Institute of
Technical Physics

Open Access Tools for the Simulation of Ultrashort-Pulse Laser Ablation

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Open Access Tools

Two-Temperature Model

$$C_e(T_e)\frac{\partial T_e}{\partial t} = \nabla[K_e(T_e)\nabla T_e] - \gamma_{ei}\cdot(T_e - T_i) + S(\vec{r},t)$$

$$C_i(T_i)\frac{\partial T_i}{\partial t} = \gamma_{ei}\cdot(T_e - T_i)$$

Simulation Setup

- Aluminum target
- Gaussian laser pulse, λ = 1064 nm
- Normal incidence
- Φ = 0.19 - 0.37 - 0.74 - 1.49 - 2.97 J/cm²
- τ = 0.05 - 0.5 - 5 ps

Example $\Phi = 0.37\ J/cm^2, \tau = 5\ ps$

IMD - Molecular Dynamics

- Open-access software [1]
- FMQ Stuttgart
- γ_{ei}, κ_e *const.*, $c_e \propto T_e$

Simulation Details

- EAM-potential [2]
- Ionization neglected in EAM potential
- Input of absorbed energy from VLL
- 20 nm x 20 nm lateral, periodic boundary
- 400 ... 850 nm thickness
- Computation time:
  450 ... 700 ps x nm / day / CPU

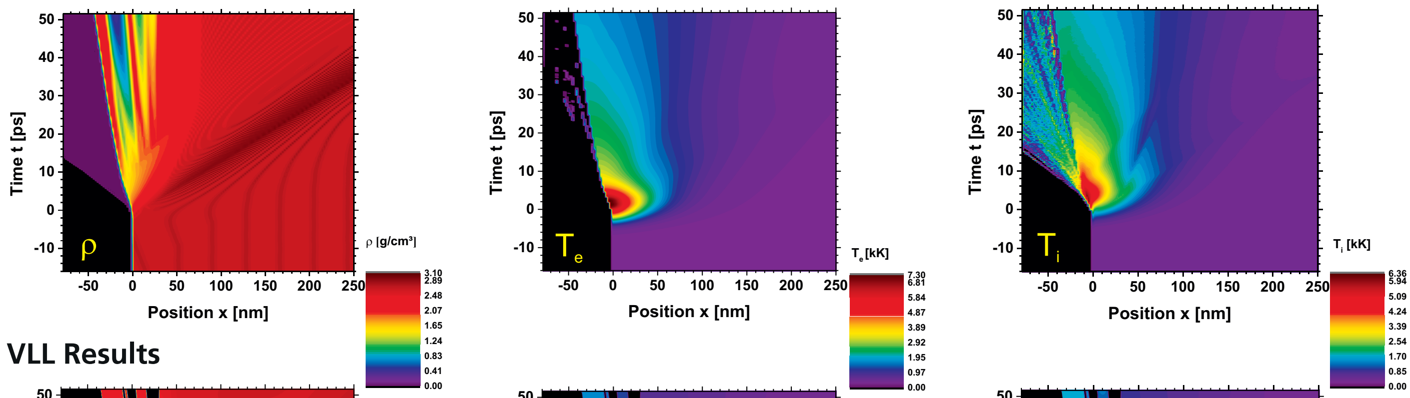
VLL Virtual Laser Lab

- Online simulations [3]
- RAS Moscow
- γ_{ei}, κ_e wide-range model [4]
- c_e and c_i from EOS [5,6]

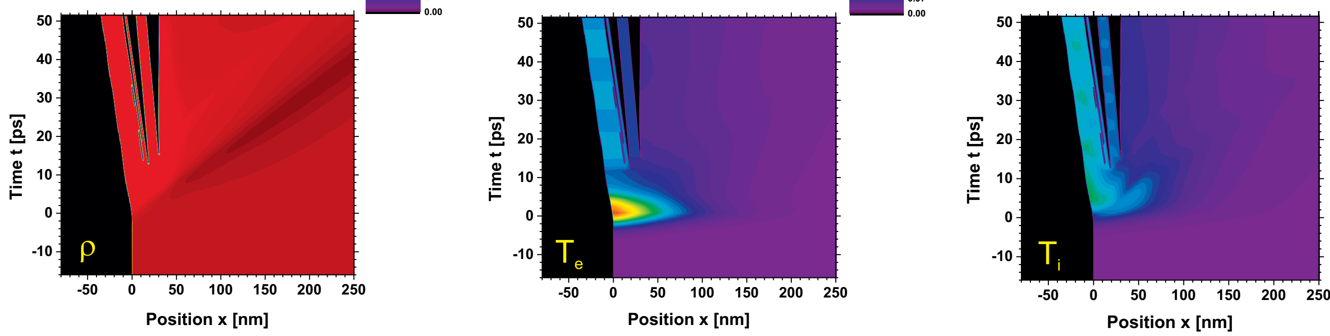
Simulation Details

- Semiempirical multiphase EOS
- Ionization considered in EOS
- Computation of absorbed laser energy
- 1D simulation
- 1 mm bulk material
- Computation time: < 2 minutes

IMD Results



VLL Results



Summary

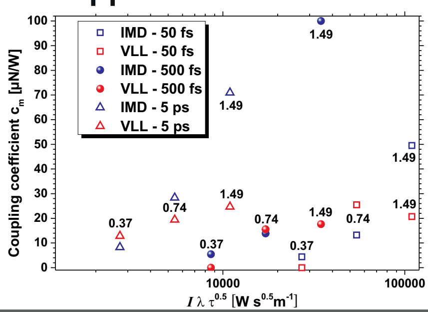
EAM potential around normal state (IMD) vs. wide-range EOS (VLL)

Φ = 0.19 ... 0.37 J/cm²
IMD: lower Φ_{th} (melt., ablation) than VLL

Φ = 0.74 ... 1.49 J/cm²
IMD: ρ equiv. VLL, T_e and T_i higher than VLL

Φ = 2.97 J/cm²
IMD: Ionization (VLL) vs. extreme T_e (IMD)

BEP Application



References

[1] J. Stadler et al., *Int. J. Mod. Phys. C* **8**: 1131 (1997)
[2] F. Ercolessi and J.B. Adams, Europhysics Letters **26**: 583 (1994)
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[4] M.E. Povarnitsyn et al., *Appl. Surf. Sci.* **258**: 9480 (2012)
[5] M.E. Povarnitsyn et al., *Phys. Rev. B* **75**: 235414 (2007)
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Knowledge for Tomorrow

Deutsches Zentrum für Luft- und Raumfahrt
German Aerospace Center

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