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Interdiffusion in the formation of thin niobium films on single-crystal silicon under vacuum annealing conditions

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Abstract

For the design of technological process for creating device structures based on niobium and single-crystal silicon with the desired properties, empirical and theoretical knowledge about the solid-phase interaction process in the system of a thin niobium film is required. The purpose of the research was a comprehensive study of the redistribution of components during the formation of thin niobium films on single-crystal silicon obtained by magnetron-assisted sputtering followed by vacuum annealing.

The structure and phase composition were studied by X-ray phase analysis, scanning electron microscopy, and atomic force microscopy. Distribution of components along the depth was determined using the Rutherford backscattering spectrometry.

The traditional experimental method for studying the process of interdiffusion of components in binary macroscopic systems is the placing of inert marks. However, the use of this method in systems containing thin films is hindered by the comparable thicknesses of the films and marks. This circumstance makes the mathematical modelling the most convenient method for the analysis of the interdiffusion process in thin-film systems.

The interdiffusion model during the formation of polycrystalline niobium film – single-crystal silicon systems, developing the Darken's theory for the limited solubility components was proposed. Grain boundary diffusion of silicon in the intergrain space of a polycrystalline niobium film was proposed. Numerical analysis of the experimental distribution of concentrations within the model established that silicon is the dominant diffusant in the studied system. The temperature dependence of the individual diffusion coefficient of silicon D_{Si} = 3.0 10^{-12}exp(-0.216 eV/(kT)) cm^2/s in the temperature range 423–773 K was determined.

The model is applicable to the description of the redistribution of components in the thin niobium film – single-crystal silicon system prior to synthesis conditions providing the chemical interaction of the metal with silicon and the formation of silicides. It illustrates the mechanism of the possible formation of silicide phases not by layer-by-layer growth at the Nb/Si grain boundary, but in its vicinity due to deep mutual diffusion of the components.

Keywords: Reactive interdiffusion, Limited solubility, Thin films, Niobium, Single-crystal silicon, Magnetron-assisted sputtering, Vacuum annealing, Rutherford backscattering spectrometry, Simulation method, Darken's theory

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1. Introduction

Thin film niobium-silicon systems are widely used in superconductors [1–2]. The high radiation resistance of layered NbC-Si and Nb-Si systems in combination with their thermal stability make their application in X-ray optics promising [3, 4]. In the technology of integrated circuits, thin layers of niobium are used as a barrier between transition metals and single-crystal silicon or silicon dioxide [5].

A feature of the Nb-Si system is the slight solubility of silicon in niobium and niobium crystallites in single-crystal silicon. According to the Nb–Si binary phase diagram (Fig. 1), the maximum solubility of Si in bulk Nb samples is 3.5–4.36 at. %, and the solubility of niobium in silicon is negligible, Fig. 2 [6]

In two-layer systems Nb-Si and Si-Nb, obtained by vacuum sputtering on single-crystal Si (100), under conditions of insignificant solubility of Si and Nb in each other (the solubility limit of Si in the Nb solid solution phase from 0.6 to 1.7 at. % [8]), mutual diffusion between Nb and Si during annealing at 200°C leading to solid-phase amorphisation of the polycrystalline Nb layer and the formation of a mixed amorphous layer was demonstrated in [7]. Mutual diffusion of layers of materials during low-temperature annealing (100–250 °C) – is commonly observed phenomenon in metal – silicon systems [9, 10]. At these temperatures, grain boundary diffusion, usually, predominates in comparison with the diffusion of vacancies through the bulk. Mutual diffusion in the Nb-Si system during annealing T = 200 °C, the authors [7] explained by the diffusion of Si atoms into the Nb layer, which was due to the presence of grain boundaries in the polycrystalline Nb layer. Thermally activated interdiffusion in nanoscale thin film systems initiates several different temperature dependent

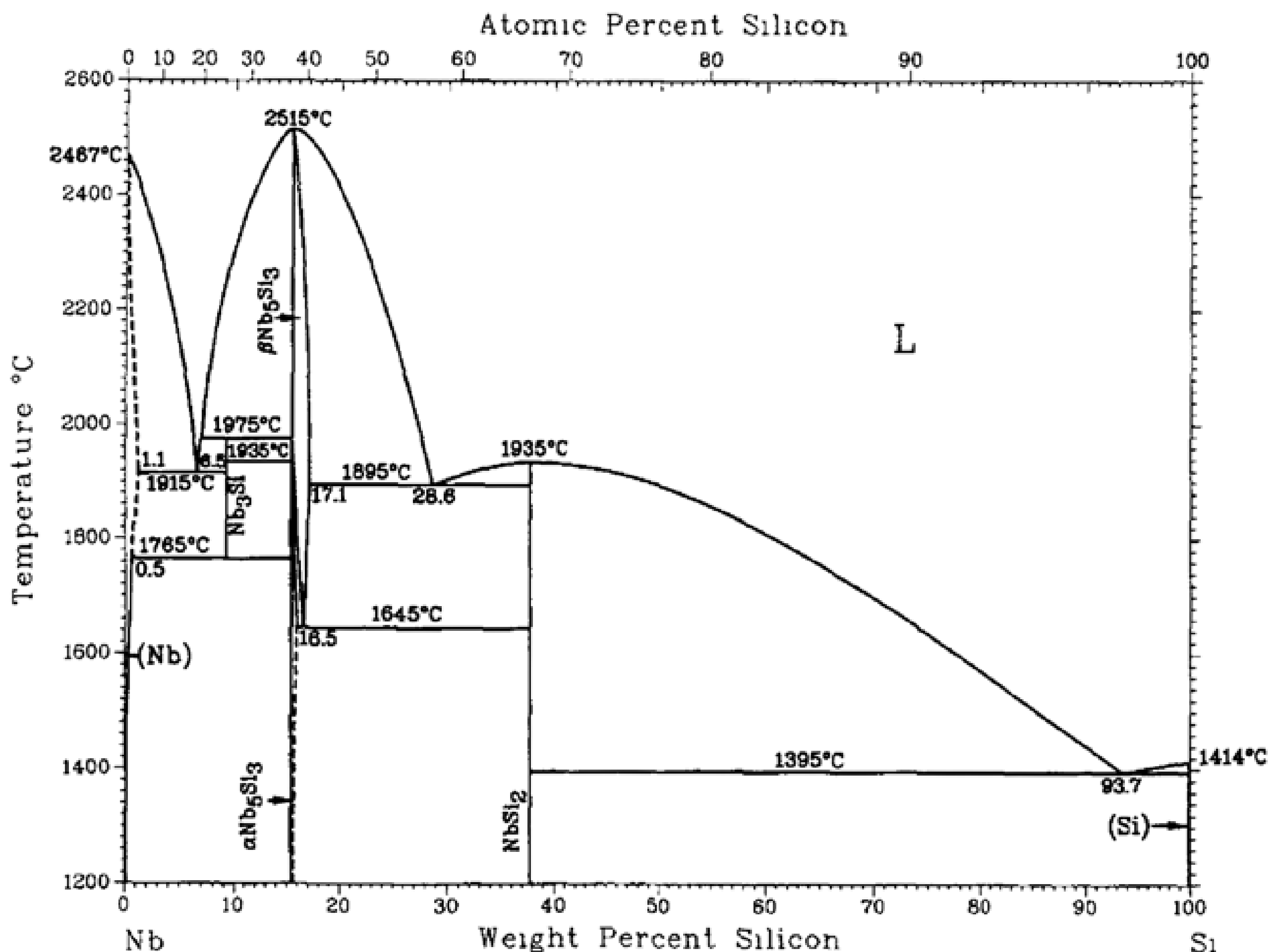


Fig. 1. Phase diagram of the niobium-silicon system [6]

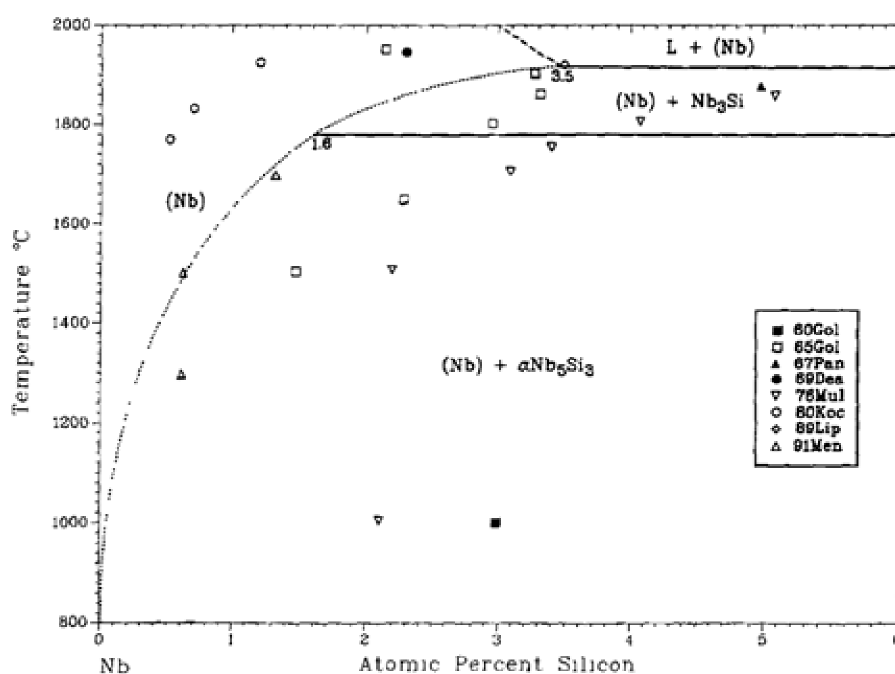


Fig. 2. The solubility of Si in Nb measured by different authors [6]

processes such as solid phase amorphisation, phase formation and crystallization.

Another feature of the Nb-Si system is that the metal film, both after deposition on single-crystal silicon and during subsequent annealing in an inert medium, has a polycrystalline character [7, 11].

According to modern concepts, the interaction of metal atoms with the silicon crystal lattice weakens the Si–Si covalent bonds and leads to the formation of free atoms in it [12]. Heat treatment can promote accelerated diffusion of mobile silicon along the grain boundaries of the metal under conditions of low solid solubility in its crystallites and the formation of solid solutions in a wide temperature range.

The process of mutual diffusion redistribution in the Nb-Si system suggests that the flow of silicon atoms into the niobium film is accompanied by an oppositely directed flow of niobium atoms into silicon. A significant difference in the intensity of these flows will lead to the displacement of the grain boundary in the diffusion pair (the Kirkendall effect) [13].

The question of the mechanisms of heterodiffusion of niobium in silicon and silicon in niobium, as well as of interdiffusion in the Nb–Si system, has not been sufficiently developed in the literature.

To design a technological process for creating device structures based on niobium and single-crystal silicon with the desired properties, empirical and theoretical knowledge about the solid-phase interaction process in the system of a thin niobium film is required. Insufficient discussion of these issues in the literature makes their comprehensive study an urgent and important task.

The purpose of this research was a comprehensive investigation into the redistribution of components during the formation of thin niobium films on single-crystal silicon under vacuum annealing conditions.

2. Experimental

Niobium films were deposited on single-crystal silicon wafers by magnetron-assisted sputtering. In the vacuum chamber, immediately before the sputtering process, a residual pressure level of $2.7\cdot10^{-3}$ Pa was reached using a diffusion pump. Then, an electric discharge was excited in high-purity argon at a pressure of $13.3\cdot10^{-2}$ Pa, discharge voltage of 430 V, and current strength of 0.7 A. The deposition rate of the niobium film was 0.67 nm/s, the sputtering time determined the thickness of the deposited films. A metal niobium target with an impurity content not higher than 0.01 at. % was used as the cathode material.

The synthesized samples were annealed using LG-220/1000 halogen lamps in a vacuum chamber at a residual pressure $R = 2.7 \cdot 10^{-3}$ Pa in the temperature range 423–773 K.

X-ray phase analysis of the thin Nb film – single-crystal Si system was carried out using an ARLX'TRA diffractometer (Switzerland). Studies were performed using radiation $K\alpha1$ emission line of copper (1.54056 Å) in automatic mode with a step displacement of 0.05°. The exposure time at each point was 1 s. The diffraction patterns were interpreted using the JCPDC database [14].

The surface relief of the films was studied by atomic force microscopy (AFM) using a Solver P47PRO microscope (Russia) in the semi-contact (intermittent-contact) scanning mode.

The microstructure and thickness of the films were studied on the sample cleavage using a JSM-6380 LV scanning electron microscope.

The concentration distributions of the components over the depth of the system were determined by the Rutherford backscattering spectrometry (RBS) on proton beams and singly charged helium ions – 4 of electrostatic generator EG-5 in the laboratory of neutron physics of the Joint Institute for Nuclear Research.

The traditional experimental method for studying the process of interdiffusion of components in binary macroscopic systems is the placing of inert marks [13]. However, the use of this method in systems containing thin films is hindered by the comparable thicknesses of the films and the marks. This circumstance makes the mathematical modelling the most convenient method for the analysis of the interdiffusion process in thin-film systems.

3. Experimental section

Micrographs of the cleavage of a thin Nb film – single-crystal Si system after deposition (a) and vacuum annealing at $T = 773$ K for 30 min (b) are shown in Fig. 3. The metal film thickness was 189 nm.

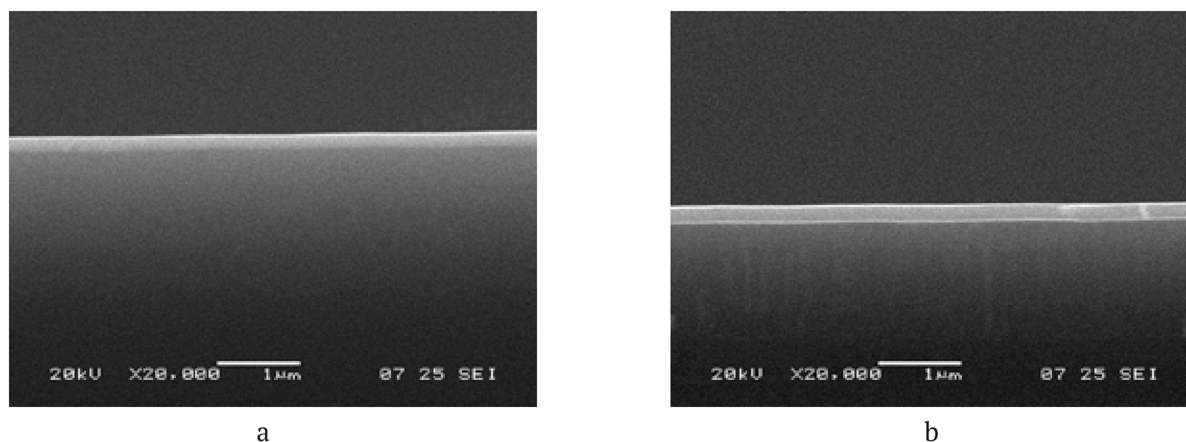
As can be seen from Fig. 3, after deposition at the niobium-silicon grain boundary, a thin transition layer was observed, and the thickness of the layer increased during subsequent vacuum annealing. Interdiffusion in the niobium-silicon system was also observed in [7].

X-ray diffraction pattern of a niobium film on single-crystal Si was shown after annealing at $T = 773$ K for 30 min is shown in Fig. 4 (the diffraction lines from the silicon wafer at $2\theta = 32.906°$ were cut off). The only phase detected in the film was cubic Nb: $2\theta = 37.14°$, $d = 2.41901$ Å (ICDD card no. 00-003-0905).

According to the Debye-Scherrer formula [15], the coherent scattering region (CSR) was estimated, and the CSR was 52 nm.

AFM images of the surface of the Nb film after vacuum annealing at $T = 773$ K are shown in Fig. 5. The film has a smooth surface with an average roughness of 0.18 nm. The distribution of heights on the histogram (Fig. 4d) allows for estimating the grain size ~ 32 nm with a height (Z) of from 0.4 to 2 nm. The phase contrast confirmed the absence of phases other than niobium (Fig. 4b).

The calculated CSR size according to the Scherrer equation (~ 52 nm), and the grain



a b

Fig. 3. Microphotographs of a thin Nb film – single-crystal Si system cleavage after deposition (a) and annealing in vacuum at a temperature at $T = 773$ K for 30 minutes (b)

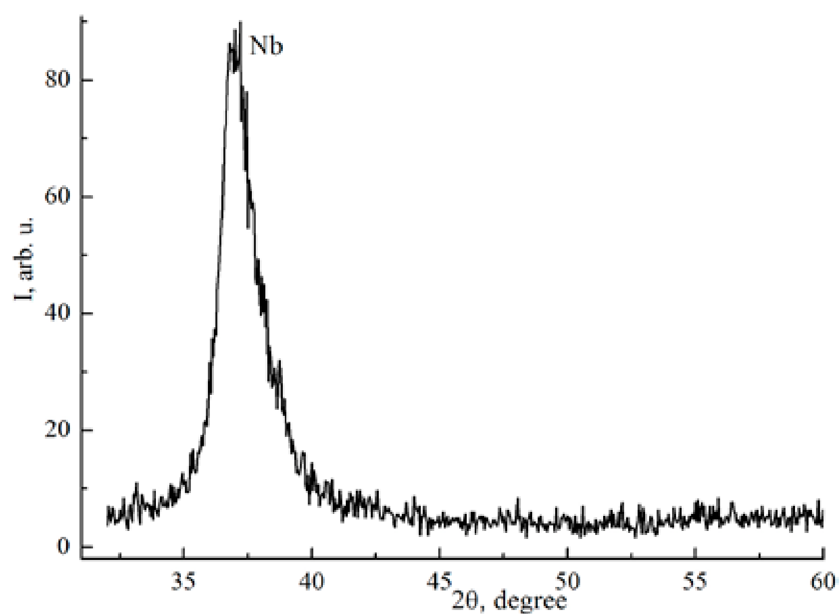


Fig. 4. X-ray diffraction pattern of thin Nb film – single-crystal Si system after annealing at T = 773 K for 30 min

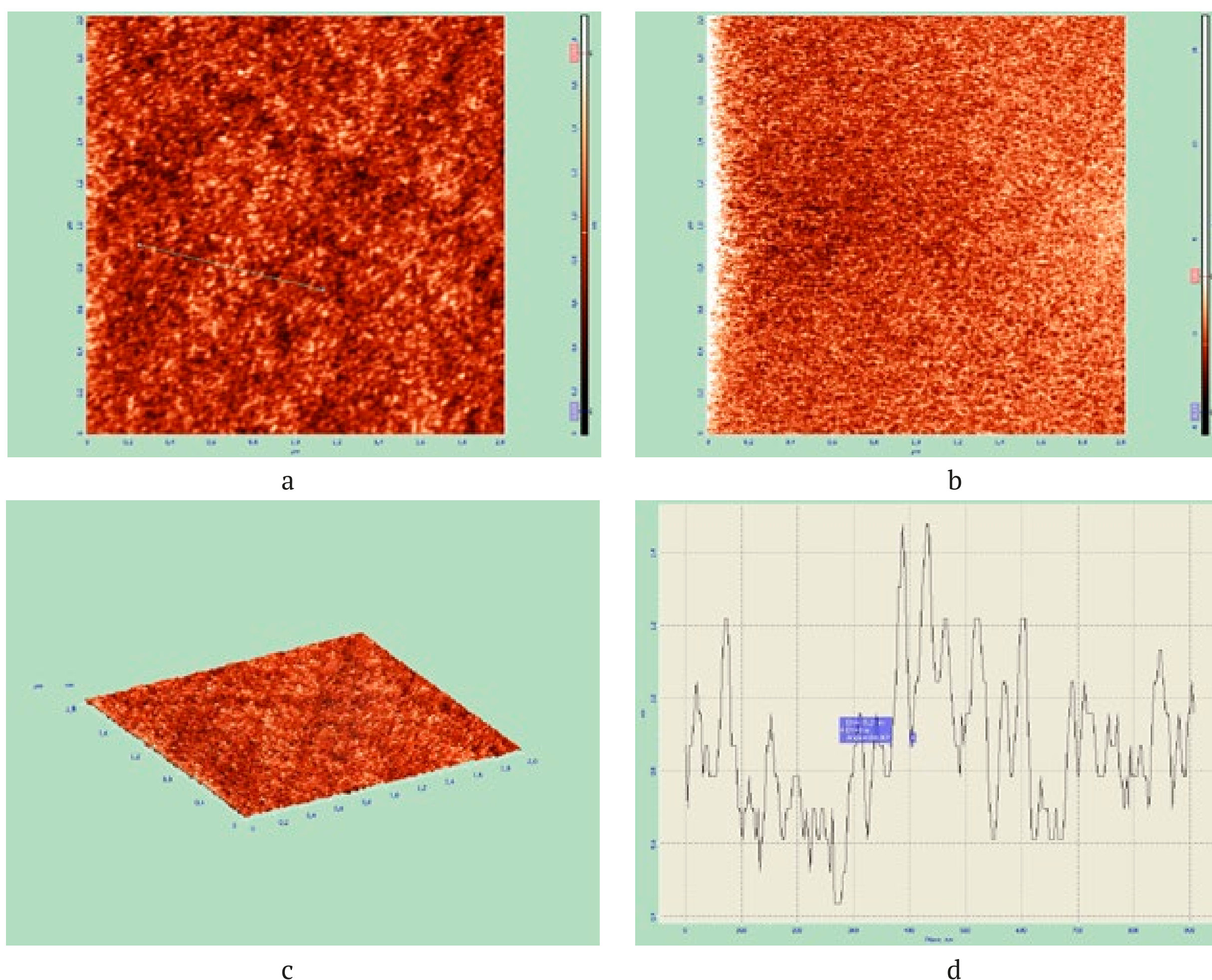


Fig. 5. AFM image of the surface of 2×2 μm films of thin Nb film – single-crystal Si system after annealing at T = 773 K for 30 min: film surface (a); phase contrast (b); 3-d image of the surface (c); surface relief section (d)

size obtained from AFM images of the surface (~ 35 nm) confirmed the nanoscale polycrystalline nature of the niobium metal film formed by magnetron-assisted sputtering followed by vacuum annealing.

The results of the analysis of samples by the RBS method are shown in Fig. 6. As can be seen from Fig. 6, in the obtained system, the Nb/Si MPB has the form of a boundary region transitional in concentration.

4. Description of the interdiffusion model in the Nb-single-crystal Si system

A qualitative nature of the process suggests that the interaction of niobium with the lattice of single-crystal silicon leads to its partial destruction. The mechanism of this destruction will be left outside the scope of the model. The consequence of this interaction is the appearance of free silicon atoms capable of migration. In the silicon lattice, they can migrate as interstitial atoms.

Silicon has low solubility in the bulk of niobium crystallites. This circumstance justifies ignoring the effect of diffusion penetration and dissolution of silicon in the bulk of niobium crystallites. However, the presence of developed grain boundaries makes the deep diffusion of silicon in a niobium film potentially possible and increases its solubility in the intergrain space.

The intergrain space of a polycrystalline niobium film contains coordinatively unsaturated bonds. Let us assume that they act as segregation trapping centres with respect to mobile silicon atoms, onto which silicon is captured with the release of free niobium. Thus, the dissolution of

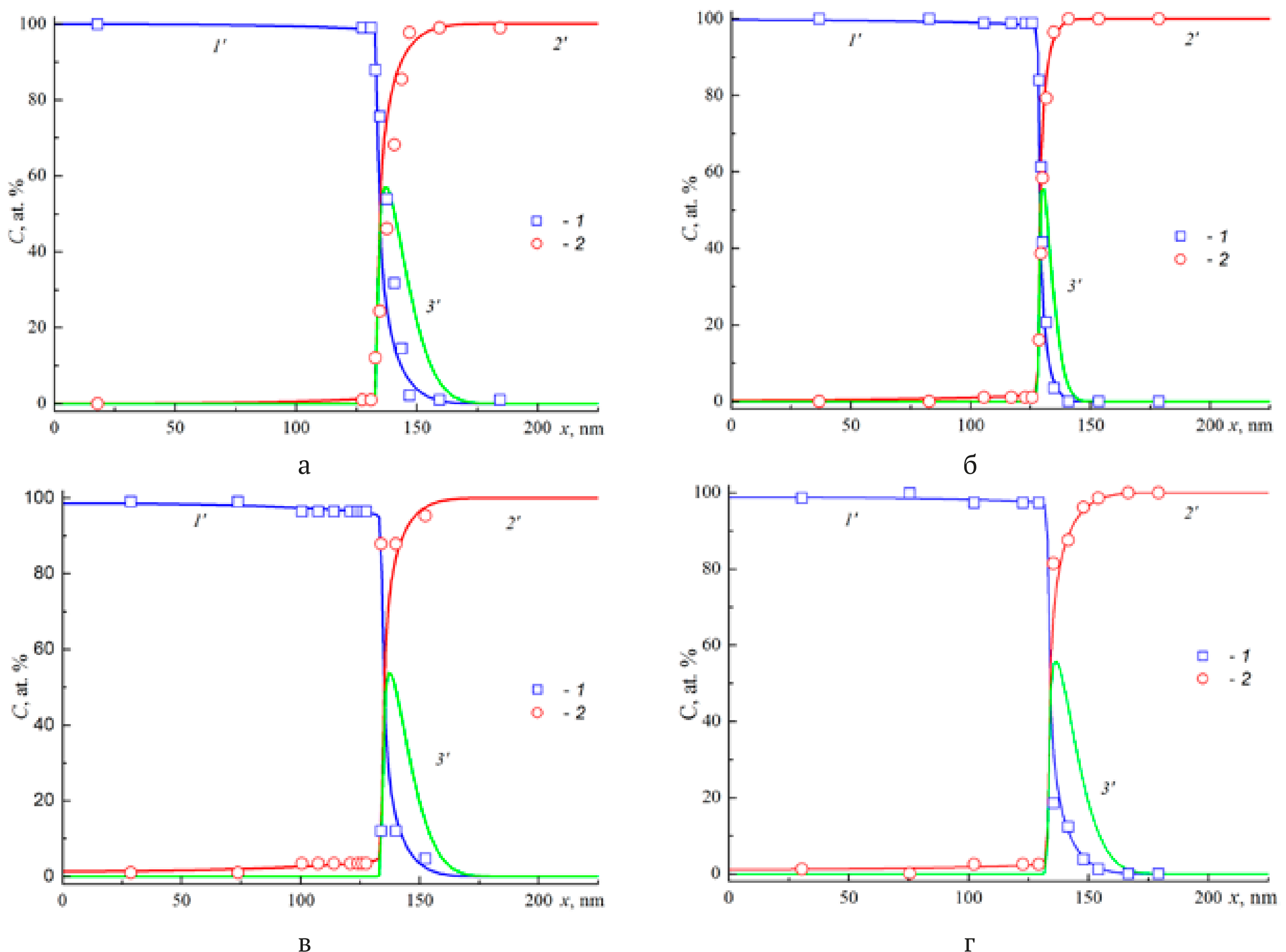


Fig. 6. Experimental (RBS method, symbols *1,2*) and calculated (curves *1'*, *2'*, *3'*) distribution over the depth of thin Nb film – single-crystal Si system of full concentration *C* of niobium (*1'*), silicon (*2'*) and its mobile part (*3'*). *1* — Nb, *2* — Si; curves: *1'*— Nb, *2'* — Si after magnetron-assisted sputtering and vacuum annealing in the T = 673 K, t = 30 min

silicon in a niobium film will be represented as the process of its reactive grain boundary diffusion in the intergrain space.

The stage of segregation capture of silicon on intergrain traps is initially carried out according to the physical sorption mechanism and is not accompanied by chemical interaction with the formation of silicides. It occurs in the volume of the metal film, has a topochemical character, and is localized in its intergrain space. The high defectiveness of the intergrain space of the film contains a sufficient free volume, which ensures the exchange sorption process with minimal energy loss for bond deformation.

The process of formation of a silicon solid solution in a niobium film will be limited by the concentration of traps, which is the fraction r from the total metal concentration.

With regard to niobium, we will assume that its diffusion and solubility as an impurity in single-crystal silicon is limited by the decomposition process of a solid niobium solution in silicon with the formation of immobile multiparticle complexes containing silicon point defects and metal atoms.

A mathematical model that describes the process of interdiffusion in a binary system with unlimited solubility of components was proposed in [16]. It assumes the invariance of the molar volume of the system and the absence of changes in its composition as a result of chemical transformations. The theory [16] suggests obtaining the distribution of concentrations of components as a solution to a boundary value problem containing two diffusion equations with one effective interdiffusion coefficient.

In [17], the model [16] was applied to the analysis of phase formation in the diffusion zone. In [18], the model [16] was developed for the description of bulk reactions of silicide formation in the Ni – SiC. In [19], the mathematical form [16] was used in a quantitative model that developed the model [16] for reactive interdiffusion in metal – second metal oxide two-layer systems with limited component solubility. In [20], it was developed for the case of reactive interdiffusion of components under vacuum annealing conditions for polycrystalline nonstoichiometric film oxide systems with limited solubility. In [21], the possibility of using the mathematical form of the model [16] for the description of the interdiffusion process in the thin polycrystalline metal film – single-crystal silicon system under conditions of limited solubility of components was demonstrated.

In our case, the qualitative nature of the solid-phase interaction in the thin Nb film – single-crystal Si system during vacuum annealing also assumes a constant molar volume. Therefore, we use the mathematical formalism of the theory [17] for the description of the reactionary interdiffusion process in it. Diffusion-reaction equations for the components of a thin Nb film – single-crystal Si system were as follows:

$$\frac{\partial C_{\mathrm{A}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{A}}}{\partial x} \right) - k_1 \cdot C_{\mathrm{C}} \cdot C_{\mathrm{A}}, \quad (1)$$

$$\frac{\partial C_{\mathrm{B}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{B}}}{\partial x} \right) + k_1 \cdot C_{\mathrm{A}} \cdot C_{\mathrm{C}} - k_2 \cdot C_{\mathrm{Ct}} \cdot C_{\mathrm{B}} - k_3 \cdot C_{\mathrm{B}} \cdot C_{\mathrm{C}}, \quad (2)$$

$$\frac{\partial C_{\mathrm{Bt}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{Bt}}}{\partial x} \right) + k_2 \cdot C_{\mathrm{Ct}} \cdot C_{\mathrm{B}}, \quad (3)$$

$$\frac{\partial C_{\mathrm{Ct}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{Ct}}}{\partial x} \right) - k_2 \cdot C_{\mathrm{B}} \cdot C_{\mathrm{Ct}}, \quad (4)$$

$$\frac{\partial C_{\mathrm{Cp}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{Cp}}}{\partial x} \right) + k_3 \cdot C_{\mathrm{B}} \cdot C_{\mathrm{C}}, \quad (5)$$

$$\frac{\partial C_{\mathrm{C}}}{\partial t} = \frac{\partial}{\partial x}\left(D^{*} \frac{\partial C_{\mathrm{C}}}{\partial x} \right) + k_2 \cdot C_{\mathrm{Ct}} \cdot C_{\mathrm{B}} - k_3 \cdot C_{\mathrm{B}} \cdot C_{\mathrm{C}}, \quad (6)$$

where t is time, x is the depth measured from the outer surface of the niobium film; C_{A}, C_{B}, C_{bt}, C_{Ct}, C_{cp}, C_{C} is the concentration of silicon (A) at the sites of the crystal lattice of silicon, mobile silicon (B), formed as a result of the interaction of niobium with silicon; silicon (Bt) trapped in the intergrain space of the niobium film; free trap centres (C_{t}) for mobile silicon in the intergrain space of the niobium film; immobile complexes (C_{p}) in silicon containing niobium and silicon atom; and mobile niobium (C), respectively.

k_1, k_2 and k_3 – are the rate constants for the generation of free silicon B, its capture by intergrain traps in niobium, and the formation of niobium-silicon complexes $\mathrm{C_p}$ respectively.

For the effective interdiffusion coefficient, the ratio was used:

$$D^* = \frac{D_B \cdot C_C + D_C \cdot C_B}{C_{tot}}, \quad (7)$$

where D_B and D_C – individual diffusion coefficients of mobile components – of free silicon B and niobium C, respectively, $C_{tot} = C_A + C_B + C_C + C_{Cp} + C_{Bt} + C_{Ct}$ – total concentration of all components of the system.

In the case when the values of the individual diffusion coefficients of the mobile components of the system differ significantly from each other, the Nb/Si grain boundary in the selected reference system will move, while the stationary components of the system will serve as inert markers in the Smigelskas and Kirkendall experiment [22].

As a boundary condition for all components of the system, the reflection condition was assumed:

$$\frac{\partial C_A}{\partial x} = \frac{\partial C_B}{\partial x} = \frac{\partial C_C}{\partial x} = \frac{\partial C_{Cp}}{\partial x} = \frac{\partial C_{Bt}}{\partial x} = \frac{\partial C_{Ct}}{\partial x} = 0 \quad (8)$$

at $x = 0$ and $x = L$

where L is the thickness of the solution region in silicon.

The following conditions were used as initial conditions:

$$C_A(x,0) = 0,\ C_{Ct}(x,0) = r \cdot N_{SC},\ C_C(x,0) = (1 - r) \cdot N_{SC}, \text{ at } 0 \leqslant x \leqslant h, \quad (9)$$

$$C_A(x,0) = N_{SA},\ C_{Ct}(x,0) = 0,\ C_C(x,0) = 0, \text{ at } h < x \leqslant L, \quad (10)$$

$$C_B(x,0) = 0,\ C_{Bt}(x,0) = 0,\ C_{Cp}(x,0) = 0 \text{ for all } 0 \leqslant x \leqslant L, \quad (11)$$

where h is the thickness of the niobium film, $N_{SA} = 4.98 \cdot 10^{22}$ cm^{-3} is the intrinsic concentration of Si atoms, $N_{SC} = 5.55 \cdot 10^{22}$ cm^{-3} is the intrinsic concentration of niobium atoms, r is the fraction of traps for silicon atoms in the intergrain space of the niobium film.

For the numerical solution of the system of diffusion-reaction equations (1)–(6) with a concentration-dependent effective interdiffusion coefficient (7), implicit conservative difference schemes and the factorization method were used [23].

The model parameters were: individual diffusion coefficients of silicon and niobium, rate constants k_1, k_2, k_3, and r.

The results of numerical simulation (curves *1′, 2′*) in comparison with the experimental distribution of concentrations of Nb and Si obtained by the RBS method over the depth of thin Nb film – single-crystal Si system (points *1, 2*) after magnetron-assisted sputtering of Nb onto single-crystal silicon and vacuum annealing during isochronous annealing at t = 30 min in temperature range T = 423–673 K are shown in Fig. 6a–c.

The experimental and calculated distributions were in good agreement for identical values $k_1 = 1 \cdot 10^{-25}$ cm^3/s, $k_2 = 1 \cdot 10^{-20}$ cm^3/s, $k_3 = 1 \cdot 10^{-19}$ cm^3/s, r = 0.028. The individual diffusion coefficient of niobium in the studied system under experimental conditions was $D_{Nb} = 4.0 \cdot 10^{-16}$ cm^2/s, and for silicon, the temperature dependence was determined (Fig. 7):

$$D_{Si} = 3.0 \cdot 10^{-12} \cdot \exp(-0.216 \text{ эВ}/(kT)) \text{ cm}^2/\text{s}. \quad (12)$$

In [24], for the study of the interdiffusion of amorphous Si–Nb multilayers during annealing in the temperature range of 423–523 K obtained by ion-beam sputtering with a repeating film thickness of 3.2 nm, the interdiffusion coefficient was determined $D^* = 2.2 \cdot 10^{-18} \exp(-0.55 \text{ eV}/(kT))$ cm^2/s. The authors explain the low value of the pre-exponential factor by the high concentration of traps in amorphous silicon [24].

As can be seen from the obtained data, the dominant diffusant in the studied system is mobile silicon (curves *3′* in Fig. 6a–d). The maximum of its distribution is localized on the Nb/Si interface.

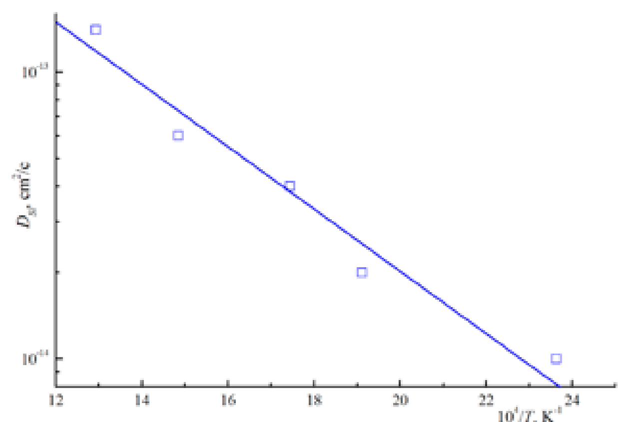


Fig. 7. Temperature dependence of the individual diffusion coefficient of silicon in thin Nb film – single-crystal Si system. Dots are the results of numerical analysis; curve was obtained by approximation using the Arrhenius equation (12)

4. Conclusions

Thin films of niobium obtained on single-crystal silicon by magnetron-assisted sputtering followed by vacuum annealing were polycrystalline with a grain size ~ of 32 nm. The Nb/Si grain boundary has the form of a transition region in terms of concentration, indicating the mutual diffusion of the components in the polycrystalline niobium film – single-crystal silicon system. This process was studied by the simulation method. A model that takes into account the limited solubility of the components was developed. The model describes the solubility of silicon in the intergrain space of niobium with its segregation on intergrain traps, as well as the solubility of the metal in silicon, limited by the complexation process. It is applicable to the description of the redistribution of components up to synthesis conditions, providing the chemical interaction of niobium with silicon and the formation of silicides.

Numerical analysis of the experimental distribution of concentrations of the components in Nb film – single-crystal Si system within the framework of the model established that silicon is the dominant diffusant in the studied diffusion pair. The values of the individual diffusion coefficients of niobium and silicon in the temperature range 423–773 K, as well as the fraction of traps for Si atoms in the intergrain space of Nb, were determined.

Contribution of the authors

The authors contributed equally to this article.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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