Available online at www.sciencedirect.com
ScienceDirect
Physica B 387 (2007) 194–202
PHYSICA B
www.elsevier.com/locate/physb

Substrate temperature evolution in ions–surface interaction processes of pulsed laser deposition

Li Guan[a,b], Duanming Zhang[a,*], Zhihua Li[a], Xinyu Tan[a], Li Li[a], Dan Liu[a], Ranran Fang[a], Dezhi Hu[a], Gaobin Liu[a]

[a]*Department of Physics, Huazhong University of Science and Technology, Wuhan 430074, China*
[b]*College of Physics Science and Technology, Hebei University, Baoding 071002, China*

Received 4 August 2005; received in revised form 1 April 2006; accepted 5 April 2006

Abstract

We established a new heat conduction model to study transient substrate temperature in the ion-irradiation surface process of pulsed laser deposition. In this process, mean number density and kinetic energy of ions can influence the imparted energy and then substrate temperature. Since we focus on the effect of large-area temperature spike produced by the simultaneous ions, the rarefaction plasma of final-stage expansion in vacuum can be assumed to divide into a series of discrete batches according to the existing space between ions in plume. Our results show that if the ion mean number density per unit volume is lower, the elevation of substrate temperature will be weak due to less input energy and the temperature spike produced by one batch of simultaneous ions has enough time to cool because of the longer distance between the batches. In comparison, at higher ion densities, the substrate temperature rise is evident, but the plume behaves more like a heat flow resulting from a smaller interval between the sequent groups. Moreover, the influence of ion kinetic energy on temperature indicates that the improved incidence energy can obviously lead to higher transient temperature. To make the temperature spike effect clear, our model is compared with a typical continuous flow model by using the same system parameters and it is found that when the interval time between the sequent groups approximately equals the lifetime of 1D thermal spike, our result is in agreement with the result calculated by the continuous flow model. In this case, if ion mean number density or kinetic energy is increased again, the continuous flow model will be more suitable to simulate temperature evolution. The difference between both models is presented in our paper.

PACS: 81.15.Fg; 85.40.Sz; 79.20.Rf; 44.10.+i

Keywords: Pulsed laser deposition; Plasma processing; Ion–surface interactions; Heat transfer

1. Introduction

Pulsed laser deposition (PLD) technique is used widely for thin film fabrication and characterized by its pulsed nature and extremely high instantaneous deposition rate (0.02–0.1 monolayer/pulse). Here, we give a brief resume of PLD process, which can be crudely split into three subsections: (i) the technique uses high-power laser pulses (10^8–10^{10} W/cm^2) to melt, evaporate and ionize material from a target; (ii) this ablation event produces a transient high-density plasma plume that expands rapidly away from the target surface; (iii) the plume is collected on a substrate upon which the thin film grows [1].

In the case of pulsed laser ablation and deposition, the plasma is considered as an ionized gas consisting of many types of species: ions, electrons, neutrals, atoms, molecules, clusters, etc. Usually, the interaction of plasma plume with substrate surfaces has been an area of great research interest for both fundamental studies and material applications because the quality of the deposited films is critically dependent on the range and profile of the kinetic energy and density of the ablated plume [2]. Especially,

*Corresponding author. Tel.: +86 02787543882; fax: +86 02787543882.
E-mail address: lguan1@163.com (D. Zhang).

0921-4526/$ - see front matter © 2006 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2006.04.004

ions as one of the main components in plasma obtain more attentions in PLD research [3–6]. Therefore, we focus on the role of ions in plasma–surface process of PLD in the present work.

At the early stage of growing film, the species impinge from the plume to a surface and transfer their kinetic energies to substrate surface, leading to atomic-scale heating, displacement and creation of mobile vacancy or interstitial, ion mixing, etc. [7,8]. Experimentally, film growth mode, crystalline quality and number of defects in the films are found to be sensitive to ion energy [9]. Recently, the influence of ion energy on substrate surface during ions–surface process has been investigated by some researchers. Tian et al. [10] described a two-dimensional fluid model to predict substrate temperature in the process of fast-pulsing plasma immersion ion implantation. By measuring the energy influx and the substrate temperature gradient, Kersten and co-workers [11] studied the influx and its influence on the thermal balance and energetic conditions of substrate surfaces during plasma processing. Akamatsu et al. [12] reported the comparison of intense pulsed ion and laser beams as a heat source for amorphous phase formation on metal surfaces. Huang et al. [13] established a model based on the energy conservation to estimate the substrate temperature during arc ion plating. Lepone et al. [14] investigated the role of the ion beam in the heating of a substrate also. The authors mentioned above studied a temperature increase of target in long-time plasma processes without considering the transient temperature evolution, namely the thermal spike effect.

On the other hand, to explain the atom-scale effects of ion energy on the substrate and investigate the instantaneous temperature in the energetic deposition process, the concept of single-ion thermal spike is used widely. The earlier articles have discussed the thermal spike effects in single-ion surface process [15,16]. On a surface, single ion bombardment causes collision with material atoms and the atoms around the bombardment position are knocked on. The kinetic energy is mostly transferred to thermal energy, leading to form pulsed high temperature called thermal spike. The different spikes will be produced by the different incident kinetic energies. When a keV or MeV species penetrates a substrate surface, the energy per unit path length along the ion track is high; therefore, the primacy effect is the cylindrical spike [17,18]. However, at low kinetic energies, the collision only occurs in near-surface region. The energy will be transferred to the atoms just local to the point of impact, so the initial thermal spike may be considered as spherical geometry centered at a point [19]. As we all know, the energy of ions on the order of 10 or 100 eV is suitable to deposit thin film. Consequently, we consider the spherical thermal spikes are formed in the deposition process of PLD. It would be significant to study the spike effect and temperature increase in ions–surface process of PLD technique and we can neglect the sputtering events during low-energy ion beam irradiation.

Although the impact of energetic ion on surface microstructure has been extensively investigated, we study the influence of pulsed ion beam on substrate surface from a new angle of view in this paper. Using a new heat conduction model, the enhancement of substrate temperature and the instantaneous spike profile are investigated. During this ions–surface process, the influences of ion mean number density and kinetic energy on temperature rise are studied in detail.

2. Theoretical model

The interaction between one pulsed plasma and substrate surface can last for some microseconds or longer time, which is determined by laser wavelength, pulse duration time, target–substrate distance, atmosphere pressure, etc. [20]. A number of energetic ions arrive at the surface at the same time and deliver their kinetic energy to surface, and therefore substrate temperature will vary with the external short-lived heat resource. Heat conduction equation can be applied to estimate the evolution of substrate temperature during energetic deposition:

$$\rho(T)C_P(T)\frac{\partial T}{\partial t} = k(T)\nabla^2 T, \tag{1}$$

where $\rho(T)$ is the mass density of substrate, $C_P(T)$ the specific heat capacity, $k(T)$ the thermal conductivity and T the substrate temperature. Here, temperature-independent values of $\rho(T)$, $C_P(T)$ and $k(T)$ are quoted in the present calculations, because the variation of temperature with the system parameters is weak, leading to a weaker variation of thermal parameters, although the thermal diffusivity was assumed to be a simple power-law function of temperature [16,21]. Employing temperature-independent thermal parameters in calculations as a useful approximation has been justified and applied to simulate temperature profile in some works [10,19,22].

Eq. (1) has been successfully applied to study single-ion thermal spike [22,23]. Nevertheless, in PLD process, it is simultaneous that lots of ions arrive at the surface, and thus a large-scale spike rather than a single-ion spike is produced. Therefore, to make approximations to simplify the calculation and estimate the overall substrate temperature evolution, a surface heat resource instead of a point resource previously used in classic thermal spike theory is applied to the present heat conduction model. In our work, the kinetic energy of ion is selected ranging from 10 to 100 eV, so the implantation depth is more or less the same as 1 nm and much less than the heat conduction length $\sqrt{2k\tau/(\rho C_P)}$, where τ is the plume pulse duration [10,24]. As a result, although three-dimensional heat diffusion would be more accurate, typical conduction lengths are much larger than the implantation depth, the volumetric effects will be ignored. Namely, if the ion penetration range is short enough, the energy deposition can be considered almost superficial [10]. In addition, it is well known that the expansion of plume is influenced by some system