroscopy, growth mechanism, three-dimensional islands, wetting layer, samarium disilicide.

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1. Introduction

As is known, Auger electron spectroscopy (AES) remains one of the most widely used methods in studies of thin film growth processes [1–4]. It can be used to obtain information not only about the elemental composition, but also about the mechanisms of growth of film structures. To achieve this, the dependences of the intensity of the Auger peaks of the film and / or adsorbent on the degree of coverage, or the amount of substance deposited on the surface of the substrate, expressed in monolayers (concentration dependences of Auger signals), are analyzed. However, such an analysis is usually qualitative character due to the lack of numerical models in most cases, with the exception of the simplest ones, in which layered (two-dimensional) films are grown according to the Frank–van-der-Merwe (FM) mechanism. Obviously, this narrows the possibilities of the AES method and does not allow it to determine many quantitative characteristics of thin films and their interfaces.

A model have been recently proposed in Ref. [5] for studying reactive film structures using AES, in which atomic mixing occurs in the substrate–film contact region, leading to the formation of diffuse interfaces. Using this model, based on the analysis of the concentration dependences of Auger signals for a number of rare earth metal (REM)–silicon systems, data on the structure and stoichiometric composition of the interfaces at room temperature were obtained, and it was also shown that these data correlate with the thermodynamic properties of adsorbates.

This article presents a development of the approach used in Ref. [5]. It offers a numerical model for studying the growth processes of films formed by three-dimensional (3*D*) islands using AES. This model can be applied to the films grown based on the Volmer–Weber (VW) or Stranski–Krastanov (SK) mechanisms, including their varieties. It allows establishing the relationship between the density of the islands, their shape and the degree of coverage, which, in turn, makes it possible to simulate the concentration dependences of Auger signals for the film and the substrate. The model can also be used to solve the inverse problem — to determine the morphological characteristics of an island film based on the available experimental AES data. The results of testing this model for samarium disilicide films on a Si(111) substrate are provided at the end of the article (for more information on the choice of this film system, see section 5).

2. Model

We assume that the film is formed by 3*D*-islands shaped like a semi-ellipsoid, and that their density ρ does not depend on the degree of N coverage. Let's select a square cell on the surface with the side $L = 1/\sqrt{\rho}$, in which the base of one island is located. Let the centers of the base of the island and the cell coincide (Figure 1). Let us introduce an analytical function to describe the totality of all points on the island's surface choosing a Cartesian coordinate system, as shown in Figure 1, and using the canonical equation of the ellipsoid $\frac{x^2}{\alpha^2(N)} + \frac{y^2}{\beta^2(N)} + \frac{z^2}{\gamma^2(N)} = 1$:

$$H(x, y, N) = \gamma(N)\sqrt{1 - \frac{x^2}{\alpha^2(N)} - \frac{y^2}{\beta^2(N)}}. \qquad (1)$$

Here $\alpha(N)$, $\beta(N)$ and $\gamma(N)$ are the half-axes of the ellipsoid, depending on the coverage. Let's find the

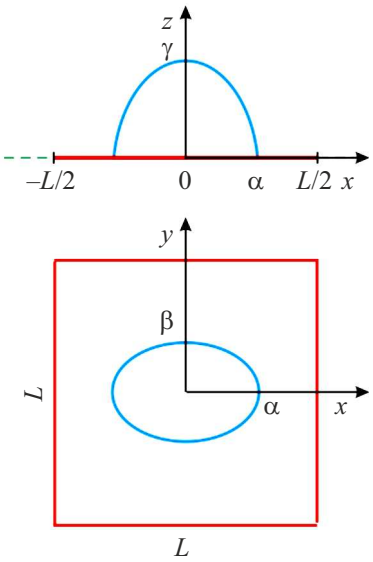

Figure 1. Image of 3*D*-island and cell $L \times L$ in two projections. The projection plane is *a*) perpendicular to the surface and *b*) parallel to the surface.

relationship between these values. To do this, we set the coefficients $n \equiv \beta(N)/\alpha(N)$ and $m \equiv (N)/\alpha(N)$, which determine the geometric shape of the island, and express the volume of the latter in terms of the coverage value:

$$V_{\text{isl}}(N) = \frac{2}{3}\pi\alpha(N)\beta(N)\gamma(N) = Nd_{\text{f}}L^2, \tag{2}$$

where d_{f} is the thickness of one monolayer of the film. Now it is possible to obtain an expression for the length of the semi-axis α of the ellipsoid from the equation (2):

$$\alpha(N) = \sqrt[3]{\frac{3d_{\text{f}}NL^2}{2\pi mn}} = \sqrt[3]{\frac{3d_{\text{f}}N}{2\pi mn\rho}}. \tag{3}$$

In the future, for simplicity, we will limit ourselves to considering the case $n = 1$. When this condition is met, the islands take the form of either an oblate (at $n > m$) or an elongated (at $n < m$) hemisphere or a hemisphere (at $n = m$). The condition $n = 1$ is not essential. A similar conclusion can be drawn for $n \neq 1$.

Now, let us consider the concentration dependences of Auger signals for the film system using the above expressions. The analysis will be carried out separately for the case when the film is grown based on the VW mechanism, and for the case when the film is formed by the SK mechanism.

2.1. VW case

The intensity of the Auger signal of the substrate is represented as the sum of two terms:

$$I_{\text{s}}^{\text{VW}} = I_{\text{s}}^{\text{unscr}} + I_{\text{s}}^{\text{scr}}. \tag{4}$$

The first of these is equal to the intensity of the signal from the part of the substrate that is free of adsorbate. Since this value is proportional to the surface area, the first term in (4) can be written as:

$$I_{\text{s}}^{\text{unscr}} = \frac{S'}{L^2} I_0, \tag{5}$$

where S' is the area of the part of the cell in Figure 1 that is not covered by an island, and I_0 is the value of the Auger signal for a substrate without adsorbate on its surface.

Let us calculate the area S' by introducing an auxiliary function

$$\sigma_{\text{s}}(x, y, N) = \\ = \begin{cases} 0, & \text{if } |x+y| + |y-x| \leq L \cap x^2 + y^2 \leq \alpha^2(N) \\ 1, & \text{otherwise.} \end{cases} \tag{6}$$

Then it can be determined using a double integral over the cell area:

$$S' = \int_{-L/2}^{L/2}\int_{-L/2}^{L/2} \sigma_{\text{s}}(x, y, N)dxdy, \tag{7}$$

and the expression (5) can be rewritten taking into account (7):

$$I_{\text{s}}^{\text{unscr}} = \frac{I_0}{L^2}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2} \sigma_{\text{s}}(x, y, N)dxdy. \tag{8}$$

The second term in (4) represents the magnitude of the Auger signal from the part of the substrate that is covered with the film (islands). It is calculated by determining the magnitude of the signal generated by a small element of the surface area $dxdy$. It is equal to $\frac{dxdy}{L^2} I_0 \varphi_{\text{s}}(x, y, N)$, where $\varphi_{\text{s}}(x, y, N)$ is a function that allows taking into account the effect of screening the substrate with a film applied to its surface. Since the value of the substrate's Auger signal exponentially decreases with the increase of the film thickness, the screening function can be expressed as follows:

$$\varphi_{\text{s}}(x, y, N) = \\ = \begin{cases} \exp\left(-\dfrac{H(x, y, N)}{\lambda_{\text{f}}}\right), \\ \text{if } |x+y| + |x-y| \leq L \cap x^2 + y^2 \leq \alpha(N)^2 \\ 0, \quad \text{otherwise.} \end{cases} \tag{9}$$

λ_{f} is the depth of the release of Auger electrons in this expression. It is determined by the free path length in the film and the angle of emergence from the surface.

Then considering (9) the second term in (4) is

$$I_{\text{s}}^{\text{scr}} = \frac{I_0}{L^2}\int_{-L/2}^{L/2}\int_{-L/2}^{L/2} \varphi_{\text{s}}(x, y, N)dxdy, \tag{10}$$

and the final expression for the value of the Auger signal of the substrate, taking into account the normalization $I_0 = 1$, will have the form

$$I_s^{VW} = \frac{1}{L^2} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \left[\varphi_s(x, y, N) + \sigma_s(x, y, N)\right] dxdy. \quad (11)$$

Let's make a similar conclusion for the Auger signal of the film. For this purpose, we select a small volume element $dxdydz$ of the island at an arbitrary point with the spatial coordinate z. It corresponds to a signal value equal to $\frac{dxdydz}{L^2 d_f} I_{ML} \varphi_f(x, y, z, N)$. Here I_{ML} is the intensity of the Auger signal from one adsorbate monolayer, and $\varphi_f(x, y, z, N)$ is a screening function similar to the function (9). Let's find an analytical expression for it. It can be written as follows by analogy with the formula (9):

$$\varphi_f(x, y, z, N) = \begin{cases} \exp\left(\frac{z - H(x, y, N)}{\lambda_f}\right), \\ \text{if } |x+y|+|x-y| \le L \cap x^2 + y^2 \le \alpha'(z, N)^2 \\ 0, \text{ otherwise.} \end{cases} \quad (12)$$

Let us turn again to the canonical equation of the ellipsoid to find $\alpha'(z, N)$ and transform it as follows:

$$\frac{x^2}{\alpha^2(N)} + \frac{y^2}{\beta^2(N)} = 1 - \frac{z^2}{\gamma^2(N)}. \quad (13)$$

Let's introduce designations

$$\alpha'(z, N) = \alpha(N) \frac{\sqrt{\gamma(N)^2 - z^2}}{\gamma(N)} \quad (14)$$

and

$$\beta'(z, N) = \beta(N) \frac{\sqrt{\gamma(N)^2 - z^2}}{\gamma(N)}. \quad (15)$$

Now, using (14) and (15), we obtain the expression

$$\frac{x^2}{\alpha'^2(z, N)} + \frac{y^2}{\beta'^2(z, N)} = 1. \quad (16)$$

It is the equation of an ellipse, which is a section of a semi-ellipsoid at a height of z in Figure 1. This explains, in particular, the physical meaning of the function $\alpha'(z, N)$: when the condition $n = 1$ is met, its value is equal to the radius of the circle, which is the section of the spheroid at a height of z.

Finally, let us obtain an expression for the value of the Auger signal of the substrate $I_f^{VW}(N)$. To achieve this, it is necessary to integrate over a three-dimensional cell with the base $L \times L$:

$$I_f^{VW}(N) = \frac{I_{ML}}{L^2 d_f} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \int_0^{\gamma(N)} \varphi_f(x, y, z, N) dxdydz. \quad (17)$$

It is necessary to find the value I_{ML} for obtaining the final answer. To do this, let us determine the signal intensity for a solid film with a thickness Nd_f. It is equal to

$$I_N = I_{ML} \int_0^{Nd_f} \frac{dz}{d_f} \exp\left(-\frac{(Nd_f - z)}{\lambda_f}\right). \quad (18)$$

Let's assume $I_N = 1$ for $N \to +\infty$ (normalization condition in AES). Then let us obtain the limit using which the value of I_{ML} can be determined:

$$\lim_{N \to +\infty} I_{ML} \int_0^{Nd_f} \frac{dz}{d_f} \exp\left(-\frac{(Nd_f - z)}{\lambda_f}\right) = I_{ML} \frac{\lambda_f}{d_f} = 1. \quad (19)$$

2.2. SK case

Let us conduct a review for the case of the SK mechanism. First, let us obtain an expression for the intensity of the Auger signal of the substrate. Since this growth mechanism is two-stage, the desired function will be piecewise continuous:

$$I_s^{SK} = \begin{cases} I_s^{wet}, & \text{if } N \le N_{wet} \\ I_s^{isl}, & \text{otherwise.} \end{cases} \quad (20)$$

Here I_s^{wet} is the value of the substrate Auger signal at the stage of wetting layer formation, i.e. before the formation of 3D-islands, and I_s^{isl} is a similar value at the stage of island film formation. The first of these values is $I_s^{wet}(N) = \exp\left(-\frac{d_f}{\lambda_f} N\right)$. As for the second value, it can be represented as $I_s^{isl} = I_s^{'scr} + I_s^{'unscr}$, where $I_s^{'scr}$ is the signal value for the part of the surface that is covered with 3D-islands, and $I_s^{'unscr}$ is the same value for the part of the surface on which there are no islands. Let us obtain the final expression for the intensity of the Auger signal of the substrate using formulas (6) and (9):

$$I_s^{isl} = \frac{1}{L^2} \exp\left(-\frac{d_f}{\lambda_f} N_{wet}\right) \times \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \left[\varphi_s(x, y, N - N_{wet}) + \sigma_f(x, y, N - N_{wet})\right] dxdy. \quad (21)$$

Now we will print the expression for the adsorbate signal. As in the case of the substrate, its intensity will have a piecewise continuous shape:

$$I_f^{SK} = \begin{cases} I_f^{wet}, & \text{if } N \le N_{wet} \\ I_f^{isl}, & \text{otherwise.} \end{cases} \quad (22)$$

Here I_f^{wet} and I_f^{isl} are the values of the Auger signal at the first and second stages of film structure formation, respectively. Let us use the relations (18) and (19) and

extend them to the three-dimensional case for finding the first part (22):

$$I_{\mathrm{f}}^{\mathrm{wet}}(N) = \frac{1}{\lambda_{\mathrm{f}} L^2} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \int_{0}^{Nd_{\mathrm{f}}} \exp\left(-\frac{Nd_{\mathrm{f}} - z}{\lambda_{\mathrm{f}}}\right) dz\, dx dy. \tag{23}$$

Now let's find the second part of the function (22). It can be represented as $I_{\mathrm{f}}^{\mathrm{isl}} = I_{\mathrm{f}}^{'\mathrm{scr}} + I_{\mathrm{f}}^{'\mathrm{unscr}} + I_{\mathrm{f}}^{'\mathrm{isl}}$, where $I_{\mathrm{f}}^{'\mathrm{scr}}$ is the magnitude of the adsorbate signal located in the part of the wetting layer that is shielded by 3*D*-islands, $I_{\mathrm{f}}^{'\mathrm{unscr}}$ is the same for the part of the wetting layer that is free of islands, $I_{\mathrm{f}}^{'\mathrm{isl}}$ is the signal value of the adsorbate located in 3*D*-islands. Now, the final expression can be derived using the formulas obtained earlier:

$$I_{\mathrm{f}}^{'\mathrm{isl}} = \frac{I_{\mathrm{f}}^{\mathrm{wet}}(N_{\mathrm{wet}})}{L^2} \times \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \left[\varphi_{\mathrm{f}}(x, y, N - N_{\mathrm{wet}}) + \varphi_{\mathrm{f}}(x, y, N - N_{\mathrm{wet}})\right] dx dy + \frac{1}{\lambda_{\mathrm{f}} L^2} \int_{-L/2}^{L/2} \int_{-L/2}^{L/2} \int_{0}^{\gamma_{\mathrm{s}}(N - N_{\mathrm{wet}})} \varphi_{\mathrm{f}}(x, y, N - N_{\mathrm{wet}}) dz\, dx dy. \tag{24}$$

As can be seen from the above, the intensity of the Auger signals of the film system is determined by two parameters characterizing the morphological structure of the insular 3*D*-film. The value L is one of such parameters which is determined by the density ρ of islands on the surface. The coefficient m is another parameter, which is equal to the ratio of the height of the island to the radius of its base (for the case of $n = 1$). Next, let us call this value the aspect ratio of the island. The impact of these parameters on the film growth process is considered in the next section.

3. Impact of L and m on the type of concentration dependences of Auger signals

Figure 2 shows the concentration dependences of the adsorbate Auger signal at different values of the parameters L and m. The calculation was made for the case when the film grows according to the VW mechanism, and metallic samarium ($\lambda_{\mathrm{f}} = 13.65$ Å and $d_{\mathrm{f}} = 3.62$ Å is its material [5]). For comparison, this figure also shows a similar dependence calculated for the case of the FM mechanism (shown as a dotted line). As follows from Figure 2, *a*, an increase of the value L of the island film, or, in other words, a decrease of the density of the islands (their shape remains unchanged), leads to the fact that the value of the Auger signal decreases, the given dependence becomes flatter, its deviation from the similar curve for a continuous film increases, and the saturation of the dependence shifts to the region of large

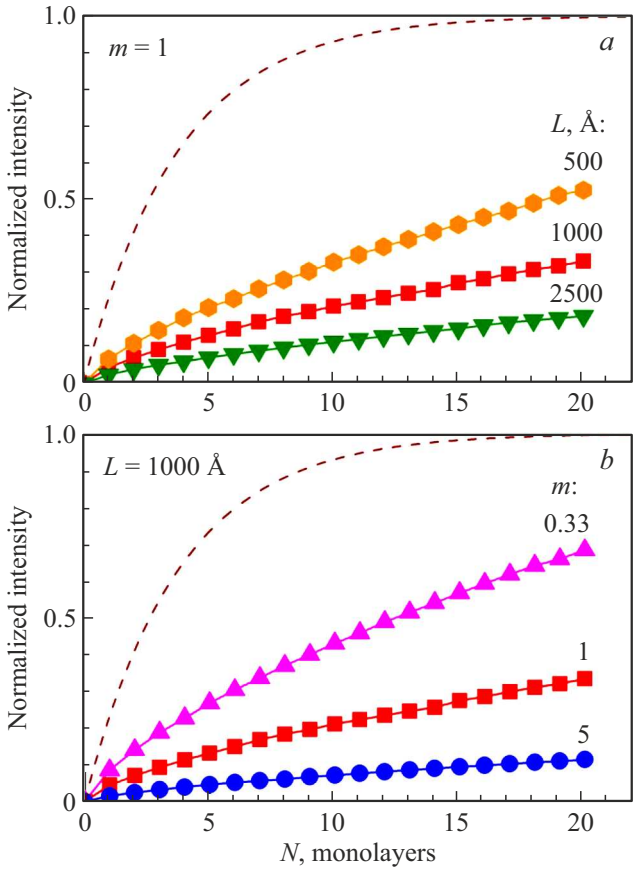

Figure 2. Type of concentration dependences of the adsorbate Auger signal intensity at different values of the parameters L and m for the VW case. The dotted line shows a similar relationship for the FM mechanism. Normalization was performed based on the magnitude of the signal for a massive solid film.

coverings. This means that the coalescence for island films should occur at an increasingly late stage of growth as L increases.

Similar conclusions can be drawn for the case when the value of L is fixed, and the shape of the islands changes. The type of adsorbate concentration dependence is very sensitive to the aspect ratio m as can be seen in Figure 2, *b*. The covering value N_{CL}, at which coalescence occurs, shifts to the region of large values as the aspect ratio increases, i. e., the islands acquire an increasingly elongated upward shape.

It should be noted that similar conclusions follow from the analysis of similar dependencies for the substrate.

4. Dependence of N_{CL} on L and m

Let us consider the results shown in Figure 3 to illustrate more clearly how the transition to the coalescence stage depends on the parameters L and m. It shows the dependences of the value of N_{CL} on the aspect ratio m for islands with different values of L. The coverage value

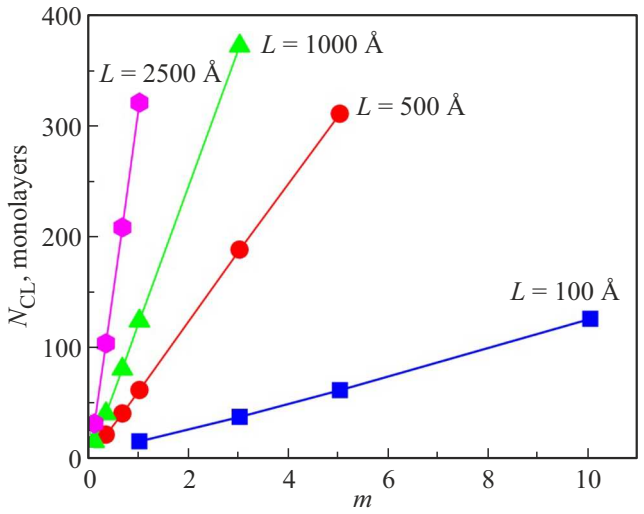

Figure 3. Dependences of the value N_{CL} on the aspect ratio m of islands with different values of L.

at which the intensity of the samarium Auger signal is 0.95 was used as the value N_{CL} to calculate these dependencies.

The following conclusions can be drawn from Figure 3.

The steepness of the dependence $N_{CL} = f(m)$ markedly increases with an increase of the value of L and a decrease of the island density. In other words, the amount of material applied to the surface required to form a continuous film at relatively low densities ρ very sharply depends on the shape of the islands. For instance, the value of N_{CL} is 32 monolayers for $m = 0.1$ and 320 monolayers for $m = 1$ with $\rho = 1.6 \cdot 10^9\,\mathrm{cm}^{-2}$ ($L = 2500$ Å).

The slope of dependence $N_{CL} = f(m)$ is relatively small at relatively low values of L and high island densities, and the fusion of 3D-islands requires smaller amounts of material deposited on the substrate. For example, the value of N_{CL} is 16 monolayers for $m = 1$ and 62 monolayers for $m = 5$ with $\rho = 1 \cdot 10^{12}\,\mathrm{cm}^{-2}$ ($L = 100$ Å). We would like to mention in passing that the model predicts that the tangent of the angle of slope of the dependence $N_{CL} = f(m)$ will approach zero with a further decrease of the parameter L, and the properties of the island film will become closer to the properties of the solid film.

Thus, the described model can be used to predict the course of concentration dependences of Auger signals of film structures for which the density and shape of 3D-islands are known.

5. System Sm–Si(111)

In practice, however, it is often necessary to solve the opposite problem, namely, to obtain information about the growth processes and morphology of films from the analysis of known experimental AES data. Let us consider such a problem in this section and use the described model to determine the parameters of island 3D-films using the concentration dependences of Auger signals. The film system Sm–Si(111) can serve as a good candidate for testing the model. This is attributable to the fact that, firstly, the mechanism of formation of this system at high temperatures is similar to the SK mechanism: after filling the wetting 2D-layer, epitaxial growth of 3D-samarium disilicide crystallites is observed [6]. Secondly, detailed AES data [7], as well as a whole range of other results, were previously obtained for it [6,8,9]. Finally, it was found in previous studies of Sm–Si(111) structures that the type of concentration dependences of Auger signals for it changes significantly during the transition from one structure of the wetting layer to another [7]. As shown below, the model proposed in this paper helps to explain the nature of this difference.

The AES data and the results of their quantitative analysis for the Sm–Si(111) system are presented in Figure 4. The symbols show the experimental curves obtained for the samarium signal in Ref. [7]. Auger peak $M_5N_{4,5}N_{4,5}$ with an energy of 816 eV was used to record these curves. The curve *1* corresponds to the case when the crystallites of a silicide film were grown on a surface reconstruction (wetting layer) of Sm–Si(111)$\sqrt{3}$ formed by coverage of ~ 0.5 monolayer of samarium atoms. The curve *2* corresponds to the case when the crystallites were created on the reconstruction of Sm–Si(111)(5×1) with metal coverage of ~ 0.3–0.4 monolayer. Figure 4 also shows the calculated dependencies for both cases. They are represented by solid lines. The mean free path in samarium disilicide was determined for modeling as the statistical sum of similar values for metallic Sm (16.6 Å) and silicon (21.0 Å) [10] with weighting coefficients 1/3 and 2/3, respectively. This approach was successfully used earlier in Ref. [5]. The calculations also took into account the geometry of the experiment in Ref. [7], namely, the angle of release of Auger electrons from the sample (42.18°). Moreover, the

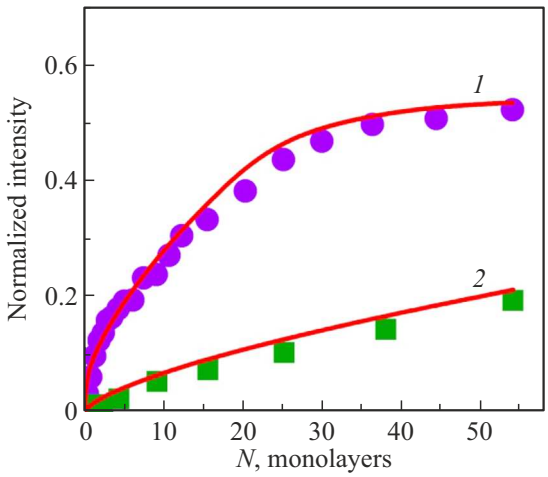

Figure 4. Concentration dependences of the samarium Auger signal for the system Sm–Si(111). Structure of the wetting layer: curve *1* — $\sqrt{3}$, *2* — (5×1). Experimental data from Ref. [7] (symbols) and modeling results obtained in this study (solid lines) are presented.

crystal structure of samarium disilicide islands was taken into account by introduction of multiplier $\theta_f = \frac{d_f}{d_f+2d_s}$ before the last term in the expression (24), which used the values $d_f = 3.62$ Å and $d_s = 1.57$ Å [5].

The results provided in Figure 4 allow for making immediate conclusions that *a*) the dependencies *1* and *2* significantly differ from each other and *b*) the model used allows for a fairly accurate replay the progress of each of them. This difference is intuitively explained in Ref. [7] on the basis of a change of the shape of 3*D*-crystallites. The calculations made in this paper fully confirm this interpretation. The calculated curve *1* was obtained with the aspect ratio of crystallites $m_1 = 0.75$. Curve *2* corresponds to the aspect ratio of crystallites equal to $m_2 = 5.55$. This means that primarily lateral growth of disilicide crystallites takes place in the case of a wetting layer with the structure $\sqrt{3}$, i. e. such islands have a relatively „flat" shape. In the case of a wetting layer with the structure (5×1), the lateral growth of crystallites is noticeably limited, and they have the form of elongated islands, with the ratio m_2/m_1 being 7.4. It should be noted that these conclusions are in full agreement with the results of diffraction observations in Ref. [7]. The crystallite density in both cases is $\rho = 2 \cdot 10^{10}\,\mathrm{cm}^{-2}$. This value correlates well with similar values for islands of REM silicides on silicon substrates in other studies [11,12].

The question inevitably follows from what has just been said: why do 3*D*-crystallites of samarium disilicide change their shape in case of the transition from one wetting layer to another? One possible reason could be the difference of the temperatures at which the silicide films were grown (900 K in the case of the wetting layer $\sqrt{3}$ and 1140 K in the case of the wetting layer (5×1) [7]). However, this difference is not so great as to explain the change in the aspect ratio of the islands by more than seven times. Therefore, this reason will not be discussed further in the article.

Another reason may be related to the alignment of the lattices of samarium disilicide and the wetting layer (surface reconstruction of silicon induced by samarium atoms). The analysis shows that in the case of reconstruction (5×1), such alignment should most likely be worse than for reconstruction $\sqrt{3}$. In principle, this should help to increase the aspect ratio of *m* islands in case of the transition from the first structure to the second one. However, the authors do not consider this reason convincing either. Indeed, the lattice alignment at the interface of the wetting layer — disilicide could play a key role if the film system was not reactive and the surface structure of the silicon and the wetting layer was not subject to rearrangement. Obviously, this condition is not fulfilled for the system Sm−Si(111).

In the authors' opinion, the most probable reason for the change of the shape of 3*D*-crystallites of silicide in case of the transition $\sqrt{3} \leftrightarrow (5 \times 1)$ can be formulated as follows. The lateral growth of the island with an increase of the coverage, i. e. an increase of its parameter $\alpha(N)$, should be accompanied by a structural restructuring of adjacent sections of the wetting layer. In fact, such a transformation involves decomposition of the surface reconstruction, the probability of which is determined by the activation energy of the process and temperature. It can be expected that 3*D*-crystallites with a lower value of parameter *m* will be formed in case of a wetting layer with lower thermal stability, and crystallites with a higher value of *m* will be formed in case of a layer with higher thermal stability. The first case corresponds mainly to the lateral growth of the island film, for which coalescence occurs at an earlier stage of formation. The second case corresponds to the growth of the film, the island character of which is more pronounced and coalescence occurs at a later stage of formation. The experimental results in Ref. [6] fully confirm this picture. The structure Sm−Si(111)(5×1) has a higher decomposition temperature and energy of removal of samarium atoms from it than the structure $\sqrt{3}$. This ultimately determines the shape of 3*D*-crystallites of samarium disilicide in Sm−Si(111) system.

6. Conclusion

A model has been developed for calculating the intensity of Auger signals of an island film and a substrate as a function of the amount of adsorbate deposited on the surface for two cases of film system growth: *a*) according to the VW mechanism and *b*) according to the SK mechanism. Typical concentration dependences of the Auger signal of a samarium metal film have been obtained and analyzed using this model. In particular, it is shown what effect the values of the parameters *L* and *m* have on the appearance of these curves. The model was also tested for the reactive system Sm−Si(111). Analysis of the experimental data obtained for it made it possible to determine the parameters of 3*D*-crystallites of samarium disilicide created on different transition (wetting) 2*D*-layers. In particular, it was found that primarily lateral growth 3*D*-crystallites of disilicide occurs on the wetting layer with the structure $\sqrt{3}$ and that their aspect ratio is $m = 0.75$. At the same time, compact, elongated crystallites are formed on the transition layer with the structure (5×1), for which the parameter *m* increases by more than seven times (5.55). Considerations concerning the physical nature of such a transformation of islands are expressed. The change of their shape is ultimately attributable to the fact that the structure (5×1) has a higher thermal stability than the structure $\sqrt{3}$, and therefore the substitution of the first of them with disilicide crystallites is less energetically advantageous than the second one. This contributes to an increase of the aspect ratio of the islands in case of the transition to the wetting layer (5×1).

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] C.J. Powell. Microscopy Today **24**, *2*, 16 (2016).
[12] W.-C. Lin, W.-C. Lo, J.-X. Li, P.-C. Huang, M.-Y. Wang. ACS Omega **6**, *50*, 34606 (2021).
[3] R.A. Vidal, J. Ferron. J. Phys. D: Appl. Phys. **48**, *43*, 435302 (2015).
[4] M. Xu, D. Fujita, J. Gao, N. Hanagata. ACS Nano **4**, *5*, 2937 (2010).
[5] V.E. Rempel, M.A. Mittsev, M.V. Kuzmin. FTT **65**, *9*, 1611 (2023). (in Russian).
[6] T.V. Krachino, M.V. Kuz'min, M.V. Loginov, M.A. Mittsev. Phys. Solid State **40**, *2*, 341 (1998).
[7] T.V. Krachino, M.V. Kuz'min, M.V. Loginov, M.A. Mittsev. Phys. Solid State **40**, *10*, 1758 (1998).
[8] F. Palmino, E. Duverger. Surf. Sci. **603**, *17*, 2771 (2009).
[9] E. Ehret, F. Palmino, L. Mansour, E. Duverger, J.-C. Labrune. Surf. Sci. **569**, *1–3*, 23 (2004).
[10] C.J. Powell, A. Jablonski. NIST Electron Inelastic-Mean-Free-Path Database, Version 1.2, SRD 71. National Institute of Standards and Technology, Gaithersburg, MD (2010).
[11] R. Hofmann, F.P. Netzer, A.J. Patchett, S.D. Barrett, F.M. Leibsle. Surf. Sci. **291**, *3*, 402 (1993).
[12] M. Kuzmin, R.E. Perälä, R.-L. Vaara, P. Laukkanen, I.J. Väyrynen. J. Cryst. Growth **262**, *1–4*, 231 (2004).

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