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Surface structure of $Gd_{20}Co_{80}$ alloy

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Abstract. $Gd_{20}Co_{80}$ alloy was studied applying experimental methods of spectral ellipsometry, atomic force and scanning tunneling microscopy. The experimental results exhibit the eutectic two-phase structure of this alloy. Clusters of a phase with a lower content had a lesser concentration of free carriers, which resulted in smaller tunnel currents during the measurements. To analyze the experimental data, a theoretical approach was developed, which was based both on the quantum-mechanical methods of configurational interaction and on three-diagonal Toeplitz matrices formalism. This approach allowed us to describe in detail the energy bands formation process in solid clusters with a relatively small quantity of atoms, which as a consequence enabled to describe the Shockley surface states as well as the existence of a surface layer with partially formed energy bands. Spectral-ellipsometric measurements of $Gd_{20}Co_{80}$ alloy thin films confirmed a significant difference between the measured optical constants for 20-nm thick films and larger films. Quantum-mechanical molecular calculus allowed to obtain optical constants for several supercells of Gd-Co chemical compounds and confirmed the acquired experimental and theoretical results.

Keywords: gadolinium cobalt alloy, Shockley surface states, configuration interaction.

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1. Introduction

Alloys of rare-earth metals with cobalt are extremely interesting both in terms of their physical properties and with regards to their applications in magneto-optics. The properties of such a rare-earth metal as Gd and the ferromagnetic transition metal when they interact in the alloy can lead to specific magnetic properties of these alloys [1], also taking into account the complex nature of the phase diagram of Gd-Co alloys [2].

In fact, the specific electronic structure of gadolinium, its unfilled inner shell, which leads to less noticeable collective properties of this metal, leads to a large number of chemical compounds on the Gd-Co alloy phase diagram. The properties of Gd_mCo_n compounds, some of which are not stable [3], depend on interaction on the contact surface of individual clusters (or layers [4]) of Gd_mCo_n with different crystal lattices [2, 5].

Previous electron-microscopic studies of Gd-Co thin films have indicated the possibility of an extremely complex cluster nanoscale structure of alloys with the possibility of the existence of separate clusters with different crystal structures and with a specific orientation of their spins [6]. It should be also noted the studied features of the structure of the alloy Gd_2Co_7. This alloy showed the presence of crystal lattices typical for Ce_2Ni_7 and Er_2Co_7 due to absorption of hydrogen by the alloy [7]. It is clear that the possibility of absorption of gas molecules from the air, which will affect the crystal structure of the samples, adds additional uncertainty in experiments with Gd_2Co_7. There are seven stable phases of Gd-Co alloys (Gd_3Co, $Gd_{12}Co_9$, $GdCo_2$, $GdCo_3$, Gd_2Co_7, $GdCo_5$ and Gd_2Co_{17}) [2, 8]. For the study, we chose the $Gd_{20}Co_{80}$ alloy, due to the existence of several types of stable phases on the Gd-Co phase diagram in the vicinity of Gd_2Co_7 phase. This allows us to study samples with different crystal clusters.

The aim of this study is to analyze experimental spectral-ellipsometric, atomic force and high spatial resolution scanning tunneling microscopy data for thin films of $Gd_{20}Co_{80}$ alloy from the viewpoint of condensed matter theory by taking into account the electronic structure properties of rare-earth metals.

2. Theory: Shockley surface states in configuration interaction formalism

Surface states can be described applying a simplified model of a one-dimensional chain of atoms. This approach is typical, when considering Shockley type surface states [9]. In this case, if we take a set of atoms with two energy levels, the levels of the chain transform to energy bands. Let us examine this point in more detail. Suppose that we have N atoms forming a one-dimensional chain – a finite one-dimensional lattice. Then, in accordance with the quantum-mechanical method of configuration interaction (CI) [10], we look the wave function of the chain in the form $\Psi = \sum_i C_i \Psi_i$ (Ψ_i – wave function of i-th atom) with the possibility to vary the coefficients C_i ($\sum_i (C_i)^2 = 1$) to minimize the energy of functional $E = \langle \Psi | H | \Psi \rangle$, which require solving a system of linear equations (including a condition of zero determinant):

$$\sum_{i=0}^{N} \left(\langle \Psi_i | H | \Psi_j \rangle - E\delta_{ij} \right) C_j = 0, \tag{1}$$

$$\det\left(\langle \Psi | H | \Psi \rangle - EI \right) = 0. \tag{1a}$$

I is a unit matrix. In fact, the second relation Eq. (1a) defines the formal procedure for finding the eigenvalues (eigenvectors) of $R = \langle \Psi | H | \Psi \rangle$ matrix. The elements of R matrix corresponding to the straight chain of atoms can be represented as the Toeplitz matrix:

$$R = \begin{vmatrix} a_0 & a_1 & a_2 & ... & a_{N-1} \\ a_1 & a_0 & a_1 & ... & a_{N-2} \\ a_2 & a_1 & a_0 & ... & a_{N-3} \\ ... & ... & ... & ... & ... \\ a_{N-1} & a_{N-2} & a_{N-3} & ... & a_0 \end{vmatrix} \approx$$

$$\approx \begin{vmatrix} a_0 & a_1 & 0 & ... & 0 \\ a_1 & a_0 & a_1 & ... & 0 \\ a_2 & a_1 & a_0 & ... & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & a_0 \end{vmatrix} = R_T(a_0, a_1) \tag{2}$$

Due to translational symmetry of the chain, the elements of the matrix Eq. (2) must be symmetrical relatively to the main diagonal $a_{i,j} = a_{i+1,j+1} \left(a_k = \langle \Psi_i | H | \Psi_j \rangle \right)$. It is also clear that the Hamiltonian matrix elements are maximal for neighboring atoms. Therefore, if we neglect the interaction of non-adjacent atoms, the density matrix can be approximately represented as the tridiagonal Toeplitz matrix R_T ($a_{i,i} \neq 0$, $a_{i\pm1,i} \neq 0$) in Eq. (2). As known [11], the spectrum of N eigenvalues of this type of matrices uniformly fills a narrow numerical interval.

Let us check out now these two energy levels for the chain of atoms as a function of the distance between atoms. In this case, the matrix R_T can be represented in the block form

$$R = \begin{vmatrix} R_T(a_0, a_1) & 0 \\ 0 & R_T(b_0, b_1) \end{vmatrix}. \tag{3}$$

The results of calculations are presented in Fig. 1. $a_1(r)/a_0(r)$ and $b_1(r)/b_0(r)$ are functions of the distance between the atoms in the chain for the main and excited energy levels. In the calculations, we considered a simplified case $a_1/a_0 = b_1/b_0$, which allowed us to more evidently present the dynamics of formation of energy bands as 2D rather than 3D curves. As one can see, the energy levels do not cross and converge forming the energy states in the forbidden energy gap (Fig. 2b, marked by circles). The finiteness of the chains of atoms results in the formation of Shockley states in the forbidden energy gap [12]. Interestingly, the upper and lower energy levels in the energy bands are the eigenvalues of the matrix corresponding to two atoms on the chain ends, *i.e.*, in our approach, these levels are associated with surface atoms. These levels converge to form surface states in the forbidden energy gap, but the process of formation of surface states is the result of the collective interaction of many atoms in the near-surface layer and not only the atoms at the chain ends. In fact, we are talking about the effect, which is localized at sample surfaces due to the ideal crystal translational symmetry violation.

If we consider an alloy that exists as an eutectic mixture of a few phases, we actually have a violation of the translational symmetry in the whole crystal bulk, namely at the phase boundaries. As a part of the configuration interaction model, let us apply Born – von Karman boundary condition for our model of a one-dimensional chain of N atoms with two energy levels with different parity:

$$\begin{aligned} &\varphi(x) = \sum_{j=0}^{N-1} C_j^g \Psi_j^g + \sum_{j=0}^{N-1} C_j^u \Psi_j^u = \exp(ikx) U(x) = \\ &U^g \sum_{j=0}^{N-1} C_j^g \exp\left(ik(x + jd)\right) + U^u \sum_{j=0}^{N-1} C_j^u \exp\left(ik(x + jd)\right) = \\ &= \Psi^g \sum_{j=0}^{N-1} C_j^g \exp\left(ik(x + jd)\right) / \exp(ikx) + \\ &+ \Psi^u \sum_{j=0}^{N-1} C_j^u \exp\left(ik(x + jd)\right) / \exp(ikx). \end{aligned} \tag{4}$$

where $\Psi^{g,u} = \Psi_0^{g,u}$. For levels with even g and odd u symmetry in respect to the $x \to -x$ operation, the condition of translational symmetry $U(x+d) = U(x)$ is also fulfilled, where d is the distance between atoms. We can rewrite the expression (4) taking into account that the even and odd components of the wave function have different complex character (the real part of $\exp(ikx)U(x)$ the relation (4) is even and complex – odd):

$$\varphi(x) = u\Psi^g(x) + wi\Psi^u(x). \quad (5)$$

In fact, we reduce the number of variables $C_j^{g,u}$ in the expression (4), using Born – von Karman boundary condition $(u = \sum_{j=0}^{N-1} C_j^g \exp(ik(x+jd))/\exp(ikx)$, $w = (-i)\sum_{j=0}^{N-1} C_j^u \exp(ik(x+jd))/\exp(ikx))$. We can use the relation (5) for description of energy levels in the forbidden energy gap. In this case, the wave function of such states is described as a mixed state of wave functions of two energy levels from the valence band and conduction band. The variables u and w are still have to be determined, but we can find the relationship between them by using the relations (4), (5) for wave functions and their derivatives at $x = \pm d/2$:

$$\begin{aligned} &u\Psi^g(d/2) + wi\Psi^u(d/2) = \\ &= \exp(ikd)\left(u\Psi^g(d/2) - wi\Psi^u(d/2)\right), \\ &u\Psi^{g\prime}(d/2) + wi\Psi^{u\prime}(d/2) = \\ &= \exp(ikd)\left(-u\Psi^{g\prime}(d/2) + wi\Psi^{u\prime}(d/2)\right). \end{aligned} \quad (6)$$

Considering the system (6) as two equations with two variable u and w, it can have solutions only at zero determinant:

$$\begin{vmatrix} \Psi^g(d/2)(1-\exp(ikd)) & i\Psi^u(d/2)(1+\exp(ikd)) \\ \Psi^{g\prime}(d/2)(1+\exp(ikd)) & i\Psi^{u\prime}(d/2)(1-\exp(ikd)) \end{vmatrix} = 0. \quad (7)$$

When solving the Schrödinger equation, we obtain solutions with a variable phase factor. When considering the relation (7), we can choose the phase factor so that at the points $x = \pm d/2$ the wave function is real. Then, by solving the relation (7), we can come to a result similar to that of Shockley's surface states:

$$(\tan(kd/2))^4 = -\frac{\left(\Psi^{g\prime}(d/2)/\Psi^g(d/2)\right)}{\left(\Psi^u(d/2)/\Psi^{u\prime}(d/2)\right)}. \quad (8)$$

The difference is in the fourth power in Eq. (8) as opposite to the second one in the original theory. When atoms converge, there is a Coulomb and exchange interaction between the electron shells of atoms, the energy levels of individual atoms change their position with forming the energy bands separated by a forbidden energy gap. Calculations based on Eqs. (1)–(3) for seven atoms with two energy levels (0.75 and 1 arbitrary energy units) are presented in Fig. 1.

An important point of the curves in Fig. 1 is that they form singularities – 14 curves do not cross similarly to the results presented for eight atoms from [13]. At the points where the curves converge, the derivative of the wave function on the coordinate of the perpendicular surface is uncertain. First, it is a consequence of direct calculations in frames of our model – seems to be the eigennumbers property of tridiagonal Toeplitz matrices.

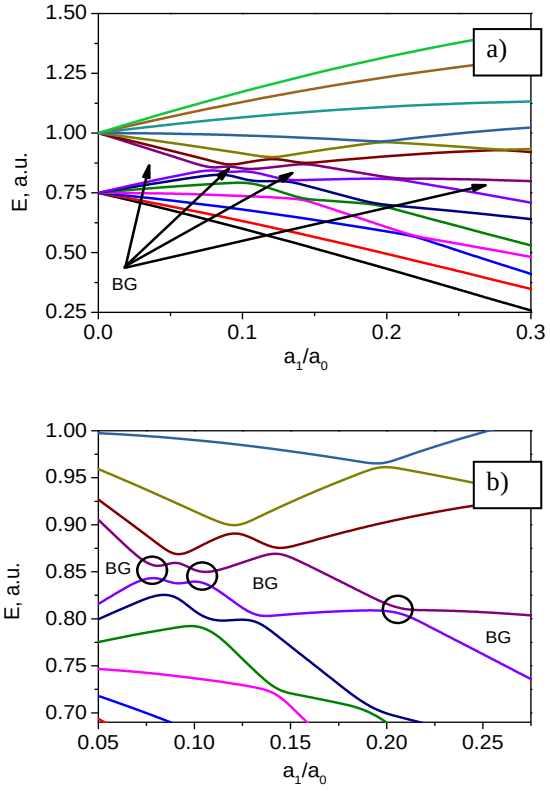


Fig. 1. a) Energy spectrum for 7 atoms one-dimensional lattice as a function of interaction coefficients between atoms, BG – forbidden energy gap. b) Enlarged part of Fig. 1a spectrum.

From the perspective of quantum-mechanical theory, the ordered eigenvalues $\lambda_1 < \lambda_2 < \ldots$ in the space of Hermitian matrices are a part of adiabatic theorem [14] related formalism. From the semi-qualitative viewpoint, two degenerate energy levels can cross and cannot, if, *e.g.*, the levels belong to different energy bands.

Shockley states are possible only with a positive right-hand side of Eq. (8). The derivative $\Psi'(d/2)$ changes its sign at the points of curves extremums, when two energy levels from the valence and conduction bands are becoming very close. Surface states in this model occur, when there is derivatives uncertainty $+\infty/-\infty$ which occurs in the right part of the relationship (8) in the vicinities of such singularities (marked by circles in Fig. 1b). These energy levels in the forbidden energy gap are located at surfaces of eutectic granules in the sample.

It should also be noted that at the points of singularity the upper and lower curves approach each other at an infinitesimal distance (in calculations, the distances between the curves in Fig. 1 are reduced with increasing the amount of points included to the curves). These results are similar to those of the semi-qualitative approach in the original theory [13].

As one can see, the quantum-mechanical configuration interaction technique can be applied for clarification of Shockley states formation by a finite number of atoms in the crystal lattice. In this case, the states can be result both of the presence of eutectic phases in the alloy and of sample surfaces.

3. Results and discussion

Spectral-ellipsometric studies were performed by measuring the elipometric parameters Ψ and Δ in a wide range of the spectrum λ = 0.24…1.0 μm with a WoollamM-2000 spectral ellipsometer.

The INTEGRA NT-MDT microscope was used for measurements in scanning tunneling microscopy (STM) and atomic force microscopy (AFM) regimes. The spatial resolution of STM in the experiments reached 4 nm. A sharp needle for STM measurements was made of 0.5 mm $Pt_{0.8}Ir_{0.2}$ wire by mechanical cutting of its end. We performed our measurements in the mode where the STM installation maintained a constant tunneling current through the needle, which was achieved by changing the position of the sample along the vertical direction. Measurements by using atomic force microscopy were performed in a semi-contact mode with a constant force of needle-substrate interaction. The needle tip diameter was about 20 nm, the needle-cantilever system oscillated at the frequency of mechanical resonance.

$Gd_{20}Co_{80}$ alloy films with the thickness between 20 to 100 nm were deposited using the ion-plasma method at a constant current in vacuum under the pressure close to 10^{-3} Pa onto glass water-cooled substrates. The results of measurements of the $Gd_{20}Co_{80}$ alloy film by using the methods of atomic force microscopy and scanning tunneling microscopy are presented in Fig. 2. We can see there two scans obtained by different methods and having similar qualitative patterns – the presence of dark clusters with tens nanometers sizes.

The pictures in Fig. 2 are presented in the halftone gradation mode of sample profile. It means that in the vicinity of the dark cluster, the cantilever needle (AFM) or $Pt_{0.8}Ir_{0.2}$ wire tip was shifted downward to maintain either constant values of the van der Waals needle-surface interaction force or tunneling current. Furthermore, in the case of atomic force microscopy, we have a relatively small contrast of the cluster pattern (displacement of the needle in the vertical direction is no higher than 8 nm). In the case of scanning tunneling microscopy, we are talking about almost an order of magnitude larger vertical displacements (60 nm). This picture can be logically explained by a much lower concentration of free carriers in these clusters on the surface, which results either in lower numbers of dipole-dipole interaction between the needle and sample surfaces or in a very large drop of tunneling currents between the sample and the wire tip.

In fact, we have a sample with the presence of two phases of gadolinium-cobalt chemical compounds. In this case, the second phase has a relatively smaller concentration and is in the form of clusters having the size of tens nanometers. This allowed us to apply the results of the theoretical part of this study. An important consequence of considering the Shockley type surface states from the viewpoint of the configuration interaction technique is the presence of two qualitatively different intervals for the distance between atoms in Fig. 1 –

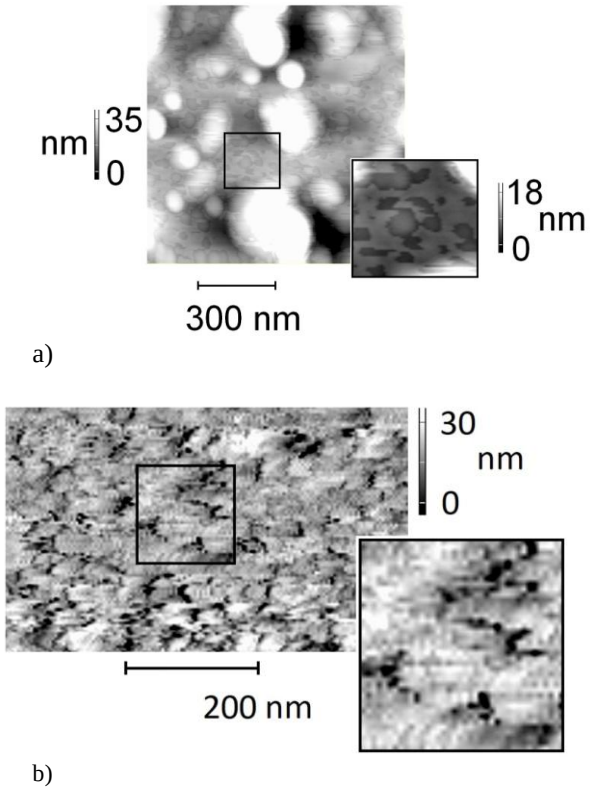


Fig. 2. a) AFM measurements of $Gd_{20}Co_{80}$ thin film. Spatial resolution 20 nm. b) STM measurements of a thin film $Gd_{20}Co_{80}$. Spatial resolution 4 nm.

$a_1/a_0 \in]0;0.078[$ and $a_1/a_0 \in]0.078;0.3[$. The limit parameter 0.78 determines the minimal value of Hamiltonian matrix elements for two neighboring atoms, which is sufficient for considering these 7 atoms as a crystal cluster with formed energy bands. Generally, a limit parameter must depend on the quantity of atoms in the cluster.

Fig. 3 shows an enlarged part of the forbidden energy gap formation for the systems of 7 and 12 atoms. The singularities between the lower level of the upper energy band and the upper level of the lower band with the minimal a_1/a_0 number are indicated with arrows. a_1/a_0 are lower at larger numbers of atoms in the chain.

Each chemical compound has specific parameters of its crystal lattice, *e.g.* the energies of interaction between neighboring atoms (having specific Hamiltonian matrix elements ratio a_1/a_0). From the viewpoint of Fig. 3 calculations, it means the existence for each substance, the minimal quantity of atoms that form a surface layer with properties (*e.g.*, Shockley surface states) differing from the rest of bulk crystal.

The relatively small number of atoms that form a chain leads to inefficient formation of energy bands (especially for rare-earth metal atoms with vacancies in inner electronic shells and, as a consequence, less pronounced collective properties). It seems to be the case for tens nanometers size clusters in Fig. 2.

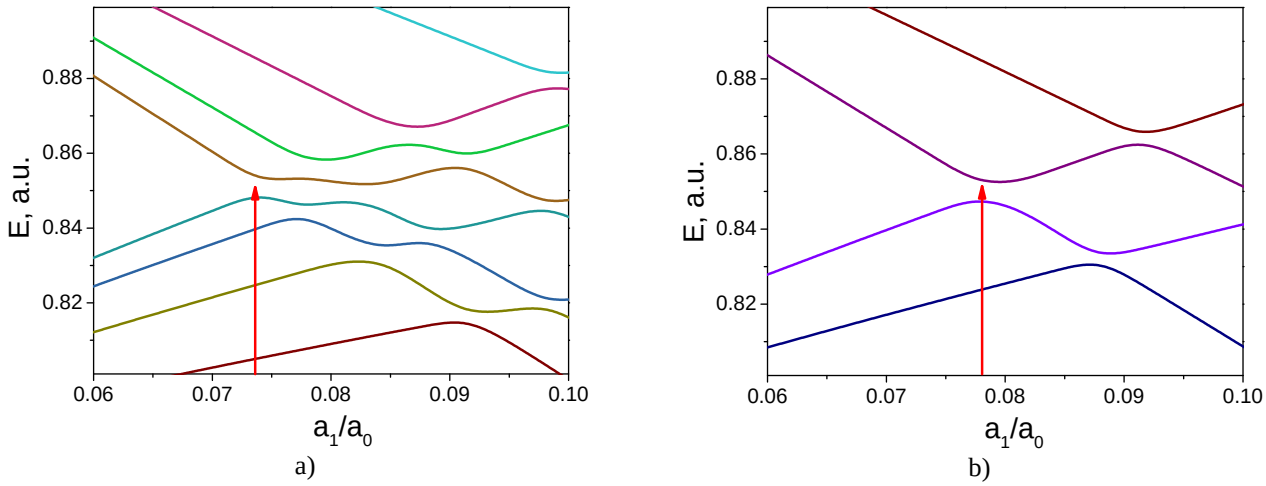


Fig. 3. Enlarged part of the energy spectrum for 12 (upper graph) and 7 (lower graph) atoms one-dimensional lattices as a function of interaction coefficients between atoms. Arrows indicate the position of the singularity with a minimum value a_1/a_0 for 12 (upper graph) and 7 (lower graph) atoms.

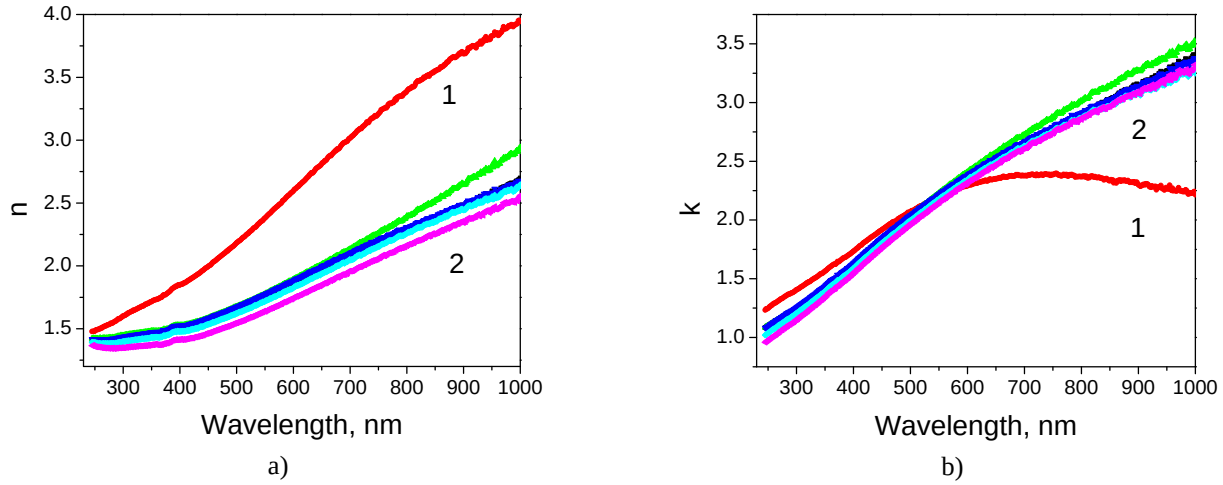
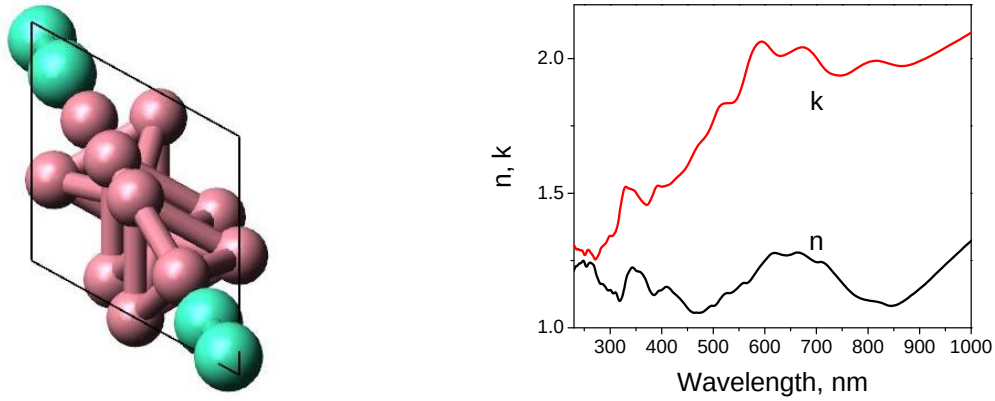


Fig. 4. Experimentally measured refractive index and absorption coefficient spectral curves for $Gd_{20}Co_{80}$ thin films with the thickness: 20 nm (*1*), 40 (*2*), 50 (*3*), 60 (*4*), 80 (*5*), 100 (*6*).

As one can see in Fig. 1a, this corresponds to a larger width of the forbidden energy gap between the lower edge of the upper system and the upper edge of the lower system of energy levels (small a_1/a_0 numbers). This leads to a lower concentration of free carriers in the conduction band, which is registered as dark spots in Fig. 2. As a consequence of our STM measurements, we can estimate the surface layer thickness of a few tens nanometers for $Gd_{20}Co_{80}$ alloy.

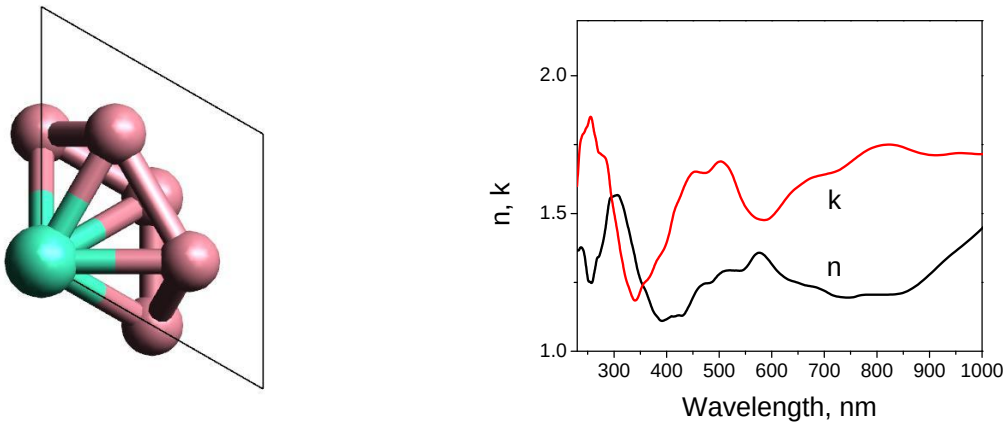
The results of spectral-ellipsometric measurements of $Gd_{20}Co_{80}$ samples with a different thickness are presented in Fig. 4. As one can see, the film with the thickness 20 nm exhibits a significant difference in the refractive indices and absorption, especially within the spectral range of intraband transitions at $\lambda > 600$ nm. The 20-nm thick film has insufficient quantity of atoms near its surface to form a completely developed energy band structure.

We present here the results of calculations of Gd-Co alloys optical properties by using the all-electron full potential linearized augmented planewave (LAPW) method implemented in optics subroutine of ABINIT software in LINUX operational system. The momentum matrix elements were evaluated in detail for the LAPW basis, and the interband as well as the intraband contributions to the dielectric tensor were taken into account. The LAPW method allowed evaluation of optical constants of supercells [15]. We calculated 9 components of dielectric tensor ε and calculated refractive indices $n+ik$ of spatial isotropic polycrystalline alloys as $\sqrt{Tr(\varepsilon)/3}$.



a) b)

Fig. 5. a) Crystal structure of the chemical compound Gd_2Co_7 (trigonal crystal system, $\bar{3}m$ point group). b) Calculated refractive index and absorption index spectral curves.



a) b)

Fig. 6. a) Crystal structure of the chemical compound $GdCo_5$ (hexagonal crystal system, 6/mmm point group). b) Calculated refractive index and absorption index spectral curves.

The results of quantum-mechanical numerical calculations of gadolinium-cobalt stable chemical compounds with smaller and larger relative values of the content of gadolinium atoms in the supercell in comparison with our sample $Gd_{20}Co_{80}$ are presented in Figs 5 and 6. Despite the differences in the shape of the curves, the values of refractive indices and absorption are approximately the same contrary to the results of spectral-ellipsometric measurements in Fig. 4 with drastically different optical constants for 20-nm thin film. This additionally verifies applicability of Shockley surface states model to analyze $Gd_{20}Co_{80}$ surface properties.

4. Conclusions

We have performed a theoretical and experimental study of the surface properties inherent to the $Gd_{20}Co_{80}$ alloy that consists of two phases with different crystal lattices. The theoretical approach is developed in this work for describing formation of energy bands by a small quantity of atoms that form some one-dimensional chain. The quantum-mechanical model of configurational interaction has been further developed for this case. The approach allowed us to obtain an approximate solution of the stationary Schrödinger equation in tridiagonal Toeplitz matrices formalism. The technique enabled to ascertain Shockley surface states in the forbidden energy gap and also to determine the surface layer thickness, which is responsible for formation of these states.

The energy band structure near $Gd_{20}Co_{80}$ alloy surface is not fully formed due to existence of a surface layer. Also the alloy consists of rare-earth element with less pronounced collective properties due to smaller values of the Hamiltonian matrix elements for neighboring atoms in the crystal lattice.

Shockley surface states can appear at cluster boundaries in the eutectic alloy and thus change the density of electronic states spectral curves. Spectral ellipsometry enables to evidently register the appearance of these states in the samples of $Gd_{20}Co_{80}$ alloys for a film with the

thickness 20 nm. Measurements by using atomic force microscopy and scanning tunneling microscopy identically confirmed the existence of the second phase in the $Gd_{20}Co_{80}$ alloy with cluster sizes of tens nanometers having a lower concentration of free carriers.

Numerical computer modeling of solutions of the Schrödinger equation allowed plotting the spectral dependences of optical coefficients for Gd-Co supercells with different specific contents of gadolinium and cobalt atoms, which allowed us to additionally verify the theoretical and experimental results obtained in this work.

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Authors and CV

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Поверхнева структура сплаву $Gd_{20}Co_{80}$

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Анотація. Сплав $Gd_{20}Co_{80}$ досліджено за допомогою експериментальних методик спектральної еліпсометрії, атомно-силової та скануючої тунельної мікроскопії. Результати експериментів показали наявність евтектичної двофазної структури сплаву. Кластери фази з меншим питомим вмістом мали меншу концентрацію вільних носіїв, що приводило до менших значень тунельних струмів при вимірюваннях. Для аналізу експериментальних даних був розвинутий формалізм у рамках квантово-механічної методики конфігураційної взаємодії із застосуванням формалізму тридіагональних матриць Тепліца. Даний теоретичний підхід дозволив у деталях описати перехідний процес формування енергетичних зон у твердому тілі з порівняно невеликою кількістю атомів, що в тому числі, як один із наслідків, включає описання поверхневих станів Шоклі та поверхневого шару твердого тіла з неповністю сформованими енергетичними зонами. Спектрально-еліпсометричні вимірювання плівок сплаву $Gd_{20}Co_{80}$ підтвердили значну відмінність виміряних оптичних констант для плівок товщиною 20 нм та більш товстих плівок. Квантово-механічні чисельні розрахунки оптичних констант різних надкомірок хімічних сполук Gd-Co підтвердили отримані експериментальні та теоретичні результати.

Ключові слова: сплав гадоліній-кобальт, поверхневі стани Шоклі, конфігураційна взаємодія.