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FINITE ELEMENTS ANALYSIS OF HETEROEPITAXIAL SiGe LAYERS GROWN BY EXCIMER LASER

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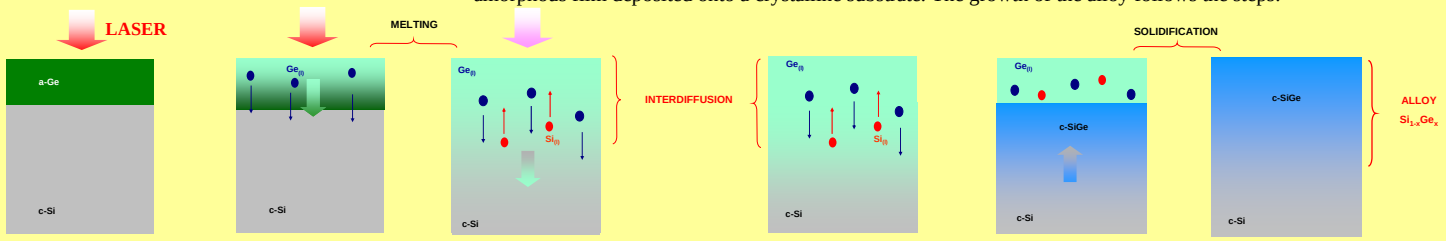
PULSED LASER INDUCED EPITAXY (PLIE)

Technique based on the application of the correct amount of the energy density to provoke the melting of the amorphous film deposited onto a crystalline substrate. The growth of the alloy follows the steps:



Excimer laser radiation impinges on a-Ge film deposited onto c-Si substrate

Melting of the a-Ge layer and c-Si substrate (partially). Melting front moves forward into the substrate.

Interdifussion of atoms among film and substrate in the liquid phase. **Maximum** melting thickness.

Solidification front moving forward to the surface.

Heteroepitaxial SiGe alloy formation.

RESULTS

Finite Elements Method: F.E.M.

Heat Conduction Differential Equation

Phase changes ⟶ Enthalpy

$$\nabla[k(T)\nabla T(r,t)] = \frac{\partial H(T)}{\partial t} \qquad H(T) = \int_{T_0}^{T} \rho(T')C(T')dT' + \mathrm{H}(T - T_l)L_i$$

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

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

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

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

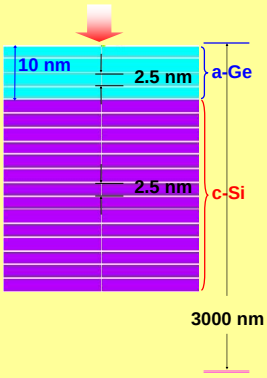
Laser parameters: $P(F,\tau) = a[F, dS(t)/dt]\,\tau Exp[-U\tau]$

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

Beer-Lambert law: $Exp(-\alpha z)$

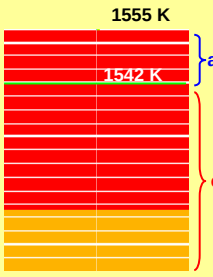
Finite Elements Analysis: ANSYS(8.0)

Geometry and Mesh

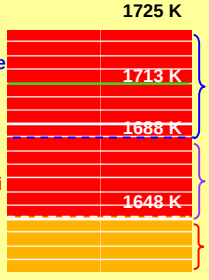


Temperature distribution on mesh

Failed epitaxial grown — Φ = 0.50 J/cm²



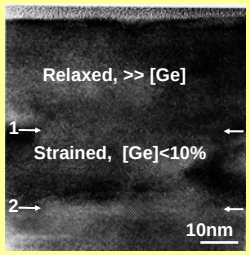
Good epitaxial grown — Φ = 0.55 J/cm²



Numerical simulation for two different laser fluences. For Φ= 0.55 J/cm², the melting temperature of silicon is reached (T_M =1685 K).

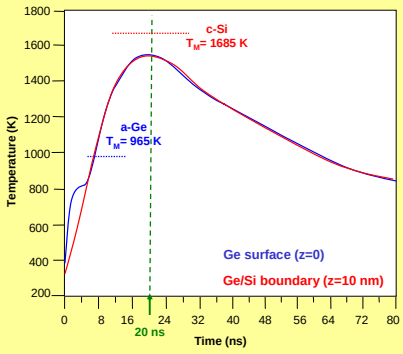
Experimental

SiGe alloy by PLIE HR-TEM image

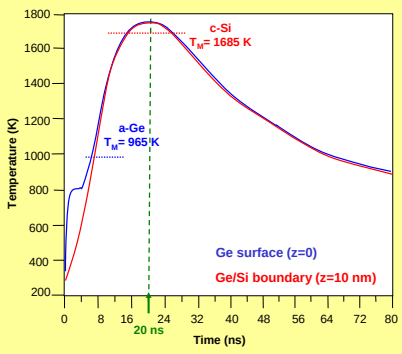


a-Ge film (10 nm) deposited onto c-Si irradiated with KrF laser (248 nm, 20 ns)

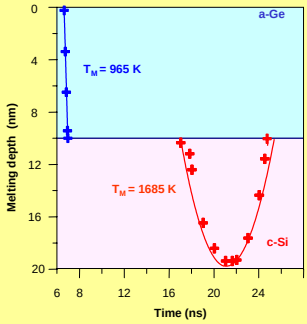
Temperature versus time



Φ = 0.50 J/cm²



Melting depth versus time



Φ = 0.55 J/cm²

CONCLUSIONS

The mathematical model developed in this study demonstrates that the laser energy density is a critical parameter in the PLIE process. Nevertheless, the intermediate layer formation can not be predicted because the diffusion effects had not been considered.

The heteroepitaxial alloys formation induced by laser has been analysed by finite elements method. Numerical simulations show that the laser energy density is a key parameter to induce the epitaxial growth. Theoretical results of melting depth and threshold energy density have successfully corroborated with the experimental data.

Acknowledgements

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