Mathematical Modeling of The Nanotubes Implementation into A Solid-State Matrix Using A Powerful Laser

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Abstract

Laser technologies are becoming increasingly widely used as a method of surface treatment of materials and the latest methods of changing the surface structure. One of the ways of using laser technology is the introduction of carbon nanotubes into a solid-state matrix. Therefore, modeling this process is relevant and important.

Keywords [1]

Laser, nanotubes, implementation, modelling

1. Introduction

Carbon nanotubes are promising materials that are widely studied for the application of various tasks in micromechanics, biology and electronics [1-3]. In nanotechnology, laser irradiation of the graphite surface in a buffer gas atmosphere is used in addition to the electric arc and focused solar method of thermal spraying of graphite to obtain nanotubes.

Implantation of nanotubes into the matrix is an important problem for their further practical use. One of the well-known methods of such implantation is the method of ultrasonic introduction.

At the same time, the matrix into which the nanotubes are inserted is in a liquid state [1-3]. The cavitation effect and the associated occurrence of a shock wave play an important role in the process of implementation.

It is of interest to study the effect of implementation carbon nanotubes into solid-state matrices with different physical parameters using a Q-switch laser, which is not only a source of heat, which allows the matrix to be converted into a liquid state, but also of a shock wave.

Thus, the use of lasers for the introduction of carbon nanotubes into materials stimulates theoretical calculations of the temperature fields of materials irradiated by powerful laser pulses in a transparent condensed medium, and the development of methods for laser formation of volumetric structures from nanotubes is an urgent task [1-3].

A peculiarity of processing materials with a nanosecond laser pulse is the occurrence of a shock wave in the material. The development of laser shock wave technology as a method of processing materials makes it necessary to study the processes that occur in materials when irradiation, with the aim of increasing the pressure of the shock wave, is carried out in a transparent condensed medium (TCM).

The shock wave which occurs in the material when powerful laser radiation acts on it is called a laser shock wave, which is understood as a sharp jump-like increase in pressure in the irradiated material, which propagates in it at supersonic speed and is resistant to small disturbances of its profile.

2. Mathematical modeling of the nanotubes implementation into a solid-state matrix using a powerful laser

This paper is devoted to the study of the implementation of carbon nanotubes into aluminum and fluoroplastic substrates and computer modeling of laser irradiation processes in a transparent condensed medium (TCM).

The materials were irradiated by a Q-switch Nd: glass laser, a flux density of ~ 10^9 W/cm^2 in a TCM, which ensured an increase in plasma pressure.

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The irradiated sample was a "sandwich": TCM, nanotubes, substrate. At the same time, reliable acoustic contact between all components of the formed "sandwich" must be ensured.

The surface of the materials (before and after irradiation) and the implementation and distribution of nanotubes on the surface were investigated by the method of electron microscopy at different magnifications. Electron microscopy of the surface of the substrate from unprotected aluminium (after irradiation in air) at different magnifications it's shown Figure 1.

Experiments have shown that:

1. The irradiated area in the centre looks uniformly melted and smooth (5k magnification). The surface relief is periodic pit-like or cylindrical structures with a diameter of 50-100 nm and a depth of up to 10 nm (50k). The wavelength of the Nd: glass laser radiation is 1060 nm. In this way, the formed structures are not the result of light interference.

2. At the radiation area edge, periodic patterns, and pores are visible (magnified from 200 to 1k times). The same relief picture as in the centre (Fig.1) in the form of influxes and patterns (magnification 50k times).

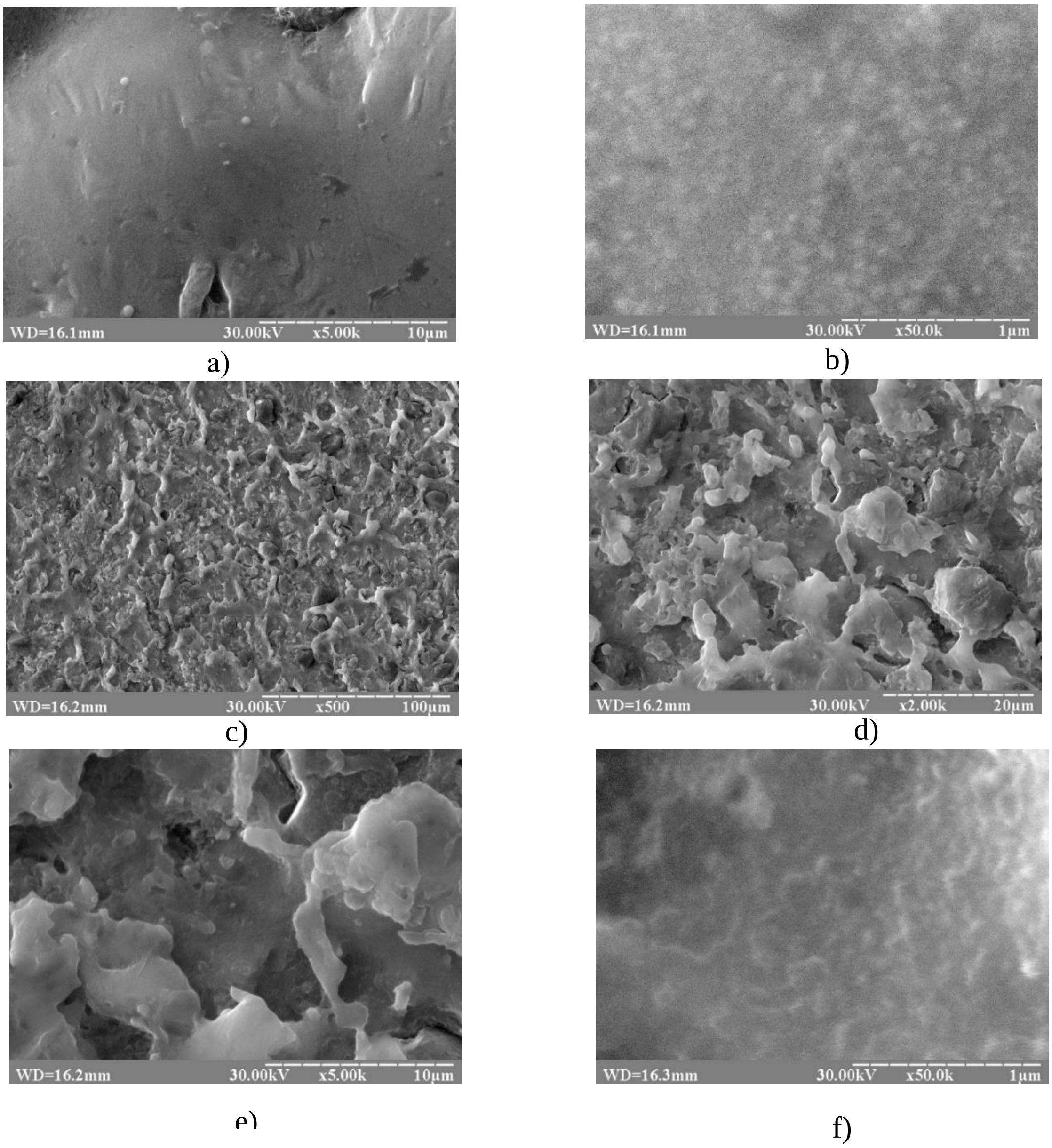

Figure1. Electron microscopy of the surface of the substrate at different magnifications

The general topography of the surface when irradiated with a smaller laser energy flux density is partially different, but generally similar to the previous one.

The surface of the sample (aluminium substrate with nanotubes) after irradiation is shown in Fig. 2.

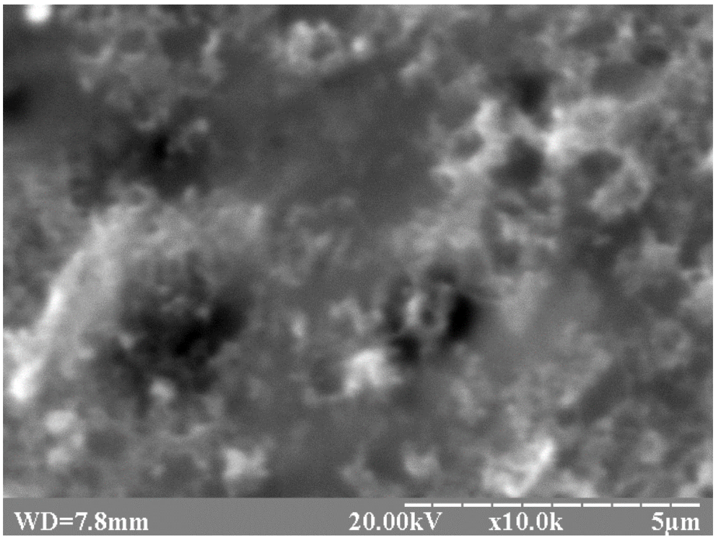

Figure. 2. The surface of an aluminum substrate with embedded nanotubes.

On the surface of aluminium, carbon nanotubes with different fusion depths are visible (magnification 10k times), fused nanotubes, as well as the glow of individual areas of the surface in the places where the nanotubes are placed.

The distribution of nanotubes on the surface is uneven. This is also confirmed by the determined chemical composition of the sample surface before and after irradiation through TCM, and confirmed by electron microscopy.

Modelling of the process of carbon nanotubes implementation into the material under the influence of laser shock waves consists of several stages and is carried out using various methods. At the first stage, the temperature field in the material is calculated under the action of a laser pulse in the shock wave generation mode. The second stage is modelling of the process of the action of TCM on the nanotube's implementation into the material. When a laser pulse hits the surface of the "sandwich" sample, which consists of a substrate on which a layer of nanotubes dissolved in toluene is deposited and covered with a layer of TCM, the near-surface layer turns into plasma, and thermal and shock waves propagate into the depth of the sample. The simulation of the temperature distribution in the material under the action of a switch laser in the TCM, requires the following conditions:

1. $r = \sqrt{a\tau}$ (r- the spot size on the surface, a - thermal conductivity, τ - pulse duration), the problem of thermal conductivity is reduced to a one-dimensional one,
2. the absorption layer $\delta = {}^{1}\!/_{\mu}$, де μ — absorption coefficient.

During the action of the laser pulse, a layer with a thickness $\delta = {}^{1}\!/_{\mu}$ absorbs energy, evaporates, turns into plasma and transfers its energy to the next layers.

The calculations showed that despite the growth of the absorption coefficient under normal conditions with an increase in temperature during the duration of the pulse, in our case, due to high laser energy flux densities (up to 10^9 W/cm^2), the surface layer reaches the plasma state in a short time (< 5 ns) for almost all studied metals and alloys. Therefore, the absorption coefficient was assumed to be constant.

For a Q-switch laser corresponding to a short duration of the laser pulse, at the initial moment of the action, the time structure of the pulse is described by a linear dependence on time for $t > 10^{-9}$ s (Fig.3).

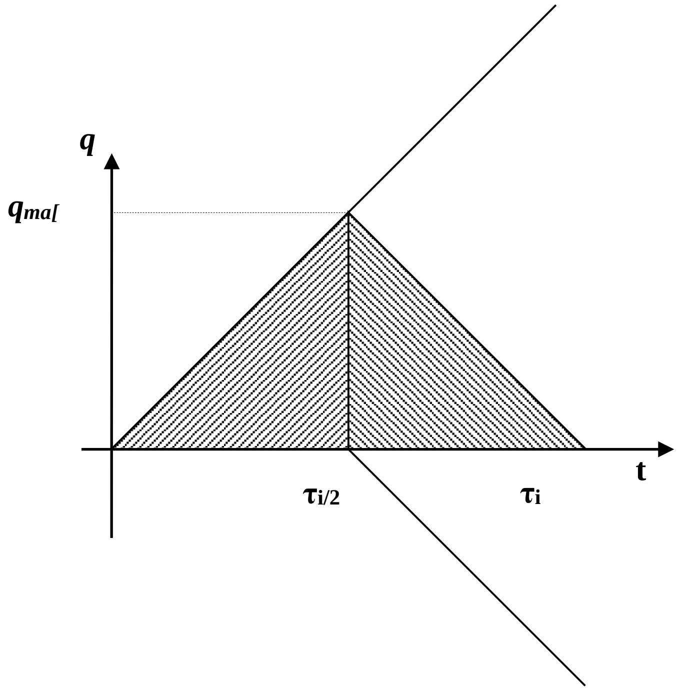

Figure.3 Time-energy structure of a Q-switch laser pulse

Computer modelling is based on solutions of the second-order differential equation

$$T(z,t)=\frac{q\sqrt{a}}{\lambda\tau_i}(4t)^{3/2}i^3erfc\frac{z}{2\sqrt{at}}$$

де T – temperature z at the moment t
λ – hermal conductivity coefficient
q – energy density
a is the coefficient of thermal conductivity

The graphical modelling method showed that the shape of the simulated laser pulse and its correspondence to the real one is influenced by the moment of switching on the fictitious source. The action of the energy source does not stop with the linear decrease of the pulse energy.

Using the theory of fictitious sources, an analytical solution was obtained:

$$T(z,t)=\frac{q\sqrt{a}}{\lambda\tau_i}\left[(4t)^{3/2}i^3erfc\frac{z}{2\sqrt{a\tau}}-(4(t-\tau))^{3/2}i^3erfc\frac{z}{2\sqrt{a(t-\tau)}}\right]$$

The experiment shows that 5% of the energy of the laser pulse, which was used in our experiments, is sufficient to start the melting of the aluminium surface. Considering the peculiarities of the process of introducing nanotubes into the material, to calculate the energy that falls on the substrate, we assumed that $E=kE_{поз}$, де k — coefficient, which is determined by the ratio of the maximum density of bulk carbon nanotubes to the density of carbon

$$k=\frac{\rho_{nanotubes}}{\rho_{\mathrm{C}}}$$

So, according to these considerations, k=0.25, and the energy falling on the surface of the substrate is ≈25% of the incident energy on the "sample – sandwich".

When the nanotubes and substrate are heated simultaneously, the substrate melts and the lower layer of nanotubes is pressed into the substrate. Since the heating process depends on the thermophysical properties of materials, during the heating of carbon nanotubes with a thickness of 2 μm, for example, a layer of aluminium with a thickness of 7 μm will warm up to the melting temperature.

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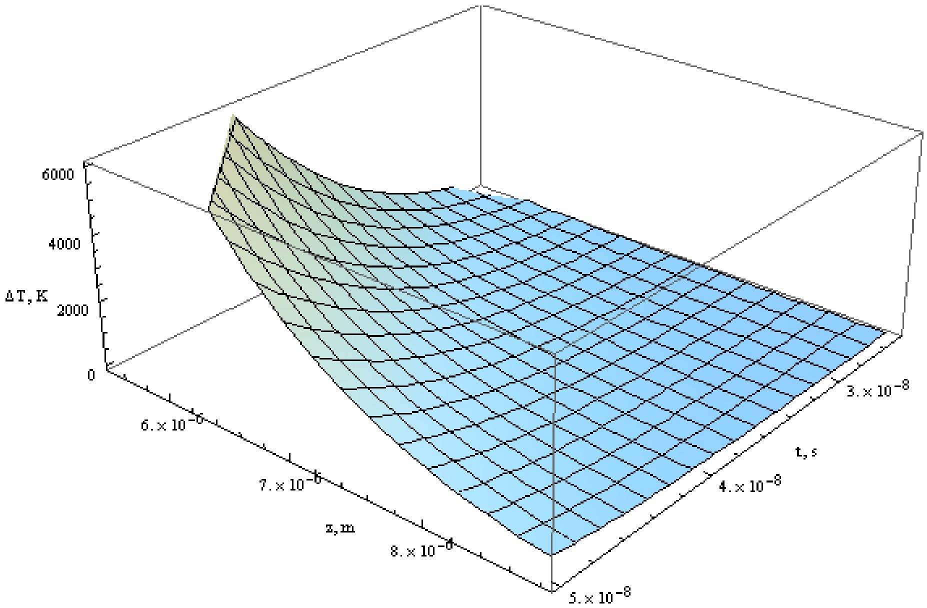
The temperature distribution in aluminium irradiated 50 ns and an energy of 10 J pulse is show on Figure 4.



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3. Conclutions

Modelling of the irradiation process for our experimental conditions showed that if the layers of nanotubes were continuous and closely abutted to each other, then the lowest layers of nanotubes, which are in direct contact with the aluminium matrix, should not heat up. However, this contradicts the picture observed in the experiment.

Therefore, when analysing the process of nanotubes implementation, the bulk nature of nanotubes and the possibility of laser radiation penetrating directly to the surface of the substrate were considerate.

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