Invited Paper

Transient analysis of thermal distortion in a silicon substrate on incidence of a single soft X-ray FEL pulse

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ABSTRACT

We discuss the dynamics of a silicon surface after incidence of a short, high energy pulse in the soft X-ray range. We focus on time-delays long enough after pulse incidence, so that the absorbed energy can be seen as a non-uniform time-dependent heat distribution in the solid. A model is developed using techniques of non-equilibrium hydro-thermodynamics, considering just the longitudinal and transverse acoustic phonon systems in the excited solid.

The general theory leads to Maxwell-Cattaneo partial differential equations for the material medium n(**r**,t) and the energy h(**r**,t) volume densities; these reduce to the diffusion equation for the temperature T(**r**,t) and the usual thermo-mechanical elastic equation for the strain **u**(**r**,t) on further simplification. Here we solve the Maxwell-Cattaneo equation for T(**r**,t) and compare to previous results where the diffusion equation was used instead; the Maxwell-Cattaneo equation predicts faster cooling at short (dozens of fs, say) time delays. Previously obtained results for the strain field are briefly recalled.

KEYWORD LIST

Thermal-distortion, LA phonon, non-equilibrium hydrodynamics, FEL, silicon

1. INTRODUCTION

The heat flow in optical surfaces subjected to intense VUV and X-ray pulses determines the surface quality and hence the performance of mirrors gratings and Bragg crystals in FEL facilities.

A detailed time-dependent calculation of surface distortion for a silicon substrate, on absorption of a VUV Gaussian pulse (wavelength 12 nm, energy 40 μJ, radius 2.0 mm, duration 1.0 fsec) has been recently reported [1,2] . The originally flat surface bulges sharply out after a delay of 200 nsec, then goes slowly back to the equilibrium flat condition. If one considers using successive pulses of a pulse train, the distortion created by the first few may unfavorably impact the focusing or spectral resolution of the succeeding pulses.

It should be realized that this is an entirely different problem from steady-state situations, where the thermal distortion of optical substrates can be discussed in terms of a space-dependent (but time-independent) temperature distribution. In fact, the complex dielectric function ε(k,ω) may change and very fast relaxation processes may take place already as the FEL pulse begins to penetrate the surface layer of the substrate; the problem falls thereby in the realm of non-equilibrium processes.

A solid under conditions of near thermodynamic equilibrium can be satisfactorily described in terms of phonon (lattice vibration) distributions, hence one hopes that suitable generalizations of this concept might also shed light on the evolution of strongly excited material systems.

We outline here how the basic concepts of non-equilibrium statistical physics can be exploited to build a "non-equilibrium phonon hydrodynamics". Within reasonable approximations, valid for times sufficiently long after excitation with a FEL pulse, the general evolution equations for the silicon substrate state-variables (temperature T(**r**,t) and local displacement **u**(**r**,t)) reduce to time- and space-dependent damped wave-equations (telegraphers equation, also

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called Maxwell-Cattaneo equation). With further simplifying assumptions, one gets the usual heat diffusion equation driven by the external energy source, and the elasticity equation driven by the gradient of the temperature.

As illustration, we solve the Maxwell-Cattaneo equation for the heat flow in silicon and compare to the previous solution of the simpler heat diffusion equation.

The result is that, at short time-delays after the incidence of the FEL pulse, the Maxwell-Cattaneo predicts faster heat flow than the heat diffusion equation. This result is physically understandable, as one can think of the Maxwell-Cattaneo equation as admitting a transient "wave-like" solution that propagates away with the speed of sound, in addition to the "diffusive" solution.

The authors are not aware of experimental measurements for heat flow or thermal distortion in the pico-second regime; it is not clear at present which one is the correct evolution equation at very short times, although the diffusion equation is known to describe slow processes quite accurately.

2. NON-EQUILIBRIUM PHONON HYDRODYNAMICS

Generalized thermo-hydrodynamics of phonons involves the description of the motion of these quasi-particles and of their energy density. The hydrodynamic equations, which couple both types of movements via thermo-striction processes, can be derived starting with a generalized Peirls-Boltzmann kinetic equation obtained in the framework of a Non-Equilibrium-Statistical-Ensemble-Formalism (NESEF), details of which will be given in a future paper.

Here we consider a system of Longitudinal Acoustic (LA) phonons in anharmonic interaction with the accompanying Transverse Acoustic (TA) phonons. The system is in contact with a thermal reservoir; an external source drives the phonon system out of equilibrium.

In order to describe the system we introduce the single-phonon dynamical operator $\nu_{\mathbf{q},\mathbf{Q}} = a_{\mathbf{q}+\mathbf{Q}/2}^{+} a_{\mathbf{q}-\mathbf{Q}/2}$ in the second-quantization representation, in reciprocal space. The average over the non-equilibrium ensemble of the quantum-mechanical Heisenberg equation of motion for the microdynamic variable $\nu_{\mathbf{q},\mathbf{Q}}$ is

$$\partial \nu_{\mathbf{qQ}}(t)/\partial t = \mathrm{Tr}\{(i\hbar)^{-1}[\nu_{\mathbf{qQ}};H]\rho_{\varepsilon}(t)\} \qquad \text{(eq. 2.1)}$$

where, for simplicity, we wrote $\nu_{\mathbf{qQ}}(t)$ for the quantum-mechanical ensemble average $\langle \nu_{\mathbf{qQ}}(t) \rangle$, H is the Hamiltonian of the system and $\rho_{\varepsilon}(t)$ is the non-equilibrium statistical operator [3]. Omitting all details, suffice it to say that going over to direct space, and conserving just linear terms, a generalization of the classical Peierls-Boltzmann equation is obtained, namely,

$$\partial \nu_{\mathbf{q}}(\mathbf{r},t)/\partial t = -\,\mathrm{div}_{\mathbf{r}}[\nu_{\mathbf{q}}(\mathbf{r},t)\,\nabla_{\mathbf{q}}\varpi_{\mathbf{q}}] - \Gamma_{\mathbf{q}}[\nu_{\mathbf{q}}(\mathbf{r},t) - \nu_{\mathbf{q}}^{0}] + \mathcal{G}_{\mathbf{q}}(\mathbf{r},t) \qquad \text{(eq. 2.2)}$$

where $\varpi_{\mathbf{q}} = \omega_{\mathbf{q}} + (\pi/\hbar^2)\,\Pi_{\mathbf{q}}$ is a renormalized frequency dispersion relation, and $\Pi_{\mathbf{q}}$, usually referred to as "self-energy correction", depends on the populations of TA phonons and the matrix element of the LA-TA phonon interaction; $\mathcal{G}_{\mathbf{q}}(\mathbf{r},t)$ accounts for external sources.

By multiplying the phonon distribution $\nu_{\mathbf{q}}(\mathbf{r},t)$, obeying eq. 2.2, into various suitable coefficients one gets the matter and energy densities and tensor fluxes of all orders.

Fluxes of high order decay in time much faster than the low order ones [4]; after a suitable delay we can use a "contracted description". Let us take as the set of basic variables only $\{n(\mathbf{r},t), \mathbf{I}_n(\mathbf{r},t), h(\mathbf{r},t), \mathbf{I}_h(\mathbf{r},t)\}$, namely, the local number of LA phonons, its flux (or current density), the local density of energy and its flux. In reciprocal space they are given by

$$n(\mathbf{Q},t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{Q},t) \qquad \text{(eq. 2.3a)}$$
$$\mathbf{I}_n(\mathbf{Q},t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{Q},t)\,\mathbf{u}(\mathbf{q}) \qquad \text{(eq. 2.3b)}$$
$$h(\mathbf{Q},t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{Q},t)\,\hbar\omega_{\mathbf{q}} \qquad \text{(eq. 2.3c)}$$

$$\mathbf{I}_h(\mathbf{Q},t) = \sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{Q},t)\, \mathbf{u}(\mathbf{q})\, \hbar\omega_{\mathbf{q}} \qquad \text{(eq. 2.3d)}$$

where $\mathbf{u}(\mathbf{q}) = \nabla_{\mathbf{q}}\omega_{\mathbf{q}}$ is the "bare" group velocity of the phonon with wave-vector $\mathbf{q}$.

The equations of motion for these four quantities are

$$\partial n(\mathbf{Q},t)/\partial t = i\mathbf{Q}\bullet\mathbf{I}_n(\mathbf{Q},t) + \mathcal{G}^n_{\mathbf{qQ}} - (1/2)\sum_{\mathbf{q}} \nu_{\mathbf{q}}(\mathbf{Q},t)[i(\Pi_{\mathbf{q}+\mathbf{Q}/2} - \Pi_{\mathbf{q}-\mathbf{Q}/2}) - (\Gamma_{\mathbf{q}+\mathbf{Q}/2} + \Gamma_{\mathbf{q}-\mathbf{Q}/2})] \qquad \text{(eq. 2.4a)}$$

$$\partial \mathbf{I}_n(\mathbf{Q},t)/\partial t = i\mathbf{Q}\bullet\mathbf{I}_n^{[2]}(\mathbf{Q},t) + \mathcal{G}^n_{\mathbf{qQ}} - (1/2)\sum_{\mathbf{q}} \boldsymbol{u}(\mathbf{q})\, \nu_{\mathbf{q}}(\mathbf{Q},t)[i\,(\Pi_{\mathbf{q}+\mathbf{Q}/2} - \Pi_{\mathbf{q}-\mathbf{Q}/2}) - (\Gamma_{\mathbf{q}+\mathbf{Q}/2} + \Gamma_{\mathbf{q}-\mathbf{Q}/2})] \qquad \text{(eq. 2.4b)}$$

$$\partial h(\mathbf{Q},t)/\partial t = i\mathbf{Q}\bullet\mathbf{I}_h(\mathbf{Q},t) + \mathcal{G}^h_{\mathbf{qQ}} - (1/2)\sum_{\mathbf{q}} \hbar\omega(\mathbf{q})\, \nu_{\mathbf{q}}(\mathbf{Q},t)[i(\Pi_{\mathbf{q}+\mathbf{Q}/2} - \Pi_{\mathbf{q}-\mathbf{Q}/2}) - (\Gamma_{\mathbf{q}+\mathbf{Q}/2} + \Gamma_{\mathbf{q}-\mathbf{Q}/2})] \qquad \text{(eq. 2.4c)}$$

$$\partial \mathbf{I}_h(\mathbf{Q},t)/\partial t = i\mathbf{Q}\bullet\mathbf{I}_h^{[2]}(\mathbf{Q},t) + \mathcal{G}^h_{\mathbf{Qq}} - (1/2)\sum_{\mathbf{q}} \boldsymbol{u}(\mathbf{q})\, \hbar\omega(\mathbf{q})\, \nu_{\mathbf{q}}(\mathbf{Q},t)[i\,(\Pi_{\mathbf{q}+\mathbf{Q}/2} - \Pi_{\mathbf{q}-\mathbf{Q}/2}) - (\Gamma_{\mathbf{q}+\mathbf{Q}/2} + \Gamma_{\mathbf{q}-\mathbf{Q}/2})] \qquad \text{(eq. 2.4d)}$$

Using perturbation expansion we can handle eq. 2.4, expressing $\nu_{\mathbf{q}}(\mathbf{Q},t)$ in terms of the basic variables defined by eq. 2.3; redefining coefficients and going back to direct $\mathbf{r}$ space, we get two pairs of equations, one involving just $n(\mathbf{r},t)$ $\mathbf{I}_n(\mathbf{r},t)$ $I_n^{[2]}(\mathbf{r},t)$ the other just $h(\mathbf{r},t)$ $\mathbf{I}_h(\mathbf{r},t)$ $I_h^{[2]}(\mathbf{r},t)$, where $I_{n,h}^{[2]}(\mathbf{r},t)$ are tensor fluxes of second order.

Invoking perturbation linear expansions, the second order tensor fluxes can also be expressed in terms of our basic set.

Combining the two equations in the "n pair", one gets for $n(\mathbf{r},t)$ the following inhomogeneous second-order partial differential equation:

$$\mathrm{div}_{\mathbf{r}}[\Lambda_n^{[2]}:\mathbf{grad}_{\mathbf{r}}n] - \partial^2 n/\partial t^2 - (\Gamma_{n1}+\Gamma_{n2})\partial n/\partial t - \Gamma_{n1}\Gamma_{n2}n = \mathrm{div}_{\mathbf{r}}[\boldsymbol{\mathcal{G}}_{In}+\boldsymbol{\mathcal{F}}_n] - [\Gamma_{n2}+\partial/\partial t]\mathcal{G}_n \qquad \text{(eq. 2.5)}$$

where $\boldsymbol{\mathcal{F}}_n$ is a thermodynamic force due to external fields or density gradients. In our case, there are no external LA phonon sources, so $\mathcal{G}_n$ and $\boldsymbol{\mathcal{G}}_{In}$ vanish. $\boldsymbol{\mathcal{F}}_n = C\,\mathbf{grad}_{\mathbf{r}}h$ does not vanish because the energy density h is not uniform.

Next [5], let $n(\mathbf{r},t)=n_0[1-\mathrm{div}_{\mathbf{r}}\mathbf{u}(\mathbf{r},t)]$; the equation for $\mathbf{u}$ becomes

$$\mathrm{div}_{\mathbf{r}}[\Lambda_n^{[2]}:\mathbf{grad}_{\mathbf{r}}\mathrm{div}_{\mathbf{r}}\mathbf{u}] - \partial^2\mathbf{u}/\partial t^2 - (\Gamma_{n1}+\Gamma_{n2})\partial\mathbf{u}/\partial t - \Gamma_{n1}\Gamma_{n2}\mathbf{u} + C\,\mathbf{grad}_{\mathbf{r}}h/n_0] = 0 \qquad \text{(eq. 2.6)}$$

The "h pair" leads to an equation for $h(\mathbf{r},t)$ of same form as eq. 2.5 (with subscripts h instead of n). Now, for the situation discussed in this paper, $\boldsymbol{\mathcal{F}}_h$ is negligible because n never significantly departs from n_0; $\boldsymbol{\mathcal{G}}_{Ih}$ vanishes identically; $\mathcal{G}_h$ is non-zero because there is a transfer of energy from the "external" radiant field into the LA phonon system (mediated by the electron system). Furthermore, one finds that $h(\mathbf{r},t)=C_V T(\mathbf{r},t)$, where C_V is the specific heat per unit volume and $T(\mathbf{r},t)$ the temperature field. The constant tensor $\Lambda_h^{[2]}$ is diagonal and eq. 2.5 reduces to the following equation for $T(\mathbf{r},t)$:

$$\Lambda_h\, \mathrm{div}_{\mathbf{r}}\mathbf{grad}_{\mathbf{r}}T - \partial^2 T/\partial t^2 - (\Gamma_{h1}+\Gamma_{h2})\partial T/\partial t - \Gamma_{h1}\Gamma_{h2}T = -\Gamma_{h2}\mathcal{G}_h/C_V \qquad \text{(eq. 2.7)}$$

Pending a detailed justification to be given elsewhere, let us point out that the terms $\Gamma_{n1}\Gamma_{n2}\mathbf{u}$ and $\Gamma_{h1}\Gamma_{h2}T$ are associated with damping of the fields $\mathbf{u}$ T. Depending on the physical situation, these effects can be neglected or can be treated by lumping them together with other related terms. Then, the resulting equations are of Maxwell-Cattaneo form.

3. ILLUSTRATION: MAXWELL-CATTANEO TEMPERATURE DISTRIBUTION

We consider the same conditions as in [1], reproduced in Table 1. At the moment t=0, a short Gaussian-shaped pulse is completely absorbed on normal incidence in an infinitely thick silicon slab occupying the half-space z>0. For t<0, z>0, the silicon temperature is $T(t,\mathbf{r})=0$. For t>0, z>0, there is EM radiant energy transfer into the material medium, which heats it up locally. This heat will flow to the cooler parts of the silicon slab and the temperature $T(t,\mathbf{r})$ will follow the differential equation

$$(1/v_h^2)\partial^2 T(t,\mathbf{r})/\partial t^2 + (1/D_h)\partial T(t,\mathbf{r})/\partial t - \nabla^2 T(t,\mathbf{r}) = W_h(t,\mathbf{r})/(C_v D_h) \qquad \text{(eq. 3.1)}$$

where v_h is a velocity, D_h is a diffusion constant, C_v is the specific heat per unit volume and $W_h(t,\mathbf{r})$ is the local power density given to the material medium. The diffusion equation is formally obtained taking the limit $v_h \to \infty$. In practice, if $D_h t << (v_h t)^2$, one considers the regime "diffusive".

This non-homogeneous equation has a particular solution of form

$$T(t,\mathbf{r}) = \iiint dt' d^3r'\, G(t,\mathbf{r},t',\mathbf{r}')\, W_h(t',\mathbf{r}')/(C_v D_h) \qquad \text{(eq. 3.2)}$$

where G is the causal Green´s function (identically zero if $t-t'<0$) which vanishes at infinity ($z\to\infty$, $t\to\infty$, $|x|\to\infty$, $|y|\to\infty$), given in the literature [6] as

$$G(t,\mathbf{r},t',\mathbf{r}') = (v_h/4\pi R)\, exp(-v_h^2\tau/2D_h)\{\, \delta(v_h\tau - R) + u(v_h\tau - R)(v_h^2 R/4D_h^2) J_1(w)/w\} \qquad \text{(eq. 3.3)}$$

$$\tau = t-t' > 0;$$
$$R^2 = (x-x')^2+(y-y')^2+(z-z')^2;$$
$$w = (R^2 - v_h^2\tau^2)^{1/2}\, v_h/2D_h$$

and where $u(s)=1$ if $s>0$, $u(s)=0$ if $s<0$; $\delta(s)$ is the Dirac delta-function; $J_n(w)$ is the cylindrical Bessel function of order n, regular at the origin. It was checked analytically that this reduces to the well known Green function of the wave equation in the limit $D_h\to\infty$, and to the Green function of the diffusion equation in the limit $v_h\to\infty$.

Let the "energy source" $W_h(t',\mathbf{r}')$ be

$$W_h(t',\mathbf{r}') = 0 \qquad z'<0,\ \text{all } t' \qquad \text{(eq. 3.4)}$$
$$= (\pi)^{1/2} U_0 (z_0/t_{FEL})\, exp[-(x'^2+y'^2)/r_0^2]\, exp(-\mu z')\, \delta(z'-ct') \qquad z'>0,\ \text{all } t'$$

In this expression, z_0 is the spatial extent of the well localized radiant pulse while t_{FEL} is its time duration, with $(z_0/t_{FEL}) = c$, while $(\pi)^{1/2} U_0 z_0 \pi r_0^2$ is the total energy in the pulse.

Integrate first in t´, then change variables $x-x' \to x''$, $y-y' \to y''$; $x'',y'' \to \rho'',\varphi''$ and taking advantage of the circular symmetry, integrate in φ''. Let $T_1(t,r,z)$ be the contribution from the δ-function and $T_2(t,r,z)$ the contribution from the unit-step-function; we get

$$T_1(t,r,z) = \tfrac{1}{2}(\pi)^{1/2}(U_0/C_v)(v_h/D_h)\, exp(-\mu z - r^2/r_0^2)\, exp\{-u[(v_h/2D_h)\alpha - \mu\alpha^2]/(1-\alpha^2)\}\ldots$$
$$\ldots \int \rho'' d\rho'' \Delta^{-1/2}\, exp\{-\rho''^2/r_0^2 + \Delta^{1/2}[(v_h/2D_h)\alpha - \mu]/(1-\alpha^2)\}\, I_0(2r\rho''/r_0^2) \qquad \text{(eq. 3.5a)}$$

$$T_2(t,r,z) = \tfrac{1}{4}(\pi)^{1/2}(U_0/C_v)(v_h/D_h)^3\, exp[-\alpha c t v_h/2D_h - r^2/r_0^2] \int \rho'' d\rho''\, exp(-\rho''^2/r_0^2)\ldots$$
$$\ldots I_0(2r\rho''/r_0^2) \int dz'\, exp[-\mu z' + \alpha(v_h/2D_h)z']\, I_1[|w'|]/|w'| \qquad \text{(eq. 3.5b)}$$

$$\alpha = v_h/c; \qquad \text{(eq. 3.5c)}$$
$$u = ct - z > 0;$$
$$\Delta = \alpha^2 u^2 - (1-\alpha^2)\rho''^2$$
$$w' = (v_h/2D_h)[v_h^2(t-z'/c)^2 - R^2]^{1/2} = (v_h/2D_h)[\alpha^2(ct-z')^2 - \rho''^2 - (z-z')]^{1/2}$$

The limits of integration, for the usual case $\alpha<1$, are: $0 < \rho'' < \rho_M$; $z_1 < z' < z_2$, with $z_p = z-[\alpha^2 u + \sqrt{\Delta}]/(1-\alpha^2)$; $z_m = z-[\alpha^2 u - \sqrt{\Delta}]/(1-\alpha^2)$; $z_1 = \text{Largest}\{z_p, 0\}$; $z_2 = \text{Smallest}\{ct, z_m\}$; $\rho_M = \alpha u$.

These limits follow from a discussion of the roots of $g(\xi,\rho) = \alpha(u-\xi) - [\rho^2+\xi^2]^{1/2}$, with $\xi = z-z'$ and from a consideration of the causality conditions $z<ct$, $z'<ct'$ and $t'<t$, which entail $-ct < \xi < ct$. The function $g(\xi,\rho)$ occurs as the argument of both the δ-function and u-function in the Green function, (eq. 3.3), after integration in t´.

For $0<\alpha<1$ $g(\xi,\rho)$ has two real roots $\xi_1 < \xi_2$ if $\Delta = \alpha^2 u^2 - (1-\alpha^2)\rho^2 > 0$. The roots are $[\alpha^2 u \pm \sqrt{\Delta}]/(1-\alpha^2)$. The smaller root ξ_1 will be negative only if $\rho < \alpha u$. Were both roots positive, z´ would be always negative, and the integral in z´ identically null because the heat source W_h is also null for $z'<0$, see (eq. 3.4); hence the definition of ρ_M.

Figure 1 shows the time-dependence of the Si surface temperature, at the center of the FEL spot, predicted by the Maxwell-Cattaneo equation for various choices of v_h. The salient feature is a continuous growth of the temperature starting from T=0 at t=0, going thru a maximum, then dropping to zero as $t\to\infty$. The dash curve shows the surface temperature according to the diffusion equation, which predicts $T\to\infty$ as $t\to 0$, with monotonic exponential decrease as $t\to\infty$. For large times, the results from both equations agree.

Regarding the value of v_h, one might argue that the sound velocity v_{Si} is the appropriate one, but the non-equilibrium theory makes v_h a function of the time-dependent variables of state hence v_h can have other values besides v_{Si}. On the other hand it is clear that the diffusion equation needs a correction at very short delay times.

Figure 2 shows T(z,r=0), the temperature depth-profile, at the center of the FEL spot, for time-delays of 10^2 10^4 … 10^{14} fsec, according to the Maxwell-Cattaneo equation (full lines) and diffusion equation (dash lines). For times 10^6 fsec or longer, the profiles predicted by both equations coincide, but for t=100 fsec, the results are significantly different.

The strain $\mathbf{u}(\mathbf{r},t)$ is related to the material density $n(\mathbf{r},t)$ thru $n(\mathbf{r},t) = n_0(1-\nabla\bullet\mathbf{u})$ where n_0 is the equilibrium density of the material medium (Silicon). The equation of motion obtained from the non-equilibrium theory reduces to the usual macroscopic thermo-elastic mechanical equation [5]

$$\partial^2\mathbf{u}(\mathbf{r},t)/\partial t^2 - c_n^2\nabla^2\mathbf{u}(\mathbf{r},t) = -(\alpha_V K/n_0)\nabla T(\mathbf{r},t) \qquad \text{(eq. 3.6)}$$

where the constants are defined in Table 2.

Once the temperature $T(\mathbf{r},t)$ has been obtained, it can be inserted in the equation above and $\mathbf{u}(\mathbf{r},t)$ can be evaluated. So far, this has been done only for the temperature field calculated using the diffusion equation. The details are given in [1,2] here we show only the results.

The boundary and initial conditions are as follows: at t=0 and t=∞, the Silicon slab is supposed to be strain-free. At all times t>0, the surface z=0 is supposed to be "free", which means all stress components normal to the surface must vanish. In order to meet these conditions it is necessary to mix the particular solution of (eq. 3.6) obtained with the appropriate Green´s function vanishing at infinity, and a solution of the associated homogeneous equation. The coefficients depend on coupled integral equations, which we have solved approximately using numerical methods. Of interest here, in connection with optical elements, is the surface normal displacement $u_z(t,z=0,r)$.

Figure 3 shows the contribution of the particular solution for the surface displacement, at the center of the FEL spot, as a function of time. A sharp maximum appears after a delay of 200 nsec, then decays in roughly exponential fashion. Figure 4 shows the radial profile of the particular solution, at the surface, for three different time delays after excitation.

Figure 5 shows the complete solution ("particular", plus "free" tailored to make the complete solution satisfy the boundary conditions at the Silicon surface) at t=200 nsec. We note that it is very laborious to obtain $u_z^{Free}(t,r)$ and this is the reason why we did it just for t=200 nsec. We believe this is illustrative of the behavior at other times, because the expression for $u_z^{Free}(t,r)$ depends on the particular solutions $u_z^{Part}(t,r)$ and $u_\rho^{Part}(t,r)$ linearly. Figure 5 shows that the maximum displacement, for the parameters of this calculation, is not large. The corresponding maximum surface figure error can be gleaned from the figure, and is about 0.02 μrad, which would be negligible considering the present status of the art in optical polishing.

However, if the experiment considers using a sequence of N pulses, equally spaced by a time interval τ, then each successive surface-bulge rides on the wake of the previous one. Say that the surface excursion changes by a factor f during the interval τ whatever the excitation history; then the excursion after the N^{th} FEL pulse is $u_z(N\tau) = u_z(\tau)\sum_{j=0}^{N-1} f^j$. One can contrive situations where $f\sim 1$, for instance if we use Figure 3 at a spacing $\tau\sim 150$ nsec. In this case, the surface excursion increases linearly with time. At N>50 pulses the surface figure error exceeds the value 1μrad, the current status of the art in polishing. Let us point out that this rather sharp surface bulge at t=200 nsec was evidenced

also in a previous calculation [7] where we solved the same equations for T and **u**, with similar sources, but using entirely different procedures. It was conjectured that this behavior was related to the propagation of some shock wave, but to investigate this question one has to look at $\mathbf{u}^{Total}(t,z,r)$, $0<z<\infty$, $0<t<\infty$, which has not been done due to numerical difficulties and excessive requirements of computer time.

We can compare the maximum surface figure error in the present calculation and in [7]. Considering that the surface bulging is a very slow process (time-scale of hundreds of nsec) compared to the FEL pulse length (femtoseconds), one expects that the incident pulse *energy per unit area* is the relevant quantity.

The energy per unit area in the present calculation is 180 $\mu J/cm^2$ and the maximum surface displacement is 0.023 nm; the "specific displacement" is 1.28×10^{-4} nm/($\mu J/cm^2$).

In [7], the incident energy was 40 $\mu J/cm^2$, the displacement was 60×10^{-5} nm and the "specific displacement" 1.5×10^{-5} nm/($\mu J/cm^2$), which is about 8 times smaller than in the present calculation.

The source in [7] had a $J_0(k\rho)$ radial dependence which implies alternate heating and cooling as the argument $k\rho$ crosses each root of the Bessel function. In fact, the total cooling roughly balances out the total heating. In the present calculation, the heat source is positive-definite, and therefore expected to be more efficient.

4. CONCLUSION

Our non-equilibrium phonon hydrodynamics, even though several linear approximations were introduced, reduces to the expected macroscopic equations for heat flow and thermo-elastic behavior under suitable conditions and points the way for corrections in these equations, which may be important at short times of order tens or hundreds of fs.

As regards time-relaxation of highly excited silicon substrates, we believe it is important to include in the analysis the electron system. This is because (i) the electrons mediate the process of light absorption and creation of the phonon populations and (ii) they control directly the optical functions of the medium which can change during the pulse and introduce wave-front aberrations even though surface figure errors as such appear only much later.

On the practical side, for absorbed energy of 40 μJ on a spot with Gaussian radius r_0=2.0 mm, considering 1 μrad as the current state of the art in optical polishing, the surface figure error is negligible after a single pulse, but due to resonant behavior can become of concern after about 50 incident pulses, depending on the spacing in the pulse train.

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Table 1 – FEL characteristics

Quantity	Symbol	Value	Unit
Photon energy	$h\nu=\nabla\omega$	100	eV
Photon wavelength	λ	124	Å
Pulse duration	Δt_{FEL}	1	fsec
Pulse total energy	W_{FEL}	40	μJ
Peak power	P_{FEL}	40	GW
# photons per FEL pulse	N_{FEL}	$2.5x10^{12}$	
Pulse Gaussian radius	r_{FEL}	$2.0x10^{6}$	nm

Table 2 – Thermo-elastic constants for silicon

Quantity	symbol	value	unit
Specific heat (per unit mass) Idem (per unit volume)	C_m $C_V = n_0 C_m$	0.702 1.635	Joule/(g ^oC) Joule/(cm^3 ^oC)
Thermal conductivity	κ	1.68	W/(cm ^oC)
Heat diffusion coefficient	D_h	0.102 1.02	nm^2/fsec cm^2/sec
Coefficient of thermal expansion (linear) Idem (volumetric)	α_l $\alpha_v = 3\alpha_l$	$3x10^{-6}$ $9x10^{-6}$	1/^{o}C 1/^{o}C
Elastic (bulk) modulus	K	$1.06x10^{12}$	g/(cm sec^2)
Shear modulus	ξ	$2.19x10^{11}$	g/(cm sec^2)
Poisson´s ratio	η	0.45	
Speed of sound	c_n	$7.21x10^{-3}$ $7.21x10^{5}$	nm/fsec cm/sec

Figure captions:

Figure 1: Temperature increase (^{0}C) at the surface of a silicon semi-infinite slab versus time elapsed after absorption of 40 μJ from a short FEL pulse in the soft X-ray range. The full lines are the result of the present calculation (Maxwell-Cattaneo equation) for three distinct values of the velocity of propagation; vsi is the speed of sound in silicon. The dash line is the result of our previously published calculation, using just the heat diffusion equation.

Figure 2: Temperature increase (^{0}C) at the surface of a silicon semi-infinite slab versus depth z, at various elapsed times after absorption of 40 μJ from a short FEL pulse in the soft X-ray range. We used for the speed of propagation the speed of sound in Si. The full line is the result of the present calculation (Maxwell-Cattaneo equation). The dash line is the result of our previously published calculation, using just the heat diffusion equation. For time-delay 10^6 fs and larger, the two equations give the same result, but at shorter times the Maxwell-Cattaneo equation predicts significantly faster cooling.

Figure 3: Contribution of the particular solution (of the thermo-elastic equation) for the surface bulge in silicon, using the temperature field predicted by the heat diffusion equation, versus elapsed time, at the center of the Gaussian light spot.

Figure 4: Contribution of the particular solution (of the thermo-elastic equation) for the surface bulge in silicon, using the temperature field predicted by the heat diffusion equation, versus radial distance, for selected elapsed times.

Figure 5: Complete solution (of the thermo-elastic equation) for the surface bulge in silicon, using the temperature field predicted by the heat diffusion equation, versus radial distance, for elapsed time 200 ns.

Figure 1

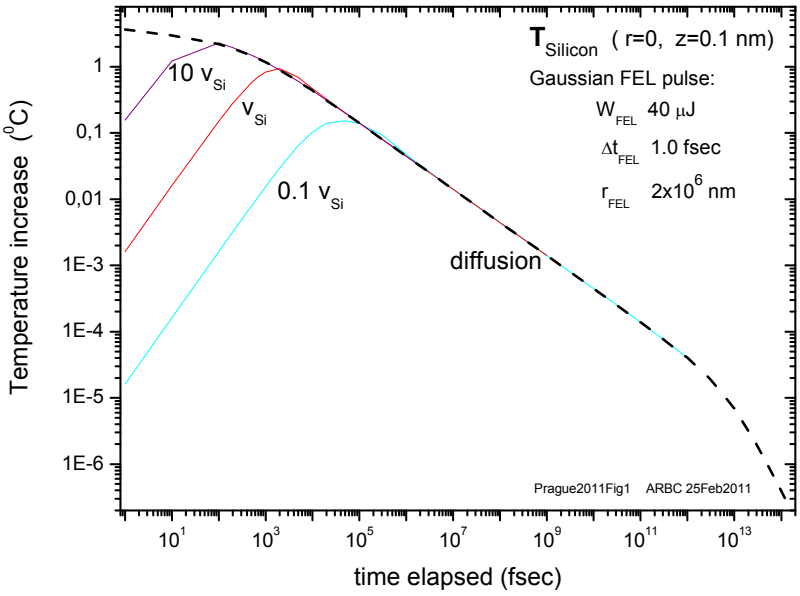

Figure 2

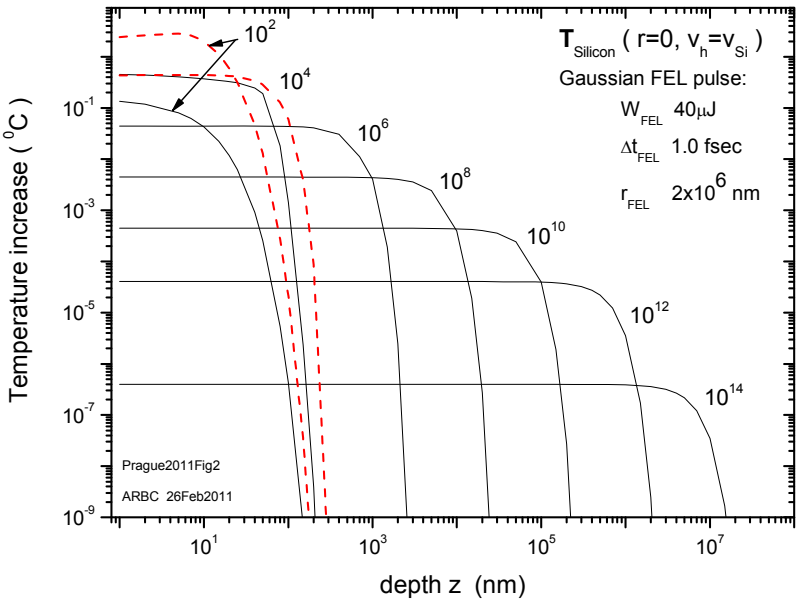

Figure 3

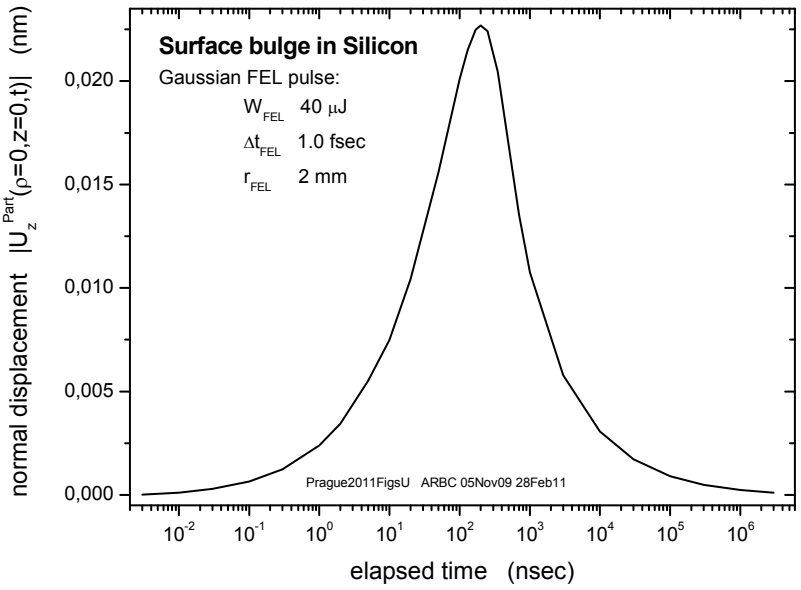

Figure 4

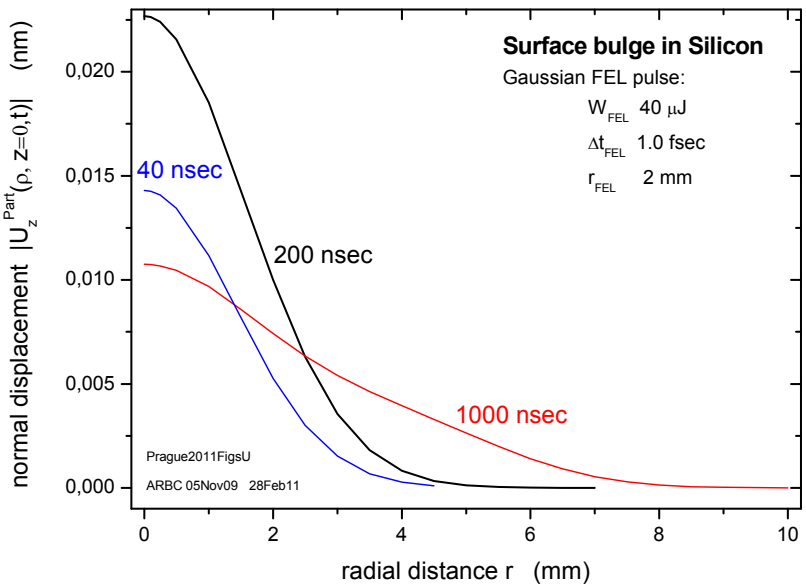

Figure 5