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A model for the prediction of radiation defect profiles in the semiconductor target (HgCdTe) subjected to high power short pulsed ion beams

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Abstract

A mathematical model to describe processes occurring during the irradiation of semiconductor materials with high power pulsed ion beams is proposed. The model takes account of recombination between vacancies and interstitial atoms and the formation of defect complexes and these processes are analysed and discussed. The effect of an inhomogeneous non-stationary temperature field and mechanical quasi-static and dynamic stress fields on radiation defect profiles is also examined. Spatial profiles of the charge carrier concentration and the implanted ion distribution are calculated and a comparison made with experimental profiles obtained for the semiconductor compound $Hg_{1-x}Cd_xTe$. The results show that the defect concentration profiles near the surface are reduced with a large rate of recombination between vacancy and interstitial atoms.

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1. Introduction

Recent years have seen an advance in the use of high power pulsed ion and electron beams as techniques for processing solid-state materials. Initial work has concentrated on understanding the effects on metals [1–4] where substrate heating, shock waves, vapourisation of the target and crater formation have been considered. These effects can also cause a change of mechanical properties, for example, microhardness and these changes have also been previously investigated [5–7].

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Because of their intrinsic importance with many different applications, processing of semiconductors by these high power pulsed ion beams (PIB) is now also being investigated. One such material which has many applications is $Hg_{1-x}Cd_xTe$, being a base material of devices of infra red (IR) optoelectronics. Photodiodes for a broad spectral region in the IR range (1-12 µm) are produced often by direct ion implantation whose profiles are dependent on the relative composition (x) of the compound. In one paper [8] the fusion and the cooling of surface layers $Hg_{1-x}Cd_xTe$ under the action of the laser pulse radiation were also studied. Experimental work carried out by the authors [9] investigated the effect of high-current pulsed ion beams on narrow gap solid solutions of mercury-cadmium-telluride ($Hg_{1-x}Cd_xTe$), concentrating on the detection of radiation defects in the semiconductor. In a previous publication [10] an initial calculation was made of some effects occurring in the semiconductor after irradiation by short high power ion pulses, and also computational profiles of the implanted atoms were compared with experimentally measured distributions.

Detailed calculation is necessary of some parameters describing the PIB effect for a more full comprehension of the processes occurring in a material. Of special importance is the distribution of temperature T(x,t) as a function of the depth, x, in the target, and its time variation t. The distribution of temperature is described by a modified parabolic heat conduction equation [11], the model for which is described in this paper.

Previous work has observed [10,12–14] an abnormal increase in diffusion when PIB are used compared to normal ion implantation. In our model we assume that the processes of diffusion occur as a combined effect of a short time thermal and mechanical process followed by longer time scale effects. For finding the distribution of implanted ions, radiation defects or their complexes the diffusion equation containing additional terms taking into account the effect field of temperature and mechanical stresses [10] is solved.

2. A model of the interaction of a high power pulse ion beam with a semiconductor target

The mathematical model describing the interaction of the high power pulsed ion beams with solid-state targets is composed of a number of differential equations describing processes in the target. All dependent variables are assumed to be functions of only on one space coordinate x and time t. The basic assumptions underlying the model are described below:

- The ballistic relocation of atoms during the collisional cascade is assumed to be decoupled from longer time scale diffusion processes.
- There is no stationary heating of the target. The propagation of the temperature T(x, t) field in the internal areas of the target is described by

$$\rho(T) \cdot C(T) \cdot \frac{\partial T(x,t)}{\partial t} = \frac{\partial}{\partial x} \left(\chi(T) \cdot \frac{\partial T(x,t)}{\partial x} \right) + \eta \cdot Q(x,t),$$
(1)

where η is a coefficient, which takes into account non-thermal energy losses of a beam, for example, Frenkel pair formation; $\rho(T)$ is the density of the target matter; C(T) is the coefficient of heat capacity; $\chi(T)$ is the thermal conductivity coefficient; Q(x, t) is the spatial distribution of heat sources in the sample:

$$Q(x,t) = s(t) \cdot \frac{1}{\tau} \cdot \sum_{i} E_i \cdot \Phi_i(x),$$

where *i* refers to the *i*th component species in the ion beam, the ion pulse duration is τ , E_i is the energy of the ion and s(t) is the time profile of the pulse; $\Phi_i(x)$ is the dose rate for the *i*th species [17–19]:

$$\Phi_i(x) = \frac{N_i}{\sqrt{2\pi} \cdot \Delta R_p} \cdot \exp\left(\frac{\left(a \cdot R_p - x\right)^2}{2 \cdot \Delta R_p^2}\right), \quad (2)$$

where *a* is a parameter describing the displacement energy profile relativity ion profile (*a* = 0.8) for the heat conduction equation (1) and a = 1 for all diffusion equations below. R_p and ΔR_p are the range and range width LSS [15]

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