Optimization of Thermal Properties
Identification of Complex Thin films
Using MATLAB® and COMSOL Multiphysics®

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Motivations

- **Study of thermal properties for thin films:**
  - AlN (Highly conductive)
  - YSZ (ceramics thin film)
  - Metals
  - Dielectric films...

- **Their applications in next generation microelectronic devices:**
  - QCL, HEMT, Thin film fuel cells

- **Fundamental knowledge of condensed matter thin film state:**
  - mesoporous Si, CNTs...
  - J.Phys.D 2011, J.A.P. 2012, ...
Principle of PhotoThermal method

- Absorption of laser pulse energy $\rightarrow$ rapid increase of temperature and then relatively slow temperature decrease
- Detector calibration curve $U(T)$ – heating support
- Experiment evaluation: $U(t) \rightarrow T(t)$
Experimental Setup

Photo-thermal nano-second

Sample holder
What is thermal identification?

Temperature of the IR detector from Ti/AlN sample surface after laser beam fluence of 4,8 mJ/cm²

Built a realistic model to fit well the experimental curves based on the multilayer system physical parameters
1- 1D analytical model for multilayer thin films (Balageas): 
Matlab Experiments gives 3 group of parameters

\[
\psi_D(t) = \frac{\theta_D(t)}{\theta_\infty} = 1 + 2 \sum_{i=1}^{2} x_i \omega_i \sum_{k=1}^{\infty} \frac{\sum_{i=1}^{2} x_i \cos(\omega_i \gamma_k)}{\sum_{i=1}^{2} x_i \omega_i \cos(\omega_i \gamma_k) - (\gamma_k \sin(\omega_i \gamma_k) - \gamma_k \sin(\omega_i \gamma_k))} \exp\left(-\frac{\gamma_k^2 t}{\eta_2^2}\right)
\]

**Eigenvalues problem**

2- Comparison with the 3D model namely for low conductive and complex thin films:
Creation of full model under Comsol:
Thin films/participating media (Heat Transfer Module)
3D Model in COMSOL – heat source

- Laser penetration into depth of sample is ruled by Beer-Lambert law

\[ I(z) = I_0 \cdot e^{-az} \]

- Optical properties:
  complex refractive index
  absorption coefficient

\[ n = n_1 + in_2 \]

\[ a = \frac{2\omega n_2}{c} = \frac{4\pi n_2}{\lambda} = \frac{2}{\delta a} \]

<table>
<thead>
<tr>
<th>Material</th>
<th>( n_1 )</th>
<th>( n_2 )</th>
<th>( a ) (m(^{-1}))</th>
<th>( \delta a ) (nm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>0.19</td>
<td>2.94</td>
<td>0.1490 \times 10^{-9}</td>
<td>13.4253</td>
</tr>
<tr>
<td>Cu</td>
<td>1.12</td>
<td>1.88</td>
<td>0.0953 \times 10^{-9}</td>
<td>20.9949</td>
</tr>
<tr>
<td>W</td>
<td>3.4</td>
<td>0.14</td>
<td>0.1444 \times 10^{-9}</td>
<td>13.8493</td>
</tr>
</tbody>
</table>
Modeling of UV laser beam absorption

Heat source distribution

1 to 3 nm
100 nm
But also the real time distribution ….

Function of laser energy

deconvolution ….

and linear variation of pics
3D Model in COMSOL: Si/YSZ/Ti

Ti: ρ1, c1, k1

YSZ: ρ2, c2, k2?

Bulk silicon: well known properties
Our new strategy:
1 - Starting 1D with Matlab (Balageas model)
2 - Then Livelink to Run Comsol.
       Running this loop until convergence of thermal fields:
3 - **Output data**: density, thermal conductivity, heat capacity
Output data: best results!

\[ \rho = 3600 \text{ kg.m}^{-3} \]
\[ c = 550 \text{ J.K}^{-1}.\text{kg}^{-1} \]
\[ k = 7 \text{ W.m}^{-1}.\text{K}^{-1} \]

Si/YSZ/Ti multilayer
Yttria-Stabilised-Zirconia (YSZ)

\[ k \text{ phonon (opaque)} = 6 \text{Wm}^{-1}\text{K}^{-1} \]

\[ k \text{ photon (STM)} = 4 \text{Wm}^{-1}\text{K}^{-1} \]

Optical parameters: \( R, n_1, n_2 \)
Conclusions

- New way for the optimization of thermal properties identification.

- But high number of loops, and long computation time.

- Is the ‘Optimization Module’ able to do faster computations using more adapted models?
THANKS
Experimental system - schematic view