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Phase field simulation of kinetic superheating and melting of aluminum nanolayer irradiated by pico- and femtosecond laser

Goal of research

To develop phase field model, which can describe kinetic superheating and melting of materials from nano-second to a few pico-second time scale.

It incorporates thermal fluctuations into Ginzburg-Landau equation and new temperature evolution equation with thermo-elastic and thermo-phase transformation coupling, as well as two-temperature model.

Phase field approach to melting

Ginzburg-Landau equation

$$\frac{1}{L}\dot{\eta} = X = J^{-1}\{-\varepsilon_{0t}p_e + 3p_e\Delta\alpha(T-T_e)\}\frac{\partial\varphi}{\partial\eta} - J^{-1}\left\{0.5\Delta K\varepsilon_{0e}^2 + \mu\boldsymbol{e}_e:\boldsymbol{e}_e + H\left(\frac{T}{T_e}-1\right)\right\}\frac{\partial\varphi}{\partial\eta} - 4A\eta(1-\eta)(0.5-\eta) + \beta\boldsymbol{\nabla}^2\eta + \zeta$$

Ref: Y.S.Hwang and V.I.Levitas, Appl. Phys. Lett. 103, 263107, 2013

Equation of motion

$$\rho\frac{d^2\mathbf{u}}{dt^2} = \boldsymbol{\nabla}\cdot\boldsymbol{\sigma}$$

Strongly coupled two temperature model (TTM)

Electron gas

$$C_e\dot{T}_e = \boldsymbol{\nabla}\cdot(k_e\boldsymbol{\nabla}T_e) + I - G(T_e - T)$$

Lattice

$$C_l\dot{T} = \boldsymbol{\nabla}\cdot(k_l\boldsymbol{\nabla}T) - 3T\{\alpha_1^m + \Delta\alpha\varphi\}\dot{p}_e + \frac{(\dot{\eta})^2}{\chi} - 3p_eT\Delta\alpha\frac{\partial\varphi}{\partial\eta}\dot{\eta} + H\frac{T}{T_{eq}}\frac{\partial\varphi}{\partial\eta}\dot{\eta} + G(T_e - T)$$

Elastic and interfacial stresses

$$\boldsymbol{\sigma} = \frac{\partial\psi}{\partial\boldsymbol{\varepsilon}} - J^{-1}\frac{\partial\psi}{\partial\boldsymbol{\nabla}\eta}\otimes\boldsymbol{\nabla}\eta = \boldsymbol{\sigma}_e + \boldsymbol{\sigma}_{st}$$

$$\boldsymbol{\sigma}_e = \{K_m + \Delta K\varphi(\eta)\}\varepsilon_{0e}\boldsymbol{I} + 2\mu\varphi(\eta)\boldsymbol{e}_e$$

$$\boldsymbol{\sigma}_{st} = \left(\tilde{\psi}_V^\theta + \psi_V^\nabla\right)\boldsymbol{I} - \beta\boldsymbol{\nabla}\eta\otimes\boldsymbol{\nabla}\eta$$

Hooke's law

$$\boldsymbol{\sigma} = \boldsymbol{C}:\boldsymbol{\varepsilon}_e$$

Ultrafast Laser induced melting

Faster heating by ultrafast laser than melting can cause superheating of material.

Superheating over 1400K was observed by femto-second laser irradiation of Al nanolayer.

Ref.: B.J.Siwick et al., Science v.302, 2003

Simulation of pico-second laser case

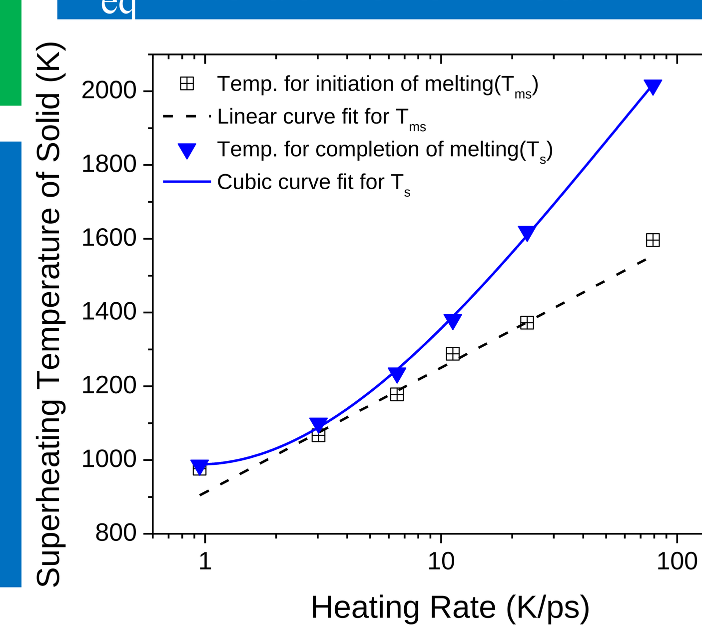
Ref: Y.S.Hwang and V.I.Levitas, Appl. Phys. Lett. 103, 263107, 2013 and paper in preparation.

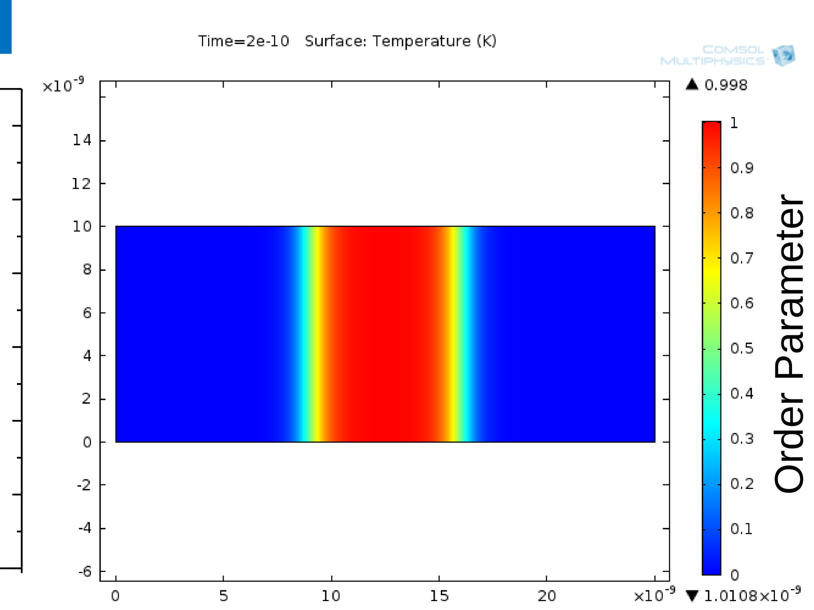
Ref. for experiment: S.Williamson et al., Phys. Rev. Lett. v.52 n.26, 1984

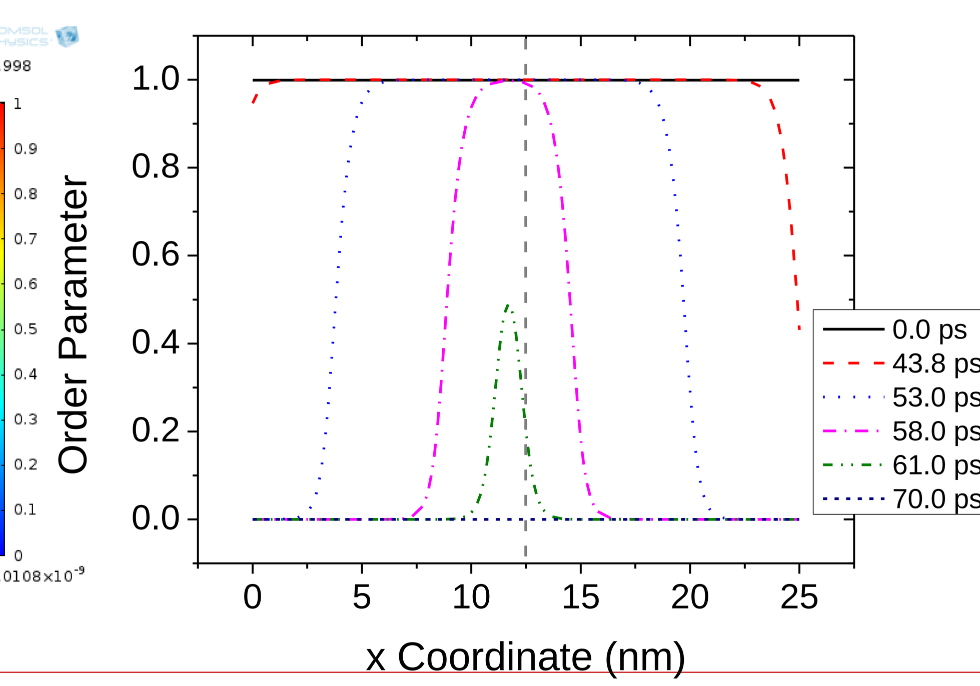
Heterogeneous melting of 25nm Al layer

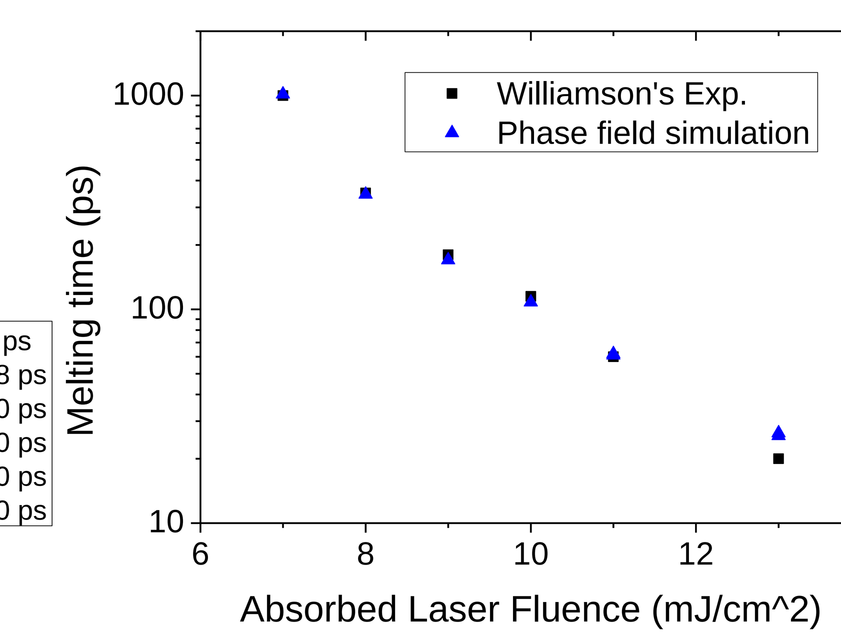
Predicted melting time shows good agreement with experimental data.

Kinetic superheating above T_{eq} was demonstrated.



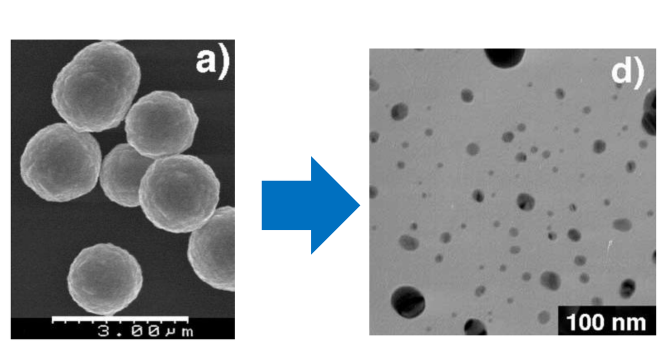






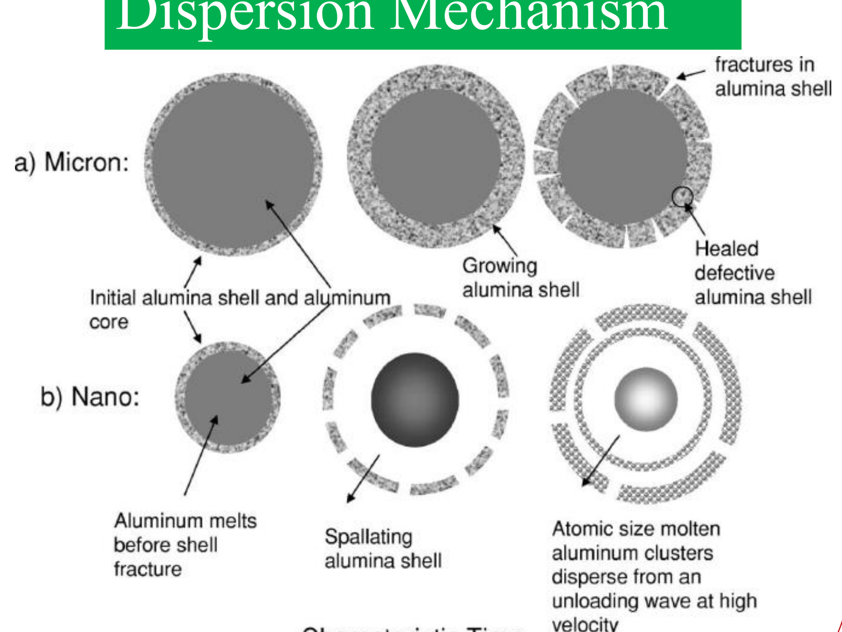
Applications

Clean generation and reformation of NP with laser



Ref.: W.T.Nichols et al., J. of Nanop. Res. n.4, 2002

NP combustion: Melt Dispersion Mechanism



Ref.: V.I.Levitas et al., J. of Appl. Phys. n.101, 2007

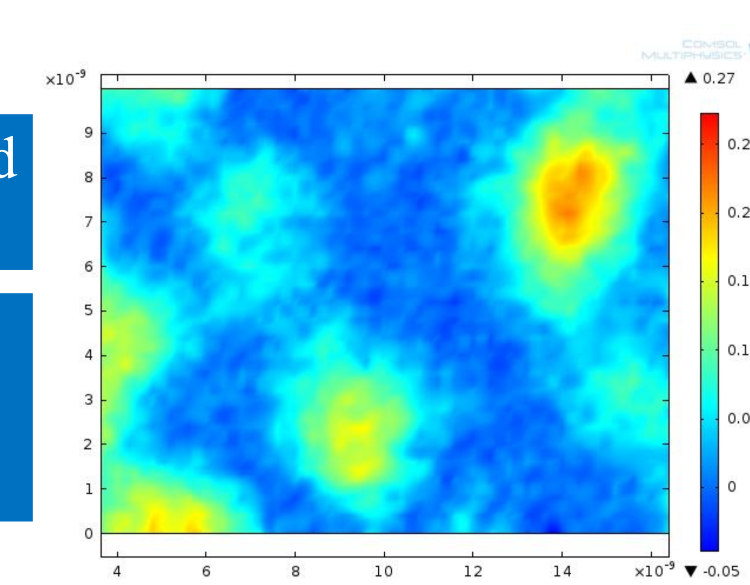
Simulation of femto-second laser case

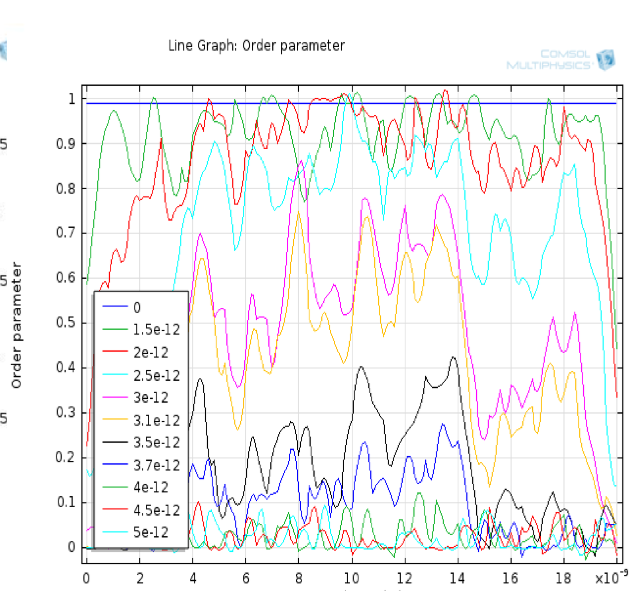
Homogeneous melting of 20nm Al layer

Predicted melting time shows good agreement with experimental data.

Thermal fluctuations are incorporated in Ginzburg-Landau equation:

$$\langle\zeta(\boldsymbol{x},t)\zeta(\boldsymbol{x}',t')\rangle = 2Lk_BT\delta(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t')$$





Ref. for simulation: Y.S.Hwang and V.I.Levitas, in preparation

t_i-2.09 ps

t_m-3.49ps

Ref. for experiment: B.J.Siwick et al., Chemical Physics 299, pp.285-305,2004

t_i-1.5~2.5 ps

t_m~3.5ps