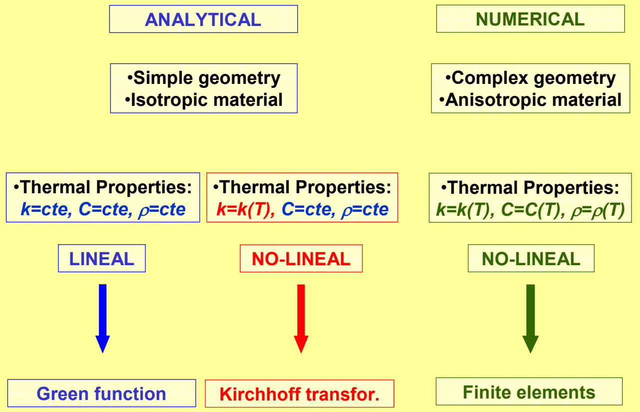
International Conference on
PHOTO-EXCITED PROCESSES & APPLICATIONS
(4-ICPEPA)
September 5-9, 2004
Contribution Mo-P22

ANALYTICAL AND NUMERICAL CALCULATIONS OF THE TEMPERATURE DISTRIBUTION ON Si AND Ge INDUCED BY EXCIMER LASERS

J.C.Conde, P.González, F.Lusquiños, S.Chiussi, J.Serra, B.León
Universidade de Vigo, Dpto. Física Aplicada, Lagoas Marcosende 9, E-36200 Vigo, Spain

Dpto. de Física Aplicada
UNIVERSIDADE DE VIGO

Mathematical Methods



ANALYTICAL

NUMERICAL

- •Simple geometry
- •Isotropic material

- •Complex geometry
- •Anisotropic material

•Thermal Properties: *k=cte, C=cte, ρ=cte* → LINEAL → Green function

•Thermal Properties: *k=k(T), C=cte, ρ=cte* → NO-LINEAL → Kirchhoff transfor.

•Thermal Properties: *k=k(T), C=C(T), ρ=ρ(T)* → NO-LINEAL → Finite elements

Heat Conduction Differential Equation

ANALYTICAL

Green function

$$\nabla^2[T(r,t)]=\frac{1}{\mathrm{D}}\frac{\partial T(r,t)}{\partial t}$$

Thermal diffusivity

$$\mathrm{D}=\frac{k}{\rho C}$$

$$-k\left.\frac{\partial T}{\partial z}\right|_{z=0}=I(r,t)$$

$$k\left.\frac{\partial T}{\partial n_i}\right|_{S_i\neq(z=0)}=0 \qquad t>0$$

$$T(r,0)=T_o \quad \text{Volume, t=0}$$

Gaussian intensity distribution

$$g_c=AI_o\,\mathrm{Exp}[-(\frac{x}{R_x})^2-(\frac{y}{R_y})^2]$$

$$I(r,t)=g_c\sum_{u=0}^{n}(-1)^n\mathrm{H}(t-ud)$$

Single pulse (*u*=1)

$$T(r,t)=\frac{AI_oR^2}{\mathrm{k}}\sqrt{\frac{D}{\mathrm{k}}}\int_{\tau=0}^{t}\frac{\mathrm{Exp}[-\frac{x^2+y^2}{4\mathrm{D}(t-\tau)+R^2}]\mathrm{Exp}[-\frac{z^2}{4\mathrm{D}(t-\tau)}]}{\sqrt{t-\tau}[4\mathrm{D}(t-\tau)+R^2]}\{\mathrm{H}(\tau)-\mathrm{H}(\tau-d)\}d\tau$$

Kirchhoff transfor.

$$\nabla[k(T)\nabla T(r,t)]=\rho C\frac{\partial T(r,t)}{\partial t}$$

$$-k\left.\frac{\partial T}{\partial z}\right|_{z=0}=I(r,t)$$

$$k\left.\frac{\partial T}{\partial n_i}\right|_{S_i\neq(z=0)}=0 \qquad t>0$$

$$T(r,0)=T_o \quad \text{Volume, t=0}$$

$$\nabla^2[V(r,t)]=\frac{1}{\mathrm{D}}\frac{\partial V(r,t)}{\partial t}$$

$$-k_o\left.\frac{\partial V}{\partial z}\right|_{z=0}=I(r,t)$$

$$k_o\left.\frac{\partial V}{\partial n_i}\right|_{S_i\neq(z=0)}=0$$

$$V(r,0)=\sum_{n=1}^{m}\frac{a_n}{n}(T^n(r,t)-T_o^n)$$

No-lineal system

$$\mathrm{D}(T)=\frac{k(T)}{\rho C}$$

Polinomial function: $k=k(\mathrm{T})=k_o\sum_{n=1}^{m}a_n\,T_{n-1}$

Lineal system

↔ $\mathrm{D}(T)=cte$

Kirchhoff transformation: $V=\int_{T_o}^{T}\frac{k(T')}{k_o}dT'$

Solution: one of the system roots. *T(r,t)* is provided for *V(r,t)*.

$$\sum_{n=1}^{m}\frac{a_n}{n}T^n(r,t)-V(r,t)=0$$

NUMERICAL (F.E.M.)

$$\nabla[k(T)\nabla T(r,t)]=\frac{\partial H(T)}{\partial t}$$

$$-k\left.\frac{\partial T}{\partial z}\right|_{z=0}=I(r,t)$$

$$k\left.\frac{\partial T}{\partial n_i}\right|_{S_i\neq(z=0)}=0 \qquad t>0$$

$$T(r,0)=T_o \quad \text{Volume, t=0}$$

Phase changes → **Enthalpy**

$$H(T)=\int_{To}^{T}\rho(T')C(T')dT'+\mathrm{H}(T-T_f)\mathrm{L_f}$$

Intensity function:
$I(r,t)=P(F,\tau)\,G(A,\theta)$

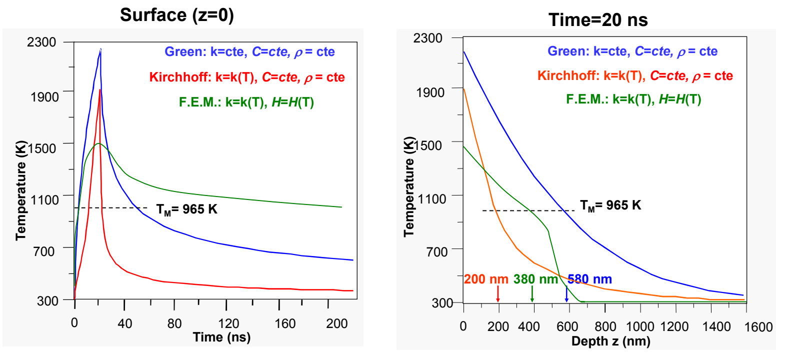
Laser parameters
$P(F,\tau)=a[F,dS(t)/dt]\,\tau\,Exp[-U\tau]$

Material Properties
$G(A,\theta)=[1-R[(n,\kappa),\theta]]\,\mathrm{Cos}\theta$

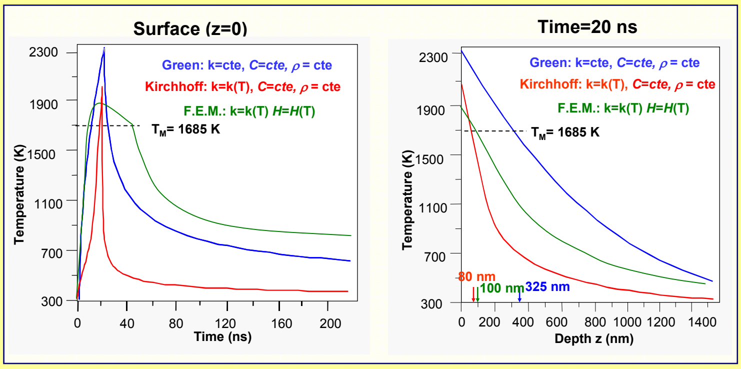
ANSYS(8.0)

Results

Amorphous germanium, Φ=0.42 J/cm^2

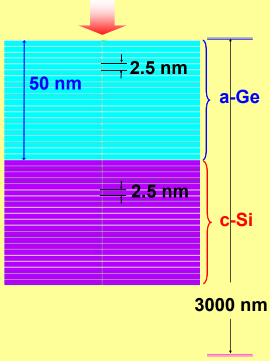


Crystalline silicon, Φ=0.93 J/cm^2

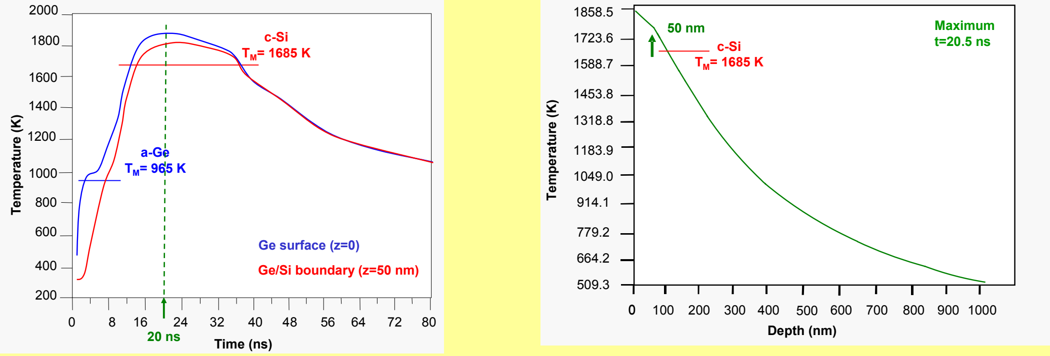


- •Profile of temperature distribution vs. time and depth obtained by the Green and Kirchhoff resolution method are similar.
- •Numerical method (F.E.M.) presents smooth transitions between heating and cooling processes due to the incorporation of material phase changes.
- •For all cases, Ge melting point is quickly reached after a few ns and maximum temperature is obtained after 20 ns (pulse length).

Application: Pulsed Laser Induced Epitaxy (PLIE)



a-Ge film (50 nm) onto c-Si substrate, Φ=0.55 J/cm^2



- •Numerical calculations by ANSYS of the temperature distribution induced by an ArF excimer laser (193 nm, 20 ns, 0.55Jcm^{-1}) on an amorphous germanium film (50 nm) deposited onto a crystalline silicon bulk.
- •Laser intensity distribution incorporates the Beer-Lambert exponential decreasing with depth.
- •a-Ge (surface) Melting temperature is reached after 3 ns; c-Si melting temperature is reached after 13 ns, and the melting depth is around 110 nm.

Conclusions

Analytical and numerical methods can be successfully applied to calculate thermal processes induced by laser irradiation. Complex physical process like PLIE should be attempted by finite elements methods.

The calculations of the temperature distributions induced by excimer lasers on semiconductors materials and thin films demonstrate the potential of these mathematical tools on the laser processing.

Acknowledgements

Xunta de Galicia

MINISTERIO DE CIENCIA Y TECNOLOGÍA

UNIVERSIDADE DE VIGO

For further information please mail to: *jconde@uvigo.es*