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Molecular Dynamics Simulation of Femtosecond Laser Interactions with Si: Interplay of Pressure and Temperature Profiles

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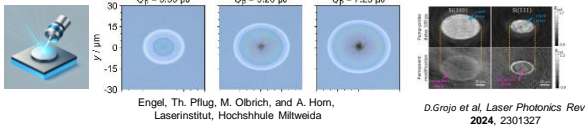
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HAL Authorization

Amorphization of Si (ANR LAMRSIM)



Fs lasers can provide numerous advantages:

- One-step processing
- Reduced heat-affected zone
- Thinner laser-modified region

Strong interest for microelectronics
(collaboration with STMicroelectronics, France)

MD-nTTM Model for fs Laser Interactions with Si

Two-Temperature Model (TTM) + additional equation for density of carriers
Drude-Lorenz model for reflectivity and free carrier absorption

$$\frac{dI(z,t)}{dz} = -(\alpha + \alpha_{FCA}(\epsilon(N_e)))I(z,t) - \beta I^2(z,t) \quad \text{Laser propagation}$$

$$\frac{\partial n_e}{\partial t} = \frac{\alpha I(z,t)}{h\nu} + \frac{\beta I^2(z,t)}{2h\nu} + \delta n_e - \gamma N_e^2 - \nabla \cdot \mathbf{j}(n_e T_e E_g) \quad \text{Free carriers excitation}$$

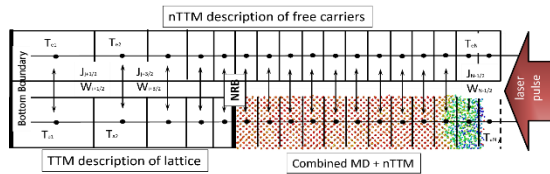
$$\frac{\partial U_e(N_e T_e E_g)}{\partial t} = (\alpha + \alpha_{FCA}(\epsilon(N_e)))I(z,t) + \beta I^2(z,t) \quad \text{Absorption}$$

$$-\nabla \cdot \mathbf{W}(N_e T_e E_g) - \frac{C_e - h(N_e T_e E_g)}{\tau_e} (T_e - T_l) \quad \text{TTM + MD}$$

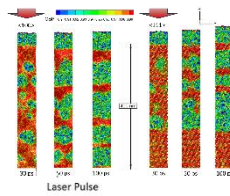
$$C_l \frac{\partial T_l}{\partial t} = \nabla \cdot (\kappa \nabla T_l) + \frac{C_e - h(N_e T_e E_g)}{\tau_e} (T_e - T_l) \rightarrow I(t) = P(1 - R(t)) \frac{1}{4} \sqrt{\frac{2}{\pi}} \exp\left(-\frac{(t-t_0)^2}{\tau^2}\right)$$

$$m_i \frac{d^2 \mathbf{r}_i}{dt^2} = -\sum_{j=1,N} \nabla U(\mathbf{r}_{ij}, T_e) + \xi m_i \mathbf{V}_i^T$$

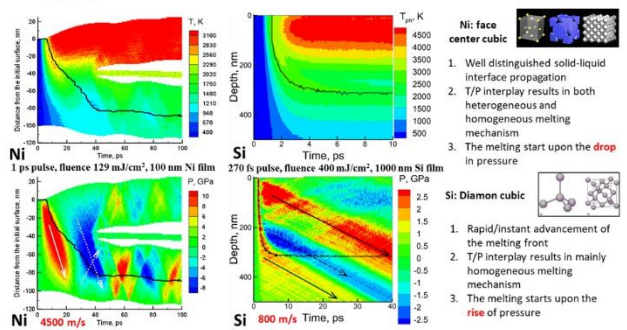
$$R = \frac{R_{\text{static}} + R_{\text{dynamic}}}{1 + \frac{\omega^2}{\omega_0^2}} \quad \text{and} \quad \alpha_{FCA} = \frac{4\pi e^2 N_e}{c} \frac{\omega_0^2}{\omega^2}$$



Melting Kinetics in Si : <001> and <111>



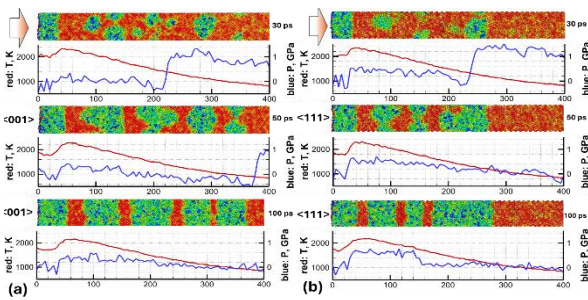
Two identical samples but <001> and <111> at 100fs, 0.3 J/cm²
Heterogeneous vs homogeneous melting mechanism
<001> results in 26% more melt
Speed of sound in <111> is 8% higher



1. Well distinguished solid-liquid interface propagation
 2. T/P interplay results in both heterogeneous and homogeneous melting mechanism
 3. The melting start upon the **drop** in pressure
- Si: Diamond cubic
1. Rapid/instant advancement of the melting front
 2. T/P interplay results in mainly homogeneous melting mechanism
 3. The melting starts upon the **rise** of pressure

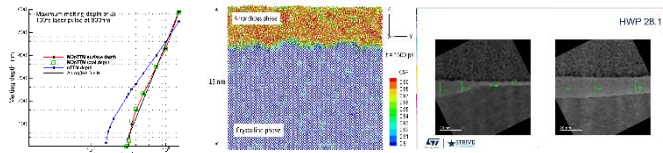
Melting Kinetics of Si (001) vs (111)

Two sets of sequences of atomic configurations illustrates the differences in the laser-induced melting process for Si samples:

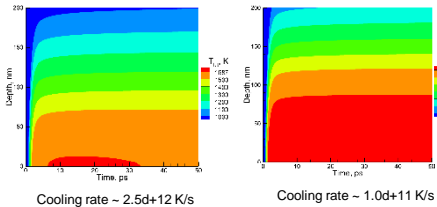


<001> (left) and <111> (right) crystal orientations. Both samples were irradiated with a 100 fs pulse at 800 nm, using the same incident fluence of 0.3 J/cm². Snapshots are presented at identical time intervals (30ps, 50ps, and 100ps) for both cases, with atoms color-coded according to the Central Symmetry Parameter (CSP), enabling the distinction between solid (CSP > 0.97) and liquid (CSP < 0.97) phases. The corresponding profiles of lattice temperature and pressure are added for a quantitative analysis.

Melting and Amorphization Mechanisms in Si



Pre-surface amorphous state of Si was achieved through a cooling process of the melted region with a certain rate. Atoms are color-coded by the Central Symmetry Parameter (CSP), indicating that amorphization occurred due to the prolonged immobility of the solid-liquid interface, even after the sample temperature dropped to 1000 K, well below the melting point of 1687 K.



See: **Ivanov D. S. and Itina T.E. Physical Chem. Chem. Phys. (2025)**

- Non-equilibrium melting and amorphization of Si have been investigated by using Molecular Dynamics simulations (MD) coupled with nTTM model and Drude-Lorentz equation.
- Working just above the melting threshold warrants the surface melting ~ 10-20nm with fastest cooling rate, which makes the amorphization possible.

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