The Numerical Simulation of Continuous Nd:YAG Laser-Annealing of InP*

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ABSTRACT

The semiconductor solid phase epitaxial model of continuous laser-annealing is used to simulate the laser-annealing process of different doping concentration of InP at the continuous Nd:YAG laser. Specially, quasi-static model is used to simulate the radial heat dissipation from radiant region to radiationless region. At the same time, thermal conductivity and optical absorption coefficient varied with temperature is also considered. The method of hidden-form different is used in solving one-dimensional, non-homogeneous, nonlinear partial differential equation of heat conduction. At the room temperature T_0=300K and the power intensity of laser I_0=800W/cm^2, the result is that the temperature of surface reaches about 1290K after 3.8sec.

Keywords: InP, laser-annealing, numerical simulation, quasi-static model.

1. INTRODUCTION

The laser-annealing is widely used in semiconductor materials and making techniques of devices. But the theory is very complicated and the process conditions are hard to grasp so that a better result can only be obtained by modulating many experiments. If the numerical calculative method can be used in the simulation of the process of laser-annealing, it will give guides in the technology of laser-annealing. In this paper, according to the semiconductor solid phase epitaxial model of continuous laser-annealing, the process of continuous Nd:YAG laser-annealing of InP has been simulated.

2. PHYSICAL MODEL

If a sample absorbs photons, carriers excited by photons heat the location of the sample by colliding. At the same time, heat will be conducted to other regions not irradiated of the sample by thermal conduction. The equation of heat conduction is expressed by:

$$c\rho\,(\partial T/\partial t)=Q_{in}-Q_{out}-\nabla\bullet\vec{F}$$

Where c is specific heat, ρ is density, T is the distribution of temperature in the sample, Q_{in} and Q_{out} is the power intensity of absorption and dissipation of the sample respectively, $\vec{F}$ is the vector of heat flow. When no scanning, $\vec{F}=-K\nabla T$. K is the thermoconductivity that is a function of temperature.

At normal conditions, the diameter 2a of a laser beam is much greater than the thickness l of a sample (ref. to Fig.1). So the three-dimensional equation of heat conduction can be reduced to a one-dimensional, non-homogeneous, nonlinear partial differential equation which has no analytical solution.

$$c\rho\,(\partial T/\partial t)-K(\partial^2 T/\partial z^2)=Q_{in}-Q_{out} \quad (1)$$

Fitting the experimental data of InP[1-2] gives: $K(T)=1.0/(-1.24356+8.9072*10^{-3}*T)$

Q_{in} depends on optical absorption coefficient. At the conditions of low power intensity of laser and photon energy lower than the band gap of InP, the free carrier absorption coefficient α is the main part of optical absorption coefficient.

$$\alpha=N_c\sigma_{FC}$$

Where N_c is the free carrier concentration and σ_{FC} is cross section. N_c is given in[3]:

$$N_c=N_0+4(2\pi kT/h^2)^{3/2}(m_e m_h)^{3/4}\exp(-Eg(T)/(2kT))$$

Where N_0 is the concentration of ionized impurities and Eg (T) is the band gap of InP given in[4]:

$$Eg(T)=1.421-23.63*10^{-4}T^2/(T+162)$$

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σ_{FC} is given in[5] $\sigma_{FC}=e^2\lambda^2/(\pi m^* n c^3 \tau)$. λ is the wavelength (1.06μm) of laser, m^* is the effective mass of carrier. For InP, electron effective mass $m^*_e=0.077m_0$, hole effective mass $m^*_h=0.64m_0$[6]. n is the refractive index, τ is the colliding time ($\tau=m^*\mu/e$). μ is the mobility of carrier in InP which is a complicated function of temperature T and doping concentration N_0. Fitting the experimental data of InP [7-9] gives the expression for μ (T, N_0):

$$\mu_n(T, N_0)=2.4*10^4(T/300)^{-1.72}/(1+(N_0/1.7*10^{-7})^{0.054})$$
$$\mu_p(T, N_0)=3.85*10^4(T/300)^{-1.53}/(1+(N_0/1.7*10^{-7})^{0.151})$$

Here, $\mu_n(T, N_0)$ is mobility of electrons and $\mu_p(T, N_0)$ is mobility of holes. In the every step of time of numerical calculation, we assume a model that the irradiated region and its around will put up steady distribution of temperature by thermal conduction. Consequently the heat dissipation of radial conduction can be evaluated. So the model is named as quasi-static model.

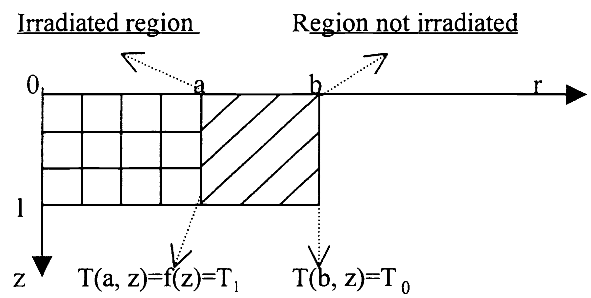

Fig. 1 The schematic diagram of quasi-static model

In the cylindrical cycle of a<r<b and 0<z<l, the temperature satisfies the Laplace Eq.: $\triangle T=0$

The boundary conditions: $\left.\frac{\partial T}{\partial z}\right|_{z=0,l}=0$; $T(a, z)=f(z)=T_1$; $T(b, z)=T_0$

Solving the Laplace Eq. gives:

$$T(r, z)=\frac{T_0\ln(r/a)+T_1\ln(b/r)}{\ln(b/a)} \quad \text{and} \quad \left.\frac{dT}{dr}\right|_{r=a}=\frac{T_0-T_1}{a\ln(b/a)} \tag{2}$$

Where b/a is 1.6 for InP. So for unit bottom area of cylinder, the dissipation of unit length of side face is given in:

$$Q_{rout}=-2\sqrt{\pi}\left(K\frac{dT}{dr}\right)_{r=a}$$

3. METHOD OF CALCULATION

A partial linear method is used to solve one-dimensional non-homogeneous nonlinear partial differential equation. In detail, we get the difference grid at the axis of space and time and assume Δz, Δt as the variations:

$$Z_k=k\triangle z \quad k=0,1,\cdots,n+1; \quad t_j=j\triangle t \quad j=0,1,\cdots m$$

The backward difference at the axis of time and the central difference at the axis of space are able to get a different form that is expressed by:

$$(\triangle_t T)_{k,j}=(T_{k,j}-T_{k,j-1})/\triangle t \tag{3.1}$$
$$(\delta^2_z T)_{k,j}=(T_{k+1,j}-2T_{k,j}+T_{k-1,j})/(\triangle z)^2 \tag{3.2}$$

Thermal conductivity K of each space layer is assumed to be constant in the partial linear method. Consequently thermal conductivity K can be extracted from the symbol of partial differential. At the point of difference grid, the equation (1) can be expressed by:

$$c\rho\,(\triangle_t T)_{k,j}-k(T_{k,j-1})(\delta^2_z T)_{k,j}=(Q_{in})_{k,j-1}-(Q_{rout})_{k,j-1} \tag{4}$$

Here $$p_{k,j}=k(T_{k,j})\triangle t/c\rho(\triangle z)^2 \tag{5}$$

Combining equation (3.1), (3.2), (4) and (5) we obtain:

$$(1+2p_{k,j-1})T_{k,j}-p_{k,j-1}T_{k-1,j}-p_{k,j-1}T_{k+1,j}=T_{k,j-1}+\Delta t/(c\rho)[(Q_{in})_{k,j-1}-(Q_{rout})_{k,j-1}] \quad (6)$$

This is a hidden-form equation.

Here $$(Q_{in})_{k,j-1}=I(1-R)(1-e^{-\alpha_k \Delta z})\Delta t\times\exp(-\Delta z\sum_{i=1}^{k-1}\alpha_i)$$

$$(Q_{rout})_{k,j-1}=-2\sqrt{\pi}\,K(T_{k,j-1})\frac{T_{k,j-1}-T_0}{a\ln(b/a)}\Delta t\Delta z$$

Where I is the power intensity of continuous Nd:YAG laser and R is the coefficient of infrared reflection. The exchange of radiative heat dissipation and the exchange of natural cooling by air convection is considered. If we select the condition of adiathermic boundary which is given in $(\partial T/\partial z)\mid_{z=0,l}=0$, the according simulation of difference is expressed by $T_{0,j}=T_{1,j}$, $T_{m,j}=T_{m+1,j}$. While we select the condition of constant temperature boundary, a condition will be changed to $T_{m+1,j}=T_0$. The initial condition is given in $T_{k,0}=T_0$.

The equations (6) and conditions constitute the complete coupled set of equations of one-dimensional nonlinear equation of heat conduction. Using these equations, we can accurately work out the distribution of temperature (T(z, t)) at the surface and in the bulk of a sample, So the thickness of recrystallization is given in [10]:

$$\xi=\xi_0\int_0^t \exp[-(E_a/K_B/T(t'))]dt'$$

Where K_b is the Boltzmann constant and E_a is the activation energy. For InP, E_a=2.03ev, $\xi_0=3.2\times10^{13}$nm/s.

4. RESULTS

The rudimentary calculated parameters are: the thickness of InP l=300 μ m, the coefficient of infrared reflection R=0.3, the step of space Δz=0.1 μ m, the step of time $\Delta t=10^{-2}$ sec, the diameter of a laser beam ra=0.2cm, the power intensity of laser $I_0=800W/cm^2$. The result is that the temperature of surface reaches about 1290K after 3.8 second.

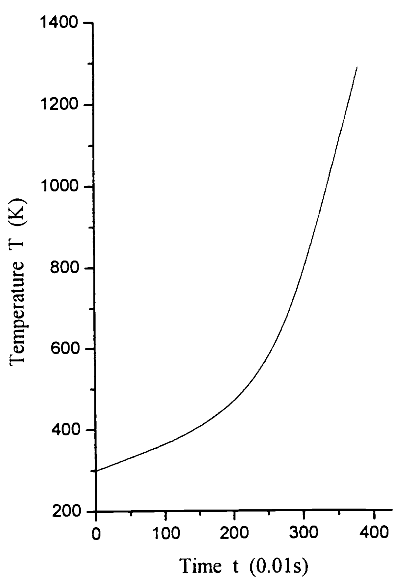

Fig. 2 Temperature versus time

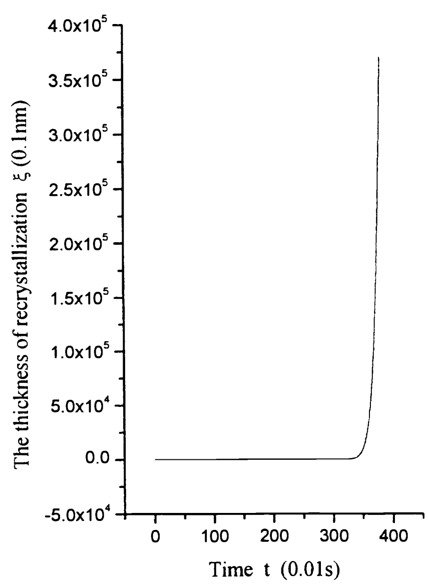

Fig. 3 The thickness of recrystallization versus time

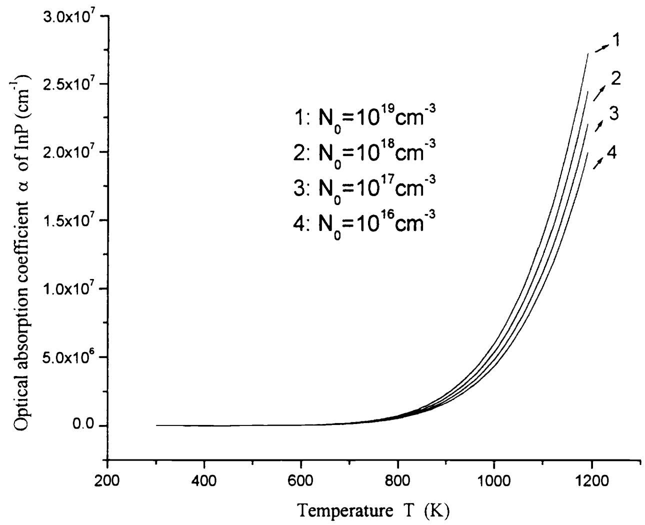

Fig.4 Optical absorption coefficient for different doping concentration (N_0) of InP versus temperature

5. DISCUSSION

Continuous Nd: YAG laser (wavelength λ=1.06μm) is used in laser-annealing. Its power intensity is 800W/cm^2. The highest temperature of InP sample is about 1290K that is lower than the melting point of InP. So the semiconductor solid phase epitaxial model is suitable.

The overt-form different equation used in laser-annealing demands the condition of $K\Delta t/C\rho(\Delta z)^2<0.5$. So it can only be used in the pulse laser-annealing. In this paper, the hidden-form different equation is used. Because it does not need this condition, the equation can be used in pulse or continuous laser-annealing.

No paper reported the optical absorption coefficient of InP varied with temperature and doping concentration until now. We use the classical formula of free carrier absorption to obtain the optical absorption coefficient at photon energy lower than the band gap of InP. From Fig.4., we find that at high temperature the excitation of band edge will dominate and the doping concentration of InP is not important. We have induced Zn into InP by Nd:YAG laser[11]. Using this paper's model and numerical simulation, good results have been obtained. The results in detail of this work will be published.

In this paper, the exchange of radiate heat dissipation and the exchange of natural cooling by air convection is considered. From the result of calculation, we find it has little influence.

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