Study of the thermal stresses during TiO_2 laser annealing on sapphire substrate

Y V Klunnikova[1], M V Anikeev[1] and A V Filimonov[2]

[1] Southern Federal University, Shevchenko 2, Taganrog, 347928, Russia

[2] Peter the Great St. Petersburg Polytechnic University, 29 Politekhnicheskaya, St. Petersburg, 195251, Russia

E-mail: jklunnikova@rambler.ru

Introduction and motivation. Oxide thin films are widely used for the design of functional devices such as photoelectric converters or sensitive elements of gas sensors. Their functionalities depend on the physical properties and on the microscopic interactions at the film/substrate interface.

The aim of our research is to investigate the thermo-elastic stresses in thin TiO_2 films on substrates obtained by laser annealing and to analyze the occurrence and evolution of thermo-elastic stresses and defects in the film-substrate structure and to determine the conditions that prevent cracks formation.

Simulation. The localization of the thermal effect during TiO_2 films laser annealing on sapphire substrate leads to a large temperature gradient in the zone of the laser beam influence, which results in thermo-mechanical stresses and possible defects. The scheme of laser radiation of TiO_2 film with a thickness of 10 μm on the sapphire surface (430 μm thickness) is presented in Fig. 1.

To calculate the temperature fields, we use a three-dimensional heat equation:

$$c\rho\frac{\partial T}{\partial t}-\left(\frac{\partial}{\partial x}k\frac{\partial}{\partial x}T+\frac{\partial}{\partial y}k\frac{\partial}{\partial y}T+\frac{\partial}{\partial z}k\frac{\partial}{\partial z}T\right)=q,$$

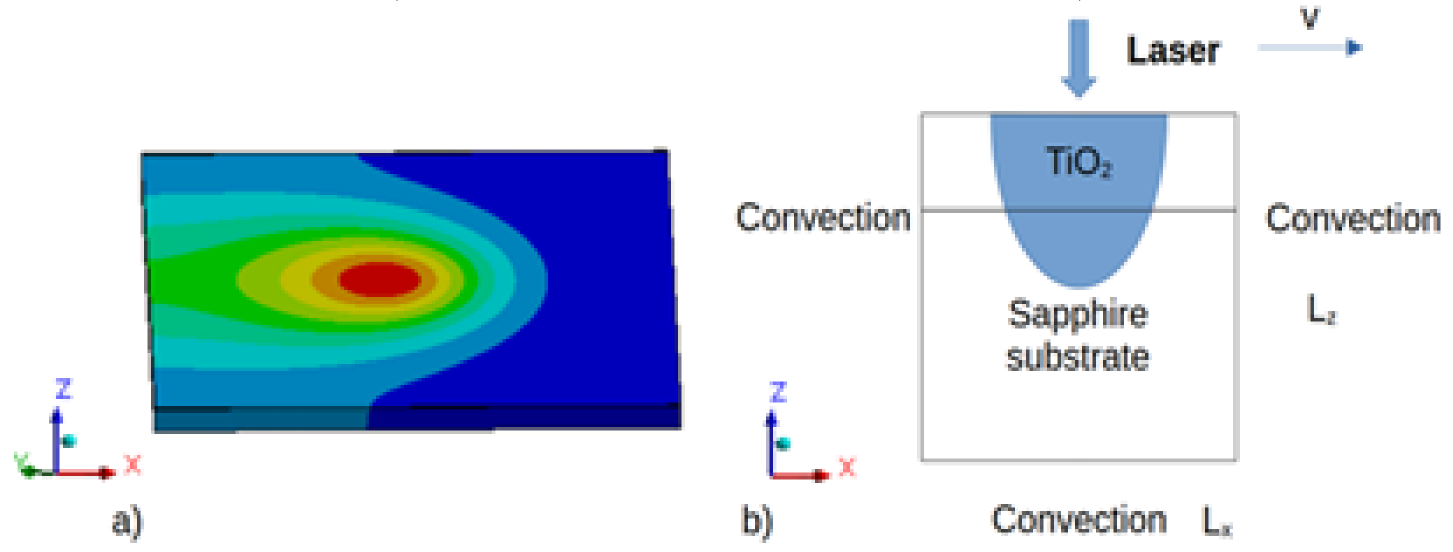

Figure 1. Right: Scheme of the TiO_2 – sapphire laser annealing, left: temperature distribution at time instant t

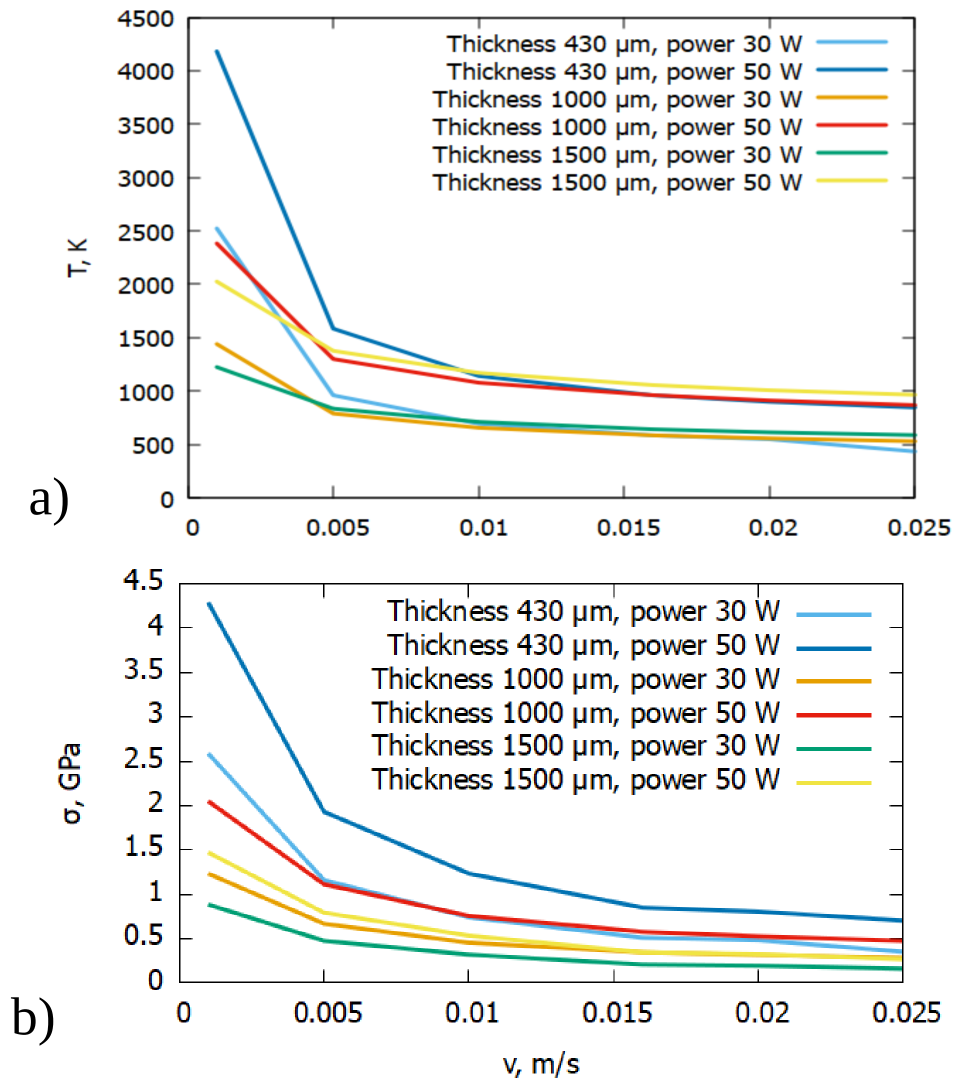

Figure 2. The influence of laser power and laser beam speed on TiO_2 film (thickness of 5 μm) laser annealing on sapphire substrate with different thicknesses a) at maximum temperatures, and b) at maximum principal stresses

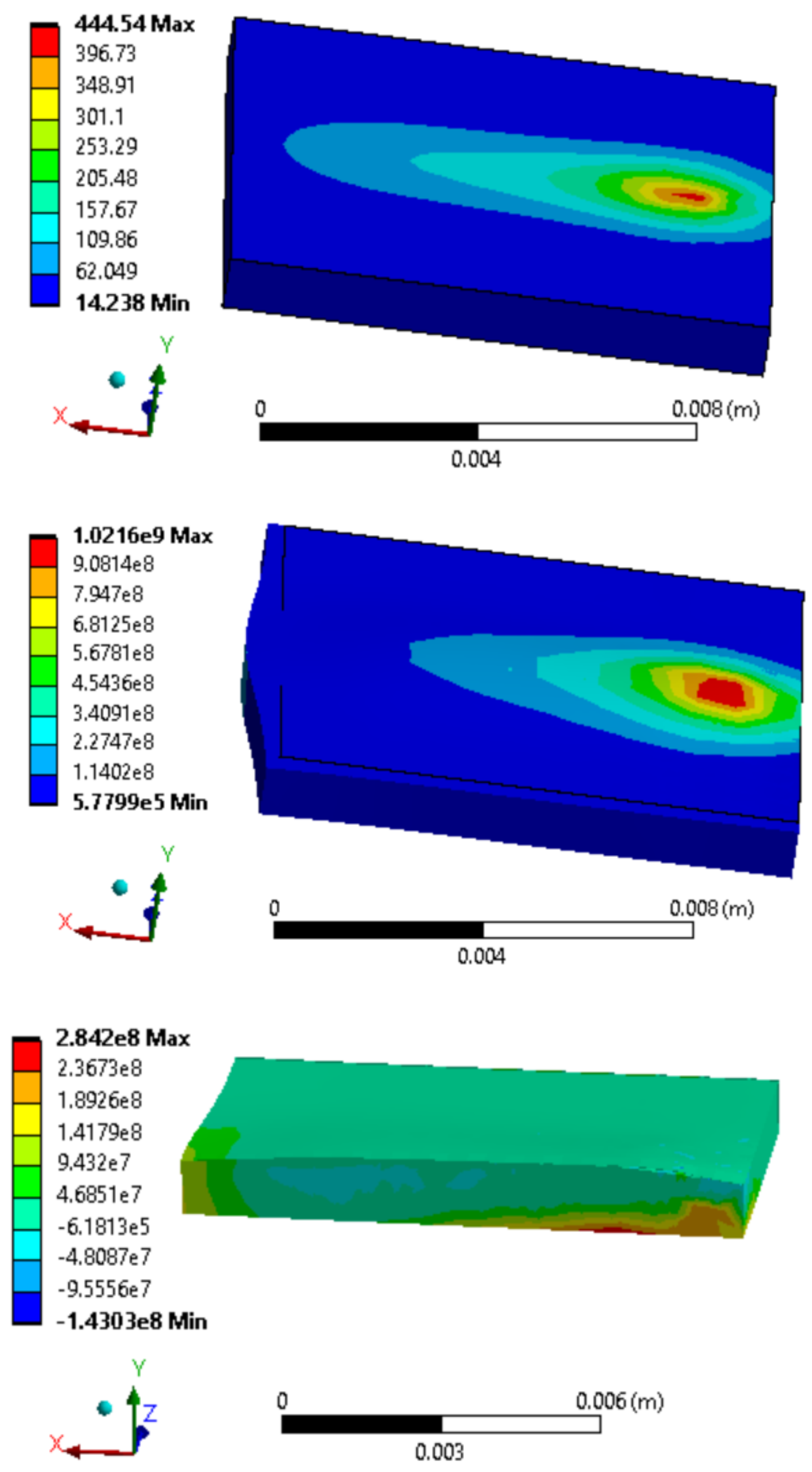

Figure 3. Maximum temperatures (first graph, in ^{0}C), equivalent von-Mises stresses (second graph, in Pa), and maximum principle stresses in a vertical section of the body (third graph, in Pa) as criteria for crack initiation during TiO_2 film laser annealing at laser scan speed of 0.025 $m\cdot s^{-1}$, laser power of 30 W, the laser direction from right to left, the film thickness of 5 μm, the substrate thickness of 1 mm, the time of laser treatment is 0.32 s

Experiments. For the experiments a thin film of tetraethoxytitanium ($Ti(OC_2H_5)_4$) was brought up onto a sapphire substrate with a thickness of 430 μm by centrifugation (centrifuge SPIN NXG-P1, rotor rotation speed of 2000-3000 rpm, application time of 30 s). After pre-drying in the oven at 100-120 °C for 15-20 minutes (the solvent and hydrolysis products have been removed from the film before) laser annealing is carried out using the radiation of a pulsed solid-state Nd:YAG laser with a wavelength of 1064 nm (film temperature of 500-600 °C, laser beam scanning rate of 1-20 mm/s, laser power of 30-90 W).

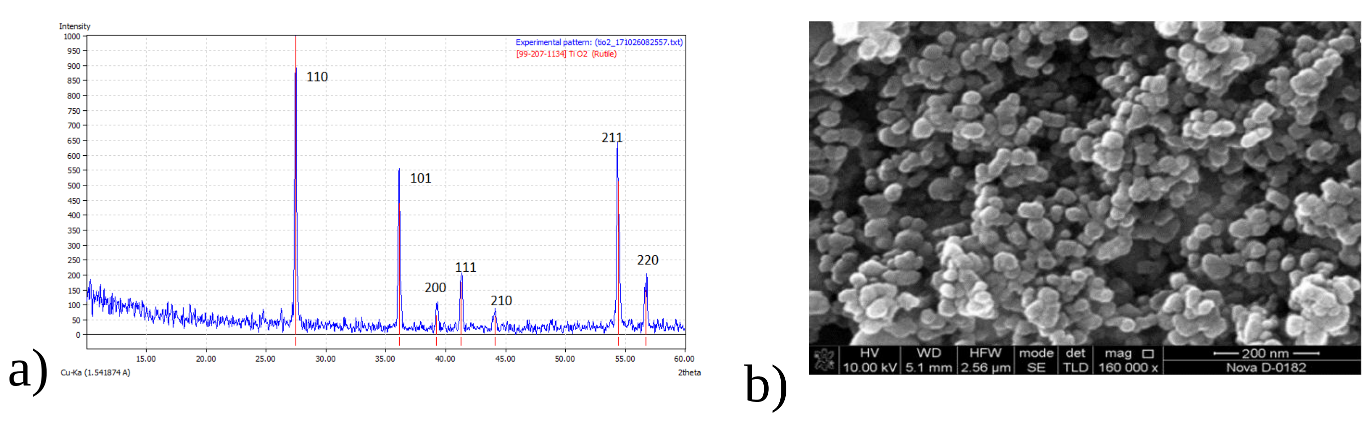

Figure 4. a) The X-ray roentgenogram of titanium oxide film obtained by laser annealing; b) the morphology of the surface of titanium dioxide (wavelength of 1064 nm) on sapphire substrate

Conclusion. We have simulated TiO_2 thin films processing on sapphire substrates and conducted related experiments. We developed a three-dimensional model for the analysis of the stress distribution in film-substrate structure. The films properties were investigated with atomic force microscopy method, scanning electron microscopy, and X-ray phase analysis.

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