ELI-ALPS Research Institute
TOWARDS THE SHARP END OF ATTOSCIENCE

LIGHT INDUCED ULTRAFAST THERMAL PROCESSES IN METAL: THERMAL EVOLUTION TO MATERIAL DAMAGE

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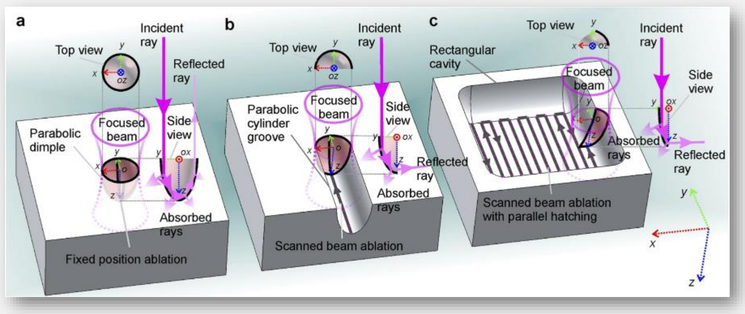
Introduction

Motivation

- Micro-machining of thin 3D materials or 2D materials with ultrafast laser pulses is currently active area of research.
- Availability of accurate models of material processing provides theoretical understanding of experimental parameters and informs avenues of future development.



Scientific Reports **8**, 17376 (2018)

- Model discussed here analyzes the effects of micro-machining materials from an oblique angle, which can be used for fluence control and creation of oblong damage craters.

Theory

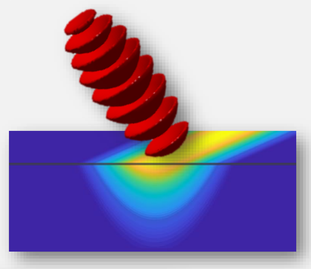
- The two-temperature model (TTM) assumes thermal energy in a material is made up of electron temperature and lattice or phonon temperature.
- TTM has been successful in describing pico- and femto-second processes in which electron and lattice temperatures are coupled but not equal, such as ultrafast laser damage.

$$C_e \partial_t T_e = \nabla \cdot [k_e \nabla T_e] - G(T_e - T_l) + Q$$
$$C_l \partial_t T_l = \nabla \cdot [k_l \nabla T_e] + G(T_e - T_l)$$

Description of Model – Source Term

Gaussian Beam

- Full Gaussian beam formalism used to find incident energy on material surface.
- 7 beam parameters: intensity, waist size, wavelength, angle of incidence, beam divergence, polarization, and pulse duration



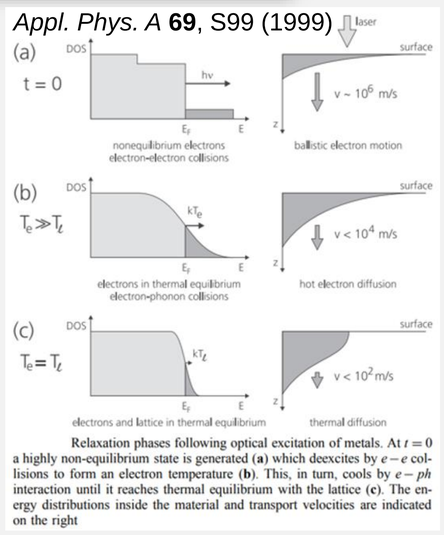
$$E(r,z,t) = A_0 \frac{\sigma_0}{\sigma(z)} \exp\left[-\left(t - \frac{r^2}{2cR(z)}\frac{z}{c}\right)^2 \frac{1}{2t_0^2}\right] \times \exp\left[-\frac{r^2}{\sigma^2(z)} + \frac{r^4}{2\sigma^4(z)}\left(\frac{\delta_0}{\omega_0}\right)^2\right] \times \exp\left\{i\omega_0\left[1 - \frac{r^2}{\sigma^2(z)}\left(\frac{\delta_0}{\omega_0}\right)^2\right]\left[t - \frac{r^2}{2cR(z)} - \frac{z}{c}\right]\right\} \times \exp[i\phi(z)]$$

$$\phi(z) = \tan^{-1}\left(\frac{z}{z_0}\right) \qquad R(z) = z\left[1 + \left(\frac{z_0}{z}\right)^2\right] \qquad \sigma^2(z) = \sigma_0^2\left[1 + \left(\frac{z}{z_0}\right)^2\right] \qquad z_0 = \frac{\pi\sigma_0^2}{\lambda_0}$$

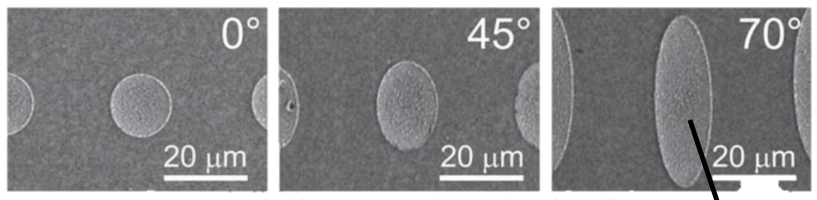
Absorption Model

- Fresnel reflection coefficients and Beer-Lambert law distribute incident energy throughout target volume.
- Oblique angle introduces polarization dependence of absorption.

Appl. Phys. A **69**, S99 (1999)



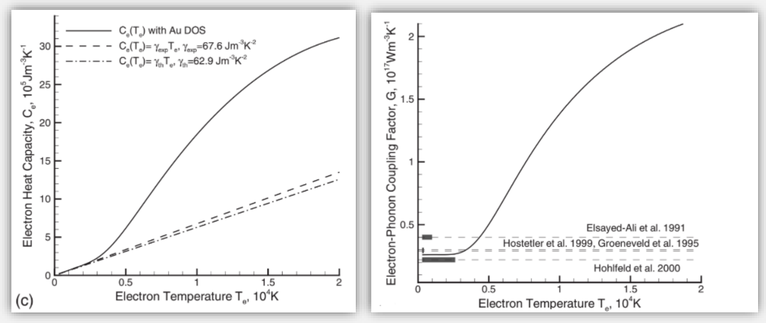
Relaxation phases following optical excitation of metals. At $t = 0$ a highly non-equilibrium state is generated (**a**) which deexcites by $e-e$ collisions to form an electron temperature (**b**). This, in turn, cools by $e-ph$ interaction until it reaches thermal equilibrium with the lattice (**c**). The energy distributions inside the material and transport velocities are indicated on the right



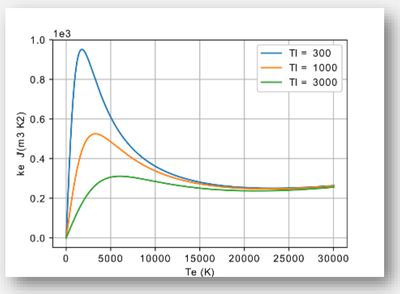
Appl. Phys. Lett. **109**, 161604 (2016)

Characteristic damage of gold

Description of Model – Thermal Properties



Physical Review B **77**, 075133 (2008)



- TTM model highly nonlinear with introduction of temperature dependent heat capacities $C_{e,l}$ and conductivities $k_{e,l}$.
- C_e and coupling term G determined by electron density of state (DOS).

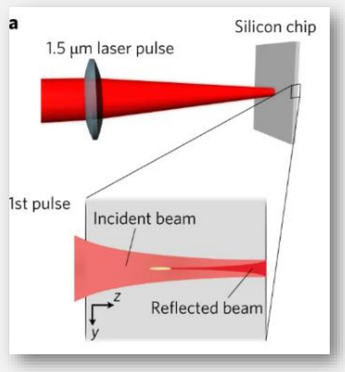
Outlook

Description of Dielectrics

- Modeling of band structure and transitions extends use of simulation beyond metals.

Subsurface Targeting

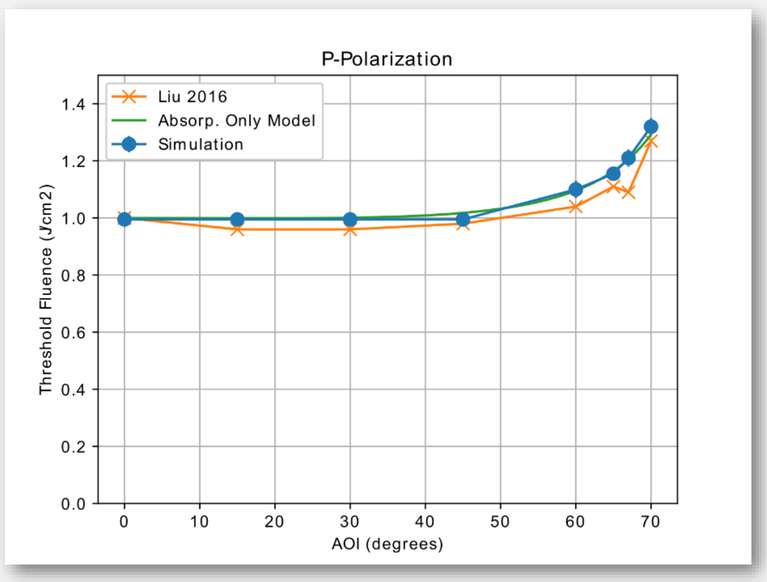
- Multilayer surfaces provide secondary reflections that can focus the beam within a material.

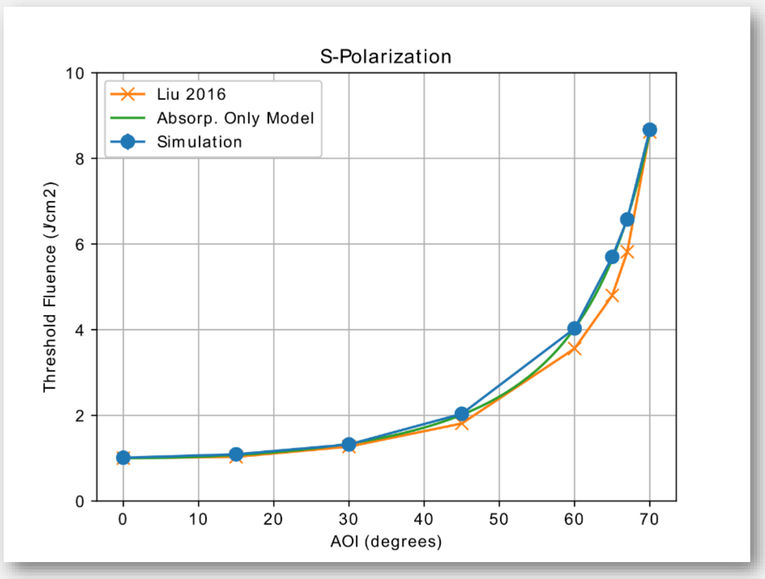


Nature Photonics **11**, 639–645 (2017)

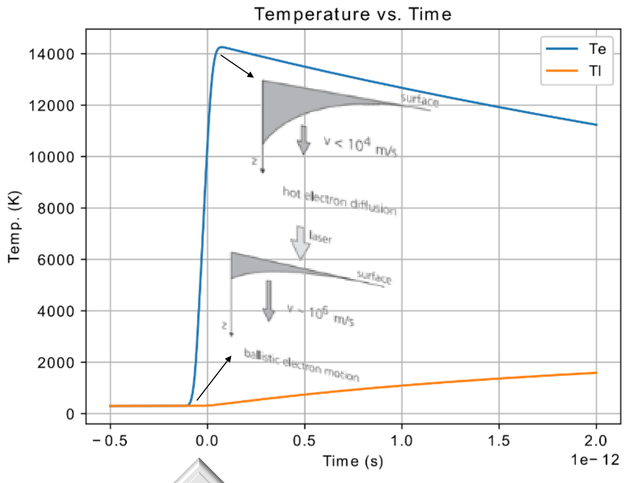
Results

- Comparison with experimental threshold fluence analysis on gold





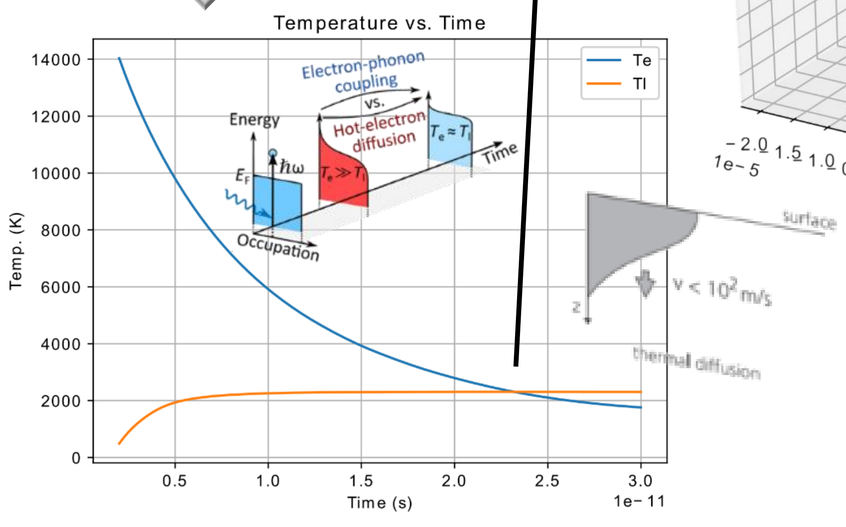
- Simulation shows good agreement with experimental results.
- Absorption only model, which accounts for only threshold changes due to increased spot size and Fresnel reflection, is responsible for most of the threshold dependence on angle.



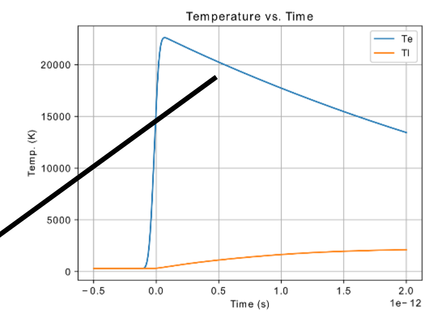
Short Scale 10-1000 fs

Long Scale 1-30 ps

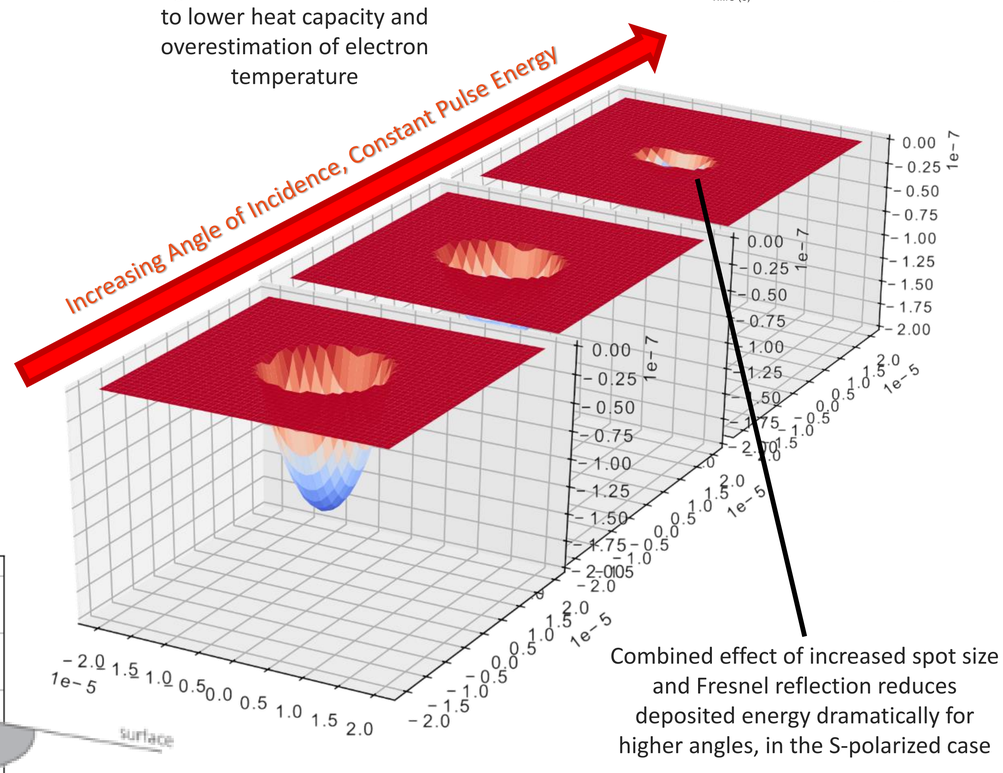
Asymptotic convergence of two temperatures initially prevented by conduction of energy away from the warmest regions of the target



Effect of *d*-Band Excitation



Neglect of electron DOS leads to lower heat capacity and overestimation of electron temperature



Combined effect of increased spot size and Fresnel reflection reduces deposited energy dramatically for higher angles, in the S-polarized case

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