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Numerical simulation on the temperature field induced by a nanosecond pulsed excimer laser in the phase-change film

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ABSTRACT

In the paper, a three-dimensional finite element model was developed to demonstrate the temperature field induced by a nanosecond pulsed excimer laser in the phase-change film. The numerical model was established with an assumed rectangular temporal profile, following the continuous medium heat conduction theory with semi-infinity heat conduction. It showed that the temperature variation followed the exponential relation in both the heating/cooling procedures, and the whole heating/cooling process was divided into four regions I–IV, namely rapid heating region I and equilibrium heating region II in the heating process as well as quick cooling region III and equilibrium cooling region IV in the cooling process. The heating/cooling rates were then fitted from the temperature variation curve. The calculated heating/cooling rates were in the scale of 10^8–10^{11} K/s for the nano-scale pulse radiance. Furthermore, the effects of laser fluence and pulse duration on the temperature field were investigated. It was noted that the effect of pulse duration was focused on regions II and III, while the heating rate in region I was mainly determined by laser fluence.

1. Introduction

Chalcogenide phase-change materials have become key components used for rewritable optical disks since 1960s [1]. During the reversible process, the optical recording bit (an amorphorized mark) is achieved by an intense and short laser pulse (ns–fs), while for the bit erasing a laser beam (ns) with the intensity sufficient to heat the material slightly above the glass-transition temperature is employed to crystallize the recording mark. Nowadays, in spite of considerable efforts made by using optical absorption [2], transmission electron microscopy [3–5], atomic force microscopy [6], Raman scattering and X-ray absorption fine structure measurement [7], a paradoxical situation exists when a device such as an optical disk is functional and commercially available, but the structural changes behind the phase transition are still unknown. That is because clear experimental information is very hard to get owing to the short phase-change timescales involved and the small length scales of actual phase-change random-access-memory (PRAM) devices [8,9].

In order to demonstrate the phase-change mechanisms of chalcogenide materials, quite a few simulations on the ab initio molecular dynamics or density functional theory models have been executed up to date [10–13]. In the calculation, two types of temperature-time profiles are usually adopted to describe the heating/cooling procedures using a series of assumed temperatures: (1) a continuous ramp (constant dT/dt) and (2) isothermal periods, interrupted by discontinuous temperature changes. In reality, the phase-change behavior induced by the short laser pulse is quite different from that based on simple temperature–time profiles [14]. Therefore, deep insights on temperature field characteristics play a vital role in elucidating the microscopic nature of the phase transition. Volkert and Wuttig [15] developed an analytical model and an axisymmetric 2D finite element model (FEM) to predict the temperature variation in optical data storage media by using the top surface loading. Nevertheless, both of the two models involved a number of simplifications relative to the real structure of the optical media so that simulated results could only provide the qualitative analysis. Park et al. [16] established a 2D FEM model to directly study the thermal stress in the PRAM structure, however, the temperature variation used in the simulation was also assumed. And Bae et al. [17] further performed a 2D FEM simulation to address the crystallization behavior of the PRAM recording layer, induced by set and re-set currents. Unfortunately, no more work has been found in systematic investigations on the temperature field in the phase-change film induced by a short pulse laser. The difficulty in the simulation analyzed by authors is given as follows: (1) the phase-change film is buried inside the optical storing media so that laser radiance is difficult to load and (2) for the simple two-layer structure of the optical media, the recording bit usually obtained is so small (~minimum 250 nm) that experimental measurements are hard to execute for verification.

The aim of this paper is to elucidate the temperature field in the phase-change film by a proposed 3D FEM model. The numerical model was developed based on the continuous medium heat conduction theory with semi-infinity heat conduction assumed. The verification was carried out by comparing the melting phenomenon between

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the experiment and simulation. Based on the model, nano-scale characteristics of the temperature field induced by single pulse laser radiance were analyzed, and the effects of laser fluence and pulse duration were further studied. The significance of the present study is not only to obtain the heating/cooling rates more accurately employed for the ab initio molecular dynamics or density functional theory simulations, but also to give a quantitative reference for the transient temperature field in order to further uncover the rapid phase-change mechanisms of chalcogenide alloys.

2. Experimental methods

The substrate, with the dimension of 60 mm in diameter and 1 mm in thickness, was monocrystalline silicon (c-Si) along [001] growth direction. The amorphous $Ge_2Sb_2Te_5$ (a-GST) film was deposited on the c-Si substrate by dc-magnetron sputtering with the stoichiometric target of GST. The working gas of Ar was employed under the pressure of 5×10^{-1} Pa. The film thickness about 70 nm was measured after deposition. Laser radiance was performed in ambient conditions by a 248 nm KrF laser with a pulse duration of 30 ns and maximum output energy of 1000 mJ, as shown in Fig. 1. The beam size, rectangular in shape (namely 1.5 cm × 3 cm), was measured by the light sensitive paper, and laser energy was uniformly distributed within the whole laser beam. The pulse laser energy adopted in the experiment was 110, 200, 300 and 400 mJ, corresponding to laser fluences of 24.4, 44.4, 66.7 and 88.9 mJ/cm^2. The single pulse radiance was performed to avoid the multi-pulse incubation effect. The photomask was employed to lessen the laser irradiation zone to a square with the side length of 1.0 mm. The surface features of the phase-change film after laser radiance were observed by scanning electron microscopy (FEI Quanta 200). The specimens were coated with gold–palladium before the SEM examination. The X-ray diffraction (XRD) analysis was carried out by using a computer-controlled diffractometer (D8 ADVANCE) (Cu Ka, $\lambda = 1.542$ Å) at room temperature. Data were collected in the range of $2\theta = 20$–38° with a step of 0.03°. The as-deposited GST films were confirmed to be amorphous by XRD analysis before laser radiance.

3. The computational approach

3.1. Formation of the 3D FEM model

The real geometry of the optical storing media is on the mm–nm scale, that is, the dimension of the substrate is on the mm-scale, while the GST film thickness is on the nm-scale, generally tens of nanometers. In order to avoid the divergence in calculation caused by the great geometry discrepancy between the substrate and GST film, a simplified two-layer 3D FEM model is developed in this paper and some assumptions are summarized as follows: (1) Different from the picosecond or femtosecond pulse laser treatment [18], pulse duration used in the experiment was on the nanosecond scale, which was much longer than the heat diffusion time from electron gas to lattice phonons (on the picosecond scale), therefore, the theory of Continuous Medium Heat Conduction was assumed to follow in the simulation; (2) laser irradiation zone was much smaller as compared to the whole geometry of the two-layer model so that heat transfer was assumed to take place under the semi-infinity heat conduction condition, which was verified in the model; (3) during the heating/cooling process, the phase-change from a-GST to crystalline GST (c-GST) or liquid state (l-GST) generally takes place [13]. However, for lack of data, latent heats for these transformations were neglected in the present study; (4) the temporal profile of laser pulse was Gaussian in shape, for simplification, it was assumed rectangular shape, as given in Fig. 2(a).

The total energy absorbed by the rectangular beam is described by

$$Q = A \cdot F \cdot S \tag{1}$$

where Q is the single-pulse energy, A is the absorption coefficient, F is the laser fluence, and S is the laser irradiation area. Temperature rise (ΔT) caused by the absorbed energy is then obtained by

$$\Delta T = \frac{Q}{C_p \cdot m} \tag{2}$$

where C_p is the specific heat, and m is the mass of laser irradiation zone. Because the heating time is short (30 ns) and thermal conductivity of a-GST is low (1.2 W/m·K) [19], we assume that the absorbed energy is totally used to heat the volume under the laser irradiation zone, as a result, mass of laser irradiation zone is expressed by

$$m = \rho \cdot S \cdot t \tag{3}$$

where ρ is the density of a-GST, and t is the film thickness. Substituting Eqs. (1) and (3) into Eq. (2), temperature rise is written as

$$\Delta T = \frac{A \cdot F}{C_p \cdot \rho} \cdot \frac{1}{t}. \tag{4}$$

According to Eq. (4), it shows that under the same laser fluence, temperature rise is inversely proportional to film thickness, in other words, the effect of the geometry of laser irradiation zone can be neglected. From this point of view, we constructed a nano-scale model with the same laser fluence as experiment. It further indicates that when laser fluence and film geometry are constant, the final temperature rise should be close to each other between the rectangular and

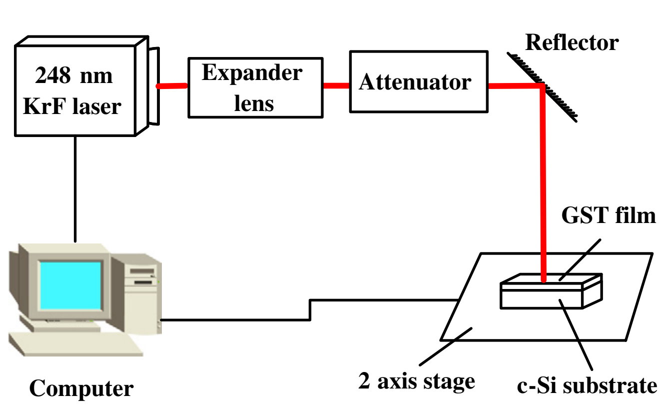

Fig. 1. Schematic illustration of the experimental set-up for the single-pulse laser radiance. Laser beam propagates along the red line.

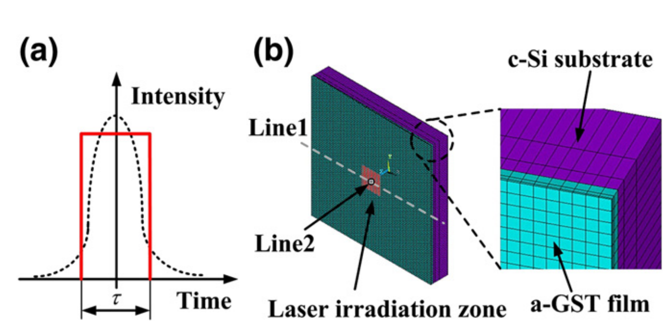

Fig. 2. Schematic of the 3D FEM model. (a) Presents the temporal profile of laser pulse, and (b) shows the construction of the FEM model. The dashed line in (a) is the Gaussian-shaped pulse, while the red solid line is the rectangular pulse for simplification. τ is the pulse duration.