INFRARED STUDY OF THERMALLY INDUCED PHASE SEPARATION IN SiO_x FILMS

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Thin SiO_x films ($x \approx 1.3$) obtained by thermal vacuum evaporation of silicon monoxide are studied. Thermally induced (annealing temperatures of 700 and 1000°C) structural transformations of the Si—O phase in SiO_x layers, which lead to the formation of amorphous or crystalline nanoinclusions, are investigated by IR-spectroscopy with the analysis of a shape of the Si—O absorption band. It is demonstrated that the thermal treatment induces the decomposition of molecular complexes of slightly oxidized Si and the formation of both Si clusters and molecular clusters containing heavily oxidized Si. The transformations of the oxide phase are almost completed after initial 5 minutes of thermal treatment. The films annealed at 700 °C contain mainly amorphous Si nanoclusters embedded in the homogeneous $SiO_{1.75}$ matrix (the volume share of the amorphous Si phase is ~ 17 %). The films annealed at 1000 °C can be represented in the form of Si nanocrystals (the volume share is ~ 20 %) surrounded by thin intermediate layers of SiO_x and embedded in SiO_2.

1. Introduction

Crystalline Si is the basic material of contemporary microelectronics. However, its application in optoelectronics is hampered due to the weak light emission in the visible spectral range caused by a non-direct band structure. Intense investigations of Si-based light emitting materials stimulated by the observation of a visible photoluminescence from porous silicon at room temperature [1], have begun in 1990th. Apart from the porous silicon, other structures with nanocrystalline Si inclusions have been developed and investigated. In particular, the composites containing Si nanoinclusions in SiO_2 (or SiO_x) matrix attract the attention of a great number of scientists as possible materials for the light-emitting Si-based structures. The advantages of Si—SiO_2 composites, as compared to porous silicon, are their mechanical and chemical stability, as well as the complete compatibility with the contemporary Si planar technology. The possibility of a practical application of such structures for light-emitting diodes, lasers, and optical amplifiers has already been demonstrated.

The process of formation of such structures usually consists of two stages. First, a layer of SiO_x is formed by various technologies, such as thermal evaporation of silicon monoxide (SiO) [2—5], implantation of Si atoms in SiO_2 layers [6, 7], CVD process [8], or co-evaporation of Si and SiO_2 [9]. At this, thermal evaporation of silicon monoxide (SiO) deserves a particular attention due to its simplicity and the possibility to obtain high-quality and homogeneous SiO_x films of variable composition. At the second stage, SiO_x layers are annealed, which results in the formation of Si clusters of nanometer sizes. The annealing temperature determines the structure of inclusions. The annealing of SiO_x layers at temperatures of 500—900 °C leads to the coagulation of Si atoms in amorphous clusters (na-Si). At the annealing temperatures above 900 °C, the amorphous Si inclusions crystallize in nanocrystals (nc-Si) with a modified electron structure due to the quantum confinement [4, 5].

In principle, the formation of Si nanoinclusions is in a good agreement with the known phenomenon of a phase separation of the SiO_x matrix into the silicon and silicon dioxide phases, which has place at elevated temperatures [10, 11]. Just because of this, the investigation of thermally induced structural and phase transformations in non-stoichiometric silicon oxides is of great

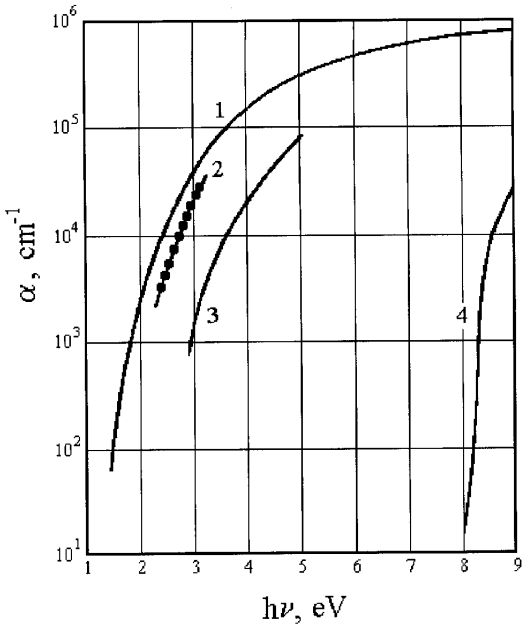

Fig. 1. Spectral dependences of the absorption coefficient for SiO films (*1*), initial SiO_x film (*2*), $SiO_{1.5}$ film(*3*), and SiO_2 film (*4*). Dependences *1*, *3*, and *4* are taken from [14]

importance for the understanding of the mechanisms of formation of Si nanoinclusions in the oxide matrix. The annealing-induced changes of the characteristics of SiO_x layers obtained by vacuum evaporation have been investigated in detail in [12, 13]. In this case, the main attention was paid to the investigation of the properties of Si nanoinclusions [3, 4]. At the same time, the analysis of thermally induced changes of the structure and phase composition of Si—O has to give the basic information on a physical mechanism of the formation of such inclusions. The purpose of this work is thus to thoroughly investigate the changes of a structural and phase state of the silicon-oxygen phase in SiO_x films due to the high-temperature thermal treatment in an inert atmosphere. IR-spectroscopy and the analysis of the shape of a band of absorption by Si—O bonds are used for the characterization of these changes.

2. Experimental Method

SiO_x layers were prepared by a thermal evaporation of SiO powder (Cerac Inc., the purity of 99.9 %) in vacuum at a residual gas pressure of 2×10^{-3} Pa. Two-side polished plates of silicon and fused silica were used as substrates. The temperature of the substrate was equal to 150 °C during all the deposition process. The deposition rate was 1.6 nm/s. The film thickness, d, was controlled *in situ* by the quartz oscillator method and was measured by an interferometer MII-4 after the deposition. It was equal to 340 nm for the studied films. The samples were annealed at 700 or 1000 °C in the argon atmosphere during 5—30 min to obtain both amorphous and crystalline nanoinclusions in the oxide matrix [4].

IR transmission spectra were measured in the range of 800—1400 cm^{-1}, using an automatic spectrometer IKS-25M. The Si substrate without oxide film was used as a reference sample. The main absorption band of SiO_x in this range (the maximum position was at 1000—1100 cm^1) is related to the asymmetric valent oscilations of bridge oxygen atoms. This band was decomposed into Gaussian-like profiles, whose key characteristics (the position and intensity of peaks) were analyzed in the framework of the random-binding model [14]. The aim of the analysis was to determine the concentration of $Si—O_y—Si_{4-y}$ ($1 \le y \le 4$) molecular complexes in the structural network of the SiO_x matrix according to the approach proposed earlier in [15]. The decomposition precision was characterized by a standard deviation of the sum of Gaussians from the experimental curve. This deviation did not exceed 10^{-2} in our experiments.

The transmission and reflection spectra in the visible and near ultraviolet regions were also measured and recorded by a spectrophotometer KSVU-23 at room temperature under the normal beam incidence.

3. Results and Discussion

In Fig. 1, the dependences of the absorption coefficient, α, on the energy of light quanta for SiO films (*1*), initial SiO_x film under investigation (*2*), $SiO_{1.5}$ film (*3*), and SiO_2 film (*4*) are shown. Curves *1*, *3*, and *4* were taken from [14], and curve (*2*) was calculated basing on the results of measurements of transmission and reflection spectra in the visible and near ultraviolet regions.

As is known, the edge of the optical absorption of homogeneous SiO_x films shifts monotonously from the near infra-red (for silicon) to the ultraviolet (SiO_2) region with the growth of x. The value of x can be estimated (according to the approach proposed in [14]), using a theoretical or experimental dependence of $E_{04}(x)$ [16], with $E_{04}(x)$ being the energy at which the absorption coefficient is equal to 10^4 cm^{-1}. Analyzing the measured absorption spectra, we have obtained $x = 1.32 \pm 0.03$ for our freshly deposited samples.

In Fig. 2, the IR transmission spectra of initial SiO_x films (*1*) and SiO_x films annealed at 700 °C (*2*) and 1000 °C (*3*), respectively, are shown. As can

be seen, the main absorption band of annealed oxides shifts considerably to higher frequencies (the maximum positions are at 1022, 1065, and 1075 cm^{-1} for the initial sample and the samples annealed at 700 and 1000 °C, respectively), and its shape essentially changes. However, the position and shape of the absorption band did not depend on the annealing duration. The increase of the annealing time from 5 to 30 min did not lead to a change of the behavior of absorption spectra both at 700 °C and 1000 °C. This result shows that the process of transformation of the oxide phase takes place at the initial stage of thermal annealing (at least during initial 5 min), which is in good accordance with the data on the formation of nanocrystalline Si inclusions in SiO_2 films implanted with silicon [7, 17].

A shift of the maximum position of the valence mode of Si—O—Si (ν_M) is usually ascribed to a change of the phase composition of the oxide film [10, 12]. Moreover, one may estimate the composition of the oxide, by comparing the ν_M value with the known experimental dependences of $\nu_M(x)$ for the oxides grown by the same technology [12, 18]. Such an estimation has shown that, for the SiO_x films under investigation, the x value was equal to 1.25, 1.75, and 1.91 before and after the thermal treatments at 700 and 1000 °C, respectively. The phenomenological linear dependence of ν_M on the stoichiometry index of the silicon-oxide phase is also known [19]:

$$\nu_M \approx (48.8x + 987)\ cm^{-1}.$$

Using this relation, we have obtained almost the same values of x for our samples: 1.28, 1.81, and 1.94, respectively.

The value of x for the initial sample obtained by IR measurements (1.25 — 1.28) is slightly lower than that obtained from the optical absorption edge position ($\sim$ 1.32). These values of x for freshly deposited films mean that SiO clusters are partly oxidized during the thermal deposition due to the presence of oxygen in the residual gases. A further change of the phase composition of the film during the thermal treatment in an inert atmosphere occurs due to the partial separation of SiO_x into the mixture of Si and SiO_2 or SiO_y ($y > x$) phases [4, 10]. This leads to an increase of the effective value of the stoichiometry index.

It should be emphasized that, although the degree of structural transformations does not depend on the time of annealing, it is determined by the annealing temperature. At higher temperatures, the bulk fraction of precipitated silicon is higher, and the matrix composition approaches that of the SiO_2 phase.

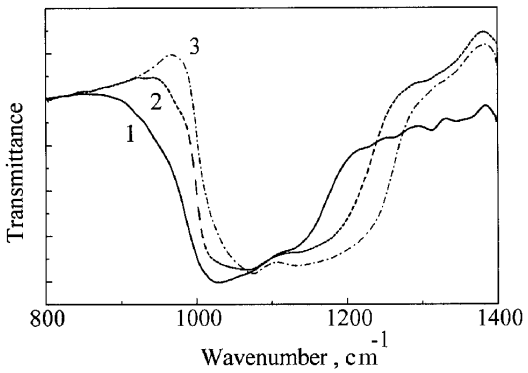

Fig. 2. IR transmission spectra of SiO_x films: freshly deposited (*1*), annealed at 700 °C (*2*), and annealed at 1000 °C (*3*)

However, even for the samples annealed at 1000 °C, the value of x remains smaller than 2. This means that the oxide separation can be described by the following equation:

$$ySiO_x \rightarrow (y - x)Si + xSiO_y\ (y > x),$$

where SiO_y consists, probably, of SiO_2 and SiO_x. Freshly deposited films are quite homogeneous, and the Raman experiments did not show any regions of a-Si or c-Si [3, 4]. Quite the contrary, the microstructure of annealed films can be described as amorphous (700 °C) or crystalline (1000 °C) Si clusters incorporated into the SiO_y matrix [4]. Using the known molecular masses and densities of the components formed and taking into account the coefficients in the reaction equation, one may easily find the volume fractions, v_{Si}, of the separated Si phase: v_{Si} = 17 % by volume for the amorphous nanoinclusions, and v_{Si} = 20 % by volume for the nanocrystalline inclusions in the $Si_{1.91}$ matrix.

The analysis of a shape of the main band of IR absorption can provide with a more detailed information on the thermally induced phase transformation of oxide. For the homogeneous SiO_x phase, such an analysis was made before [15], which did not contradict to the statistics within the random-binding model. This approach was used in this work for the freshly deposited samples. However, the mathematical decomposition of the absorption band into Gaussian profiles is a rather problematic task in the case of annealed films. The phase separation at elevated temperatures can, in principle, lead to the formation of a mixture of SiO_2 and SiO_x with different values of x. Hence, the analysis of a shape of the main absorption band of annealed films should be carried out using the known data for the SiO_2 and SiO_x phases [15, 20] in three cases: (1) a homogeneous SiO_x phase; (2) a homogeneous SiO_2 phase; (3) a mixture of

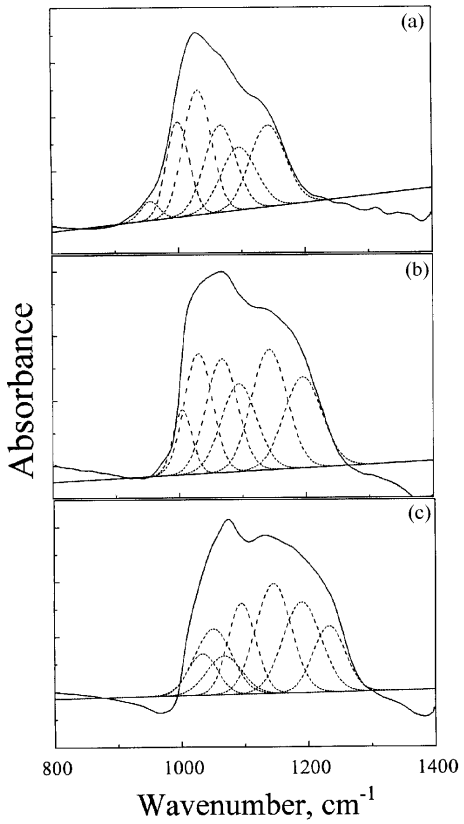

Fig. 3. Examples of the mathematical decomposition of the bands of the optical density of oxide films into the Gaussian components: a — initial sample, b — sample annealed at 700 °C during 30 min, and c — sample annealed at 1000 °C during 30 min

SiO_x and SiO_2 phases. It is worth mentioning that the absorption band of the films annealed at 700 °C cannot be described mathematically by a sum of Gaussians typical of the SiO_2 phase. Thus, these films consist of the SiO_x phase or the mixture of SiO_x and SiO_2 phases. As distinct from this, the absorption band of the films annealed at 1000 °C can be described by a sum of elementary Gaussian components typical of the SiO_2 and SiO_x phases, as well as their mixture, with practically the same precission. So, the question on the structure of these films remains open. For the following analysis of the structure and composition of annealed oxides, we treated the samples in a 5% HF solution. Such a solution etches the SiO_2 phase, but does not etch SiO_x. The oxide film annealed at 700 °C remained unchanged after etching during 10 min, in contrast to the film annealed at 1000 °C, whose etching rate was 20 nm/min. At the same time, the reference film of thermally grown SiO_2 was etched with the rate of 50 nm/min. This experiment allowed us to conclude that the oxide phase in the films annealed at 700 °C can be presented, most likely, as the homogeneous SiO_x with x greater than that for freshly deposited samples.

The oxide phase for the samples annealed at 1000 °C consists of the SiO_2 or the mixture of SiO_x and SiO_2. Taking into account that these samples contain Si nanocrystals and that a transient layer of non-stoichiometric oxide must exist between the oxide phase and the Si inclusions [21], one may finally conclude that, after the treatment at 1000 °C, the oxide phase is, most probably, the SiO_2 with SiO_x inclusions surrounding the Si nanocrystals. The presence of such inclusions should decrease the etching rate in hydrofluoric acid, comparing to that of the pure SiO_2 phase in thermally grown silicon dioxide.

Taking into account the remarks presented above, we have carried out the ultimate decomposition of the absorption bands into Gaussian-like profiles (Fig. 3). The parameters of the obtained elementary components are presented in the table.

One may see that the main absorption band of oxide is mainly represented by the sum of eight profiles related to the valence oscillations of the bridge oxygen atoms [15, 22, 23]. The transverse and longitudional oscillations are related to the bands 1—5 and 6—8 (see the Table), respectively [15, 23, 24]. A weak band with a maximum at 955 cm^{-1} related to the SiOH complexes [25] is not shown in the table. This band is observed only in the spectrum of a freshly deposited film, and its contribution to the total area of absorption bands is equal to 2.7 %. The ratio of the LO and TO modes (the ratio of the total area of LO bands to the area of TO bands) increases from 0.28 for freshly deposited films up to 0.64 and 1.04 for the films annealed at 700 and 1000 °C, respectively. Thus, it can be seen that the thermal treatment of SiO_x layers leads to an essential redistribution of the intensities of elementary bands and influences the ratio of the TO and LO modes. The temperature seems to be the determining factor in the processes under consideration.

The contributions of the TO and LO modes to the IR absorption are not equivalent. While the intensities of the transverse bands are mainly related to the concentration of the bridge oxygen in the respective structural units [according to the random-binding model, in molecular complexes Si—O_y—Si_{4-y} ($1 \leq y \leq 4$)], the intensities of the bands related to the longitudional mode depend strongly on the polarization of the matrix (i.e., on the value of x), the homogeneity of oxide, and the experimental conditions [26—28]. Thus, the transverse mode seems more acceptable for the analysis of the

structural transformations in SiO_x films. The content of molecular complexes of each kind in the oxide network can be estimated from the contribution of the respective component to the total area of the TO mode (these values are shown in three last columns of the table). It can be seen that the contribution of the band related to the $SiOSi_3$ complexes decreases considerably after the annealing at 700 °C and completely disappears after the treatment at 1000 °C. In contrast to this, the portion of the oscillations related to the bridge oxygen atoms in SiO_4 complexes increases with temperature. After the annealing at 1000 °C, the relative area of the bands related to SiO_4 tetrahedra increases by 3 times comparing to that of freshly deposited films. The contribution of the band related to SiO_2Si_2 complexes in the films annealed at 700 °C remains almost unchanged, but the relative area of the bands related to SiO_3Si and SiO_4 clusters increases. These facts show that the thermal treatment of SiO_x layers leads to the decomposition of the molecular complexes of weakly oxidized silicon and to the formation of both Si clusters and the clusters containing strongly oxidized silicon (Fig. 4).

It is natural to accept the the contributions of SiO_2Si_2 and SiO_3Si complexes decrease considerably after the thermal treatment at 1000 °C. Really, for the formation of SiO_4 tetrahedra, the Si atoms which leave $SiOSi_3$ complexes must interact with other Si—O elements. Only SiO_2Si_2 and SiO_3Si clusters can be such elements. Some of these clusters which stay in the oxide matrix belong, most likely, to the interface SiO_x layers between the Si nanocrystals and the SiO_2 phase. We can estimate the volume fraction of this interface phase for the samples annealed at 1000 °C. According to [21], the thicknesses of Si-enriched interface suboxide layers are 0.4—0.6 nm. Assuming that the mean diameter of spherical Si nanocrystals is 3 nm and using the v_{Si} value, we can obtain the volume fraction of the SiO_x phase:

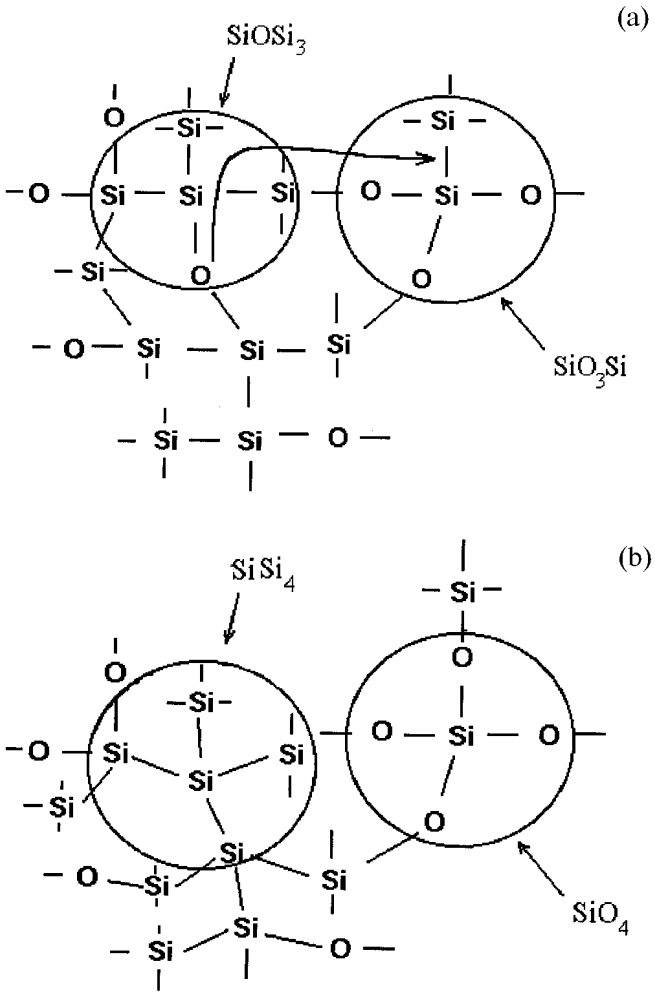

Fig. 4. Schematic view of the formation of Si nanoinclusions upon the thermally induced decomposition of the SiO_x phase

$v_{SiO_x} = 21 \div 35$ % by volume. These values agree with the contributions of the bands, related to SiO_2Si_2 and SiO_3Si clusters, to the total area of the TO mode which is equal to 34 % (see the Table).

Parameters of elementary absorption bands

Band	Maximum position, cm^{-1}	Mode	Structural component	Band area (normalized relative to the total area of the bands for TO and LO modes, respectively), %		
				Freshly deposited	Annealed at 700 °C	Annealed at 1000 °C
1	1000	TO	$SiOSi_3$	22	11	—
2	1031	TO	SiO_2Si_2	29	30	16
3	1050	TO	SiO_4	—	—	31
4	1067	TO	SiO_3Si	27	32	18
5	1095	TO	SiO_4	22	28	35
6	1142	LO		100	53	39
7	1195	LO		—	47	38
8	1233	LO		—	—	23

It is well known [28] that the SiO_4 tetrahedra join to various types of rings in the silicon dioxide network, most probable of which are the 4- and 6-fold rings. The angle of a Si—O—Si bond, θ, depends on the type of a ring: $\theta \sim 144°$ and $\theta \sim 130°$ are inherent in 6- and 4-fold rings, respectively [15, 29]. Bands 3 and 5 from the table are related to the oscillations of bridge oxygen atoms with the angles of Si—O—Si bonds $\theta \sim 130°$ and $\theta \sim 144°$, respectively, in the case of the SiO_2 lattice [15]. In other words, when the SiO_2 phase is already formed, the area of these bands shows the content of the 4- and 6-fold rings of tetrahedra. It was found before [30] that the relative areas of the mentioned bands depend on the thickness of a silicon dioxide film. In particular, the 4-fold rings of SiO_4 tetrahedra are prevalent in the lattice of ultrathin films. In our case, the ratio of the areas of Gaussians 3 and 5 is almost equal to 1 (see the Table). Taking into account that band 5 is related to SiO_4 tetrahedra both in the SiO_2 phase and the SiO_x phase of transient layers, one may expect that this value should be significantly greater than 1 for SiO_2 phase. Such a value is typical of the ultrathin (< 20 nm) films of silicon dioxide [20, 30].

Summarizing all the above-said, we can state that the films annealed at 1000 °C are the Si nanocrystals surrounded by SiO_x interface layers and are built in the SiO_2 matrix. The structure of the SiO_2 phase is typical of that for the ultrathin SiO_2 films. On the other hand, the samples annealed at 700 °C contain amorphous Si nanoclusters built into the homogeneous glassy $SiO_{1.75}$ matrix.

A significant increase of the intensities of the bands of longitudional optical phonon (LO) bands as a result of thermal treatment was observed before [3, 13]. Such an influence can be related to the inhomogeneity of annealed films due to the formation of the phases of a varying composition.

4. Conclusion

The thermal treatment of thermally evaporated SiO_x films leads to structural transformations and influences their physical properties. The transformations of the oxide phase occur at the very beginning of the action of temperature (during 5 initial minutes) both for the annealings at 700 and 1000 °C. Such a treatment leads to the decomposition of the molecular complexes of weakly oxidized silicon and to the formation of the Si inclusions and the clusters containing strongly oxidized Si. The concentration of strongly oxidized clusters depends on the treatment temperature.

The structure of the films annealed at 700 °C can be presented as amorphous Si nanoclusters built into the homogeneous SiO_x matrix with x greater than that of initial films. The films annealed at 1000 °C contain Si nanocrystals surrounded by interface SiO_x layers and built into the SiO_2 matrix. The structure of the SiO_2 phase in such films is similar to that of ultrathin SiO_2 films.

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ДОСЛІДЖЕННЯ ТЕРМОСТИМУЛЬОВАНОГО ФАЗОВОГО РОЗДІЛЕННЯ У ПЛІВКАХ SiO_x МЕТОДОМ ІЧ-СПЕКТРОСКОПІЇ

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Р е з ю м е

Досліджено тонкі плівки SiO_x ($x \approx 1{,}3$), отримані термічним вакуумним випаровуванням монооксиду кремнію. Використовуючи ІЧ-спектроскопію з аналізом форми смуги поглинання на зв'язках Si—O, було досліджено термостимульовану (температури відпалу 700 та 1000 °C) структурну трансформацію фази Si—O у шарах SiO_x, яка приводить до утворення аморфних або кристалічних кремнієвих нановключень. Показано, що термічна обробка веде до розпаду молекулярних комплексів слабкоокисленого кремнію та формування як кластерів кремнію, так і молекулярних кластерів, що містять сильноокислений кремній. Перетворення оксидної фази відбувається майже повністю вже у перші 5 хв термічної обробки. Плівки, відпалені при 700 °C, в основному містять аморфні кремнієві нановключення, вбудовані у гомогенну матрицю $SiO_{1,75}$ (об'ємна частка аморфної фази Si становить близько 17 %). Плівки, відпалені при 1000 °C, можуть бути представлені як кремнієві нанокристали (об'ємна їх частка становить близько 20 %), оточені тонкими проміжними шарами SiO_x та вбудовані в SiO_2.