Conference Paper

Physical and Technological Fundamentals of Sapphire Substrates Production for Devices of Solid-state Electronics

Y V Klunnikova and S P Malyukov

Southern Federal University, Department of Electronic Apparatuses Design, Taganrog, Nekrasovsky, 44, Russia

Abstract

The results of numerical simulation allow to investigate the thermal conditions received by active heaters influence on the thermoelastic stresses and gas inclusions in sapphire. We carried out the experiments for defects detection in sapphire crystals. We suggest the recommendations about sapphire crystals growth and processing improvement for profitability increase in sapphire substrates production for microelectronics.

Received: 10 February 2018
Accepted: 14 April 2018
Published: 7 May 2018

Publishing services provided by Knowledge E

Selection and Peer-review under the responsibility of the RFYS Conference Committee.

1. Introduction

Success of modern microelectronics largely depends on solving problems in the field of dielectric materials physics and technology, and also in development of new generation of integrated circuits. The integrated circuits elements are received by films sedimentation on dielectric substrates. These substrates are the mechanical basis on which surface forms integrated circuits structures according to the set topological scheme.

Nowadays borosilicate glass, alumina ceramic like Polikor, quartz glass, sitall, sapphire are most widely used for integrated circuits substrates production [1-3]. Taking into account technical and physical properties of different materials of microelectronics, we can conclude that sapphire has unique properties. Sapphire is one of constructional materials in optical systems in which the important requirement is resistance to mechanical influences, temperatures and radiation.

Despite variability of sapphire growth methods, sapphire single crystals have similar physical and chemical properties. However sapphire crystals received by different methods have different technical characteristics which are necessary for application in microelectronics [4, 5]. The sapphire crystals growth by horizontally directed crystallization is one of the promising methods. It allows to receive high structural quality

crystals without high-temperature annealing, which is important for integrated circuits substrates production in microelectronics.

High quality of sapphire surface and treatment accuracy are required in integrated circuits production. The quality of substrates surface considerably affects structural perfection of epitaxial layer; therefore the substrates surface is grinded and polished. For each material there is an approximate range of possible values of surface roughness depending on the processing type. At any surface processing method, which is designed to improve substrate structural quality, it is necessary to detect defects (pores, cracks) that appear in processing in due time in order to decide whether further processing is needed. This allows to increase profitability of substrates production in microelectronics.

The purpose of this work is to develop methodical basis for sapphire substrates production technology as the constructional elements of micro- and nanoelectronics.

2. Simulation of Sapphire Crystals Growth

Physical and technological processes of sapphire growth and treatment can lead to defects formation [5].

We simulated sapphire crystal growth by horizontally directed crystallization in order to increase accuracy of technological parameters control and improve sapphire crystals quality [6].

The numerical simulation allows to study the influence of thermal conditions made by active heaters on thermoelastic stresses and gas inclusions in sapphire. The equations of thermoelasticity and heat conductivity for simulation of different stages of sapphire crystals growth is presented in the following form [6-10]:

$$\begin{cases} \frac{\partial}{\partial x}\mu\frac{\partial u}{\partial x}+\frac{\partial}{\partial y}\mu\frac{\partial u}{\partial y}+\frac{\partial}{\partial z}\mu\frac{\partial u}{\partial z}+\frac{\partial}{\partial x}(\lambda+\mu)\frac{\partial u}{\partial x}+\frac{\partial}{\partial x}(\lambda+\mu)\frac{\partial v}{\partial y}+\frac{\partial}{\partial x}(\lambda+\mu)\frac{\partial w}{\partial z}=-\frac{\partial(\alpha T)}{\partial x}, \\ \frac{\partial}{\partial x}\mu\frac{\partial v}{\partial x}+\frac{\partial}{\partial y}\mu\frac{\partial v}{\partial y}+\frac{\partial}{\partial z}\mu\frac{\partial v}{\partial z}+\frac{\partial}{\partial y}(\lambda+\mu)\frac{\partial u}{\partial x}+\frac{\partial}{\partial y}(\lambda+\mu)\frac{\partial v}{\partial y}+\frac{\partial}{\partial y}(\lambda+\mu)\frac{\partial w}{\partial z}=-\frac{\partial(\alpha T)}{\partial y}, \\ \frac{\partial}{\partial x}\mu\frac{\partial w}{\partial x}+\frac{\partial}{\partial y}\mu\frac{\partial w}{\partial y}+\frac{\partial}{\partial z}\mu\frac{\partial w}{\partial z}+\frac{\partial}{\partial z}(\lambda+\mu)\frac{\partial u}{\partial x}+\frac{\partial}{\partial z}(\lambda+\mu)\frac{\partial v}{\partial y}+\frac{\partial}{\partial z}(\lambda+\mu)\frac{\partial w}{\partial z}=-\frac{\partial(\alpha T)}{\partial z}, \\ \mathrm{div}(k_i \mathrm{grad} T_i(x,y,z))=0. \end{cases} \quad (1)$$

where u, v, w are the displacement components; λ,$\mu$are Lame constants; α is the thermal volume-expansion coefficient; k_i are the coefficients of thermal conductivity

in crystal, melt and powder; i = 1,2,3 are the crystal, melt and powder accordingly, T_i are the temperatures.

For the equations set (1), boundary conditions can be written in the form of correlations for temperature (2) – (4) and displacements (5):

$$k_1 \frac{\partial T_1(x_T, y, z)}{\partial x} = k_2 \frac{\partial T_2(x_T, y, z)}{\partial x}, \tag{2}$$

$$k_2 \frac{\partial T_2(x_T + \Delta x, y, z)}{\partial x} = k_3 \frac{\partial T_3(x_T + \Delta x, y, z)}{\partial x}, \tag{3}$$

$$q_{s_1} = q_{s_2} = q_{s_3} = \sigma\beta(T^4 - T_{hot}^4), \tag{4}$$

$$u = v = w = 0, \tag{5}$$

where $\phi = \{u, v, w\}$; σ is the Stefan-Boltzmann constant; T_{hot} is a function that defines the temperature distribution on the heaters; Δx is the melt width; x_T is the boundary crystal – melt; β is the emissivity.

The equation (1) and boundary conditions (2) – (5) allow to develop the procedure of calculation of temperatures, displacements, strains and stresses in the system crystal – melt – powder.

In order to test the proposed procedure, we carried out the three dimensional numerical simulation of the temperatures, displacements, strains, and thermoelastic stresses distribution at different stages of sapphire crystal growth by the control volumes method on the unstructured grid taking the temperatures distribution in the sapphire crystals growth process into account. The simulation program was developed in C++ in Microsoft Visual Studio 2008 [6].

Figure 1 shows the results of stresses calculation in sapphire crystals.

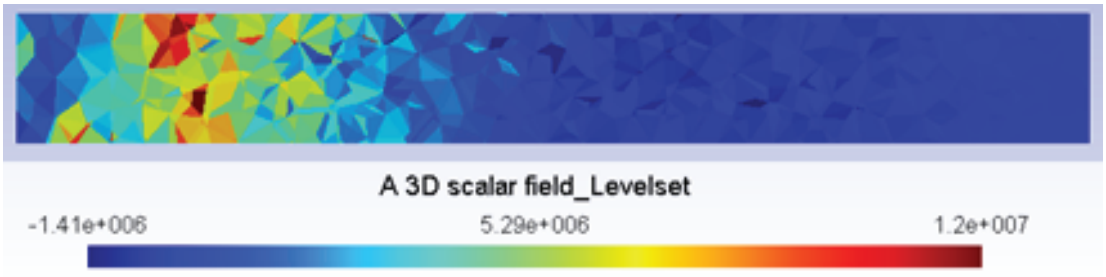

Figure 1: The results of stresses σ_x calculation in crystal in the system crystal-melt-powder in vertical cross-section of crystal (the scale is in Pa).

Considering the kinetics of the initial and subsequent stages of sapphire crystals formation process, we can conclude that not only thermal and physical parameters of

the material have significant impact on the process, but also the crystal form factor. During the whole process the temperature difference between the surface of the transformation and the "back" side of the crystal remains constant. As a result, the stresses in the crystal can be formed. Their intensity is determined by the temperature distribution [11]:

$$\xi = E\alpha_T \Delta T_s, \tag{6}$$

where ξ is the thermoelastic stresses; ΔT_s is the temperature difference between the surface phase transformations and back side of the crystal; $E$is the material Young's modulus; α_T is the coefficient of thermal expansion.

Thus, the developed models for sapphire crystal growth by horizontal directional crystallization allow us to investigate the crystallization process and related thermal stresses in the crystal on various stages of the process, the hydrodynamics of the melt and its influence on defects formation.

3. Experimental Investigation Defects in Sapphire and Their Influence on Crystal

We used various methods for experimental determination of defects in sapphire substrates (size and location of pores and microcracks) obtained by influence of different thermal conditions during sapphire growth: a method of surface acoustic wave (SAW), vibroacoustic method, as well as optical and thermal methods [12].

The frequency dependence of the complex coefficient S11 at different distances from the defect and the Fourier transform of the measured frequency dependence are shown in Figure 2.

In the transmitted electromagnetic signal and the signal reflected from the input (output) SAW transducer, interference occurs, that leads to the appearance of multiple maximum and minimum S11 parameter depending on the frequency (Figure 2).

The method of surface acoustic wave allows to determine the location, depth and length of surface cracks, scratches and their boundaries. The method of SAW can be widely used for the detection, monitoring and analysis of defects in subsurface and surface layer of sapphire, which are almost impossible to identify by other methods. The investigation of sapphire wafers was carried out by means of transmission complex coefficients meter "Obzor-103" in the laboratory of Mechanics and Physics of New Materials and Devices, Institute of Mathematics, Mechanics and Computer Sciences by Vorovich I.I., Southern Federal University [12].

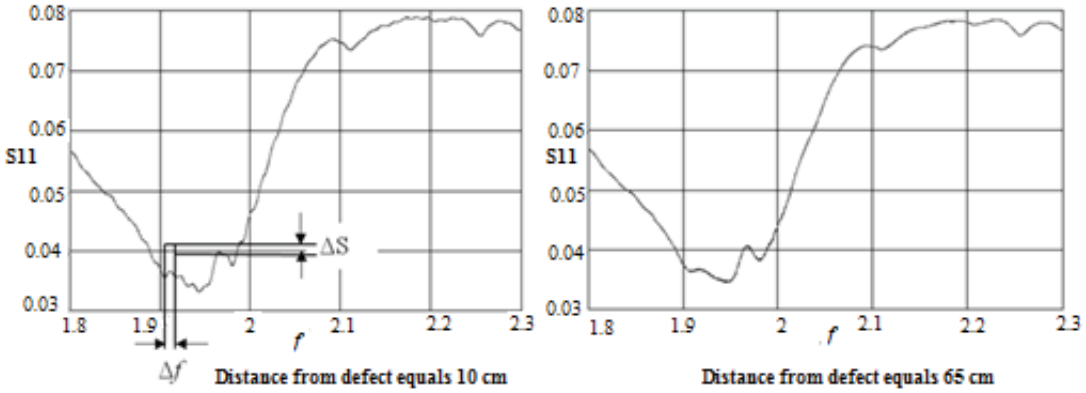

Figure 2: The typical dependences refection coefficient S11 on frequency.

The vibration-based diagnostics method gives the opportunity to define the latent defects in sapphire because the harmonics of appropriate frequencies appear in the spectrum of vibration and noise in the case of defects presence (gas bubbles, cracks) in sapphire structure. The sapphire sample was investigated by the thermal method (thermal imager Flir i5) which allowed more accurately determine expected defects [12].

Thus, the distribution of sapphire defects was determined by using different experimental methods (SAW method, vibroacoustic method, optical and thermal methods). It allows to define the structure morphology and sapphire defects change.

The experimental investigation of mechanical treatment of sapphire surface was carried out for sapphire defects quantity reduce in the surface layer. The modes of mechanical treatment significantly affects the defects distribution concentration [11, 12]. The depth of the damaged layer was calculated. It can be the basis for sapphire crystals treatment optimization and also it allows to receive the recommendations for the sapphire surface layers properties determination and crystal quality improvement.

4. The investigation results

We offer methodological fundamentals for technological processes of sapphire substrates production for elements of micro- and nanotechnology. We studied different stages of sapphire growth and treatment and offered improvements to the production technology. They make the growth of sapphire crystals more reproducible and the sapphire substrate production more efficient.

The sapphire (or sapphire substrates) surface study allows to predict the quality of sapphire products.

The calculations and the developed models can be taken into account in the design of new equipment for sapphire crystals growth by horizontal directed crystallization method.

Acknowledgments

This research is supported by the Federal Target Program of the Ministry of Education and Science of Russian Federation No. 14.587.21.0025, the project ID is RFMEFI58716X0025.

References

[1] Teplova T B, Samerhanova A S 2006 *Mining Informational and Analytical Bulletin***339**

[2] Bogdanov Y, Kochemasov V, Hasyanova E 2014 *Pecatniy Montazh***204**

[3] Akselrod M S, Bruni F J 2012 *J. Cryst. Growth***134**

[4] Dobrovinskaya E R, Lytvynov L A, Pishchik V V 2002 *Sapphire and Other Corundum Crystals* (Kharkiv: Institute of Single Crystals)

[5] Dobroviskaya E R, Lytvynov L A, Pishchik V V 2009 *Sapphire. Material, Manufacturing, Applications*(New York: Springer)

[6] Malyukov S P, Klunnikova Y V, Kirillova E V 2016 IOP Conference Series: Materials Science and Engineering151(1),012022

[7] Madency E, Oterkus E 2014 *Predynamic Theory and Its Application*(New York: Springer)

[8] Abgaryan A A 2001 *Matematicheskoe Modelirovanie***20**

[9] Malyukov S P, Klunnikova Y V 2014 Advanced Materials *Complex Investigations of Saphhire crystals Production (Springer Proceedings in Physics* vol 152) (Switzerland) chapter pp 55–69

[10] Lykov A V 1967 *Theory of Thermal Conductivity*(Moscow: High School)

[11] Malyukov S P, Klunnikova Y V, Cherednichenko D I 2013 Sapphire: Structure, Technology and Applications *Heat-Physical Processes at the Sapphire Crystals Growth by Horizontal Directed Crystallization*(USA: Nova Science Publishers) chapter pp 101–118

[12] Malyukov S P, Klunnikova Y V, Parinov I A 2014 Advanced Nano- and Piezoelectric Materials and Their Applications *Investigation of Defects Formation During Sapphire Growth*(USA: Nova Science Publishers) chapter pp 89–108