Some Thoughts on Optics for 4th Generation X-ray FEL Sources

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Part 1: Damage to Crystal Monochromators from X-ray FEL Beams

The time scale on which a crystal *lattice* responds to an intense laser pulse depends on the pulse duration and the total energy (see table on next page). From the work with short-pulse (sub-picosecond) lasers, the general rule of thumb is:

A. If the absorbed power is great enough such that about 10% of the bonding electrons are excited to anti-bonding states, then "nonthermal" melting can occur. (This has been observed with fs lasers, and structural changes on timescales of less that 100 fs have been observed.)

B. If the absorbed power is less than that required to excite 10% of the bonding electrons in a given volume, then the energy from those excited electrons is transferred to the lattice on the order of 1 - 10 ps at which time thermal expansion (and eventually thermal melting) can occur.

The 200 fs pulses expected from an x-ray FEL might be capable of producing nonthermal damage. From the following calculation, however, it seems that not enough energy is deposited per unit volume to have non-thermal melting and we need to consider only thermal effects.

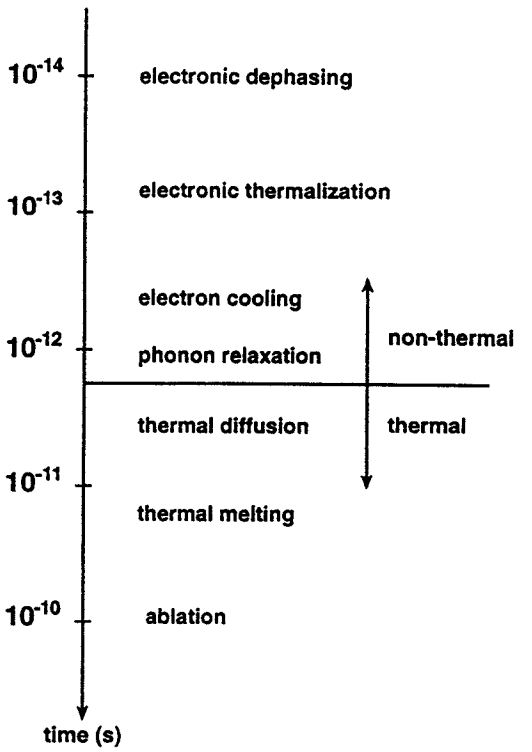

Fig. 2. Time scale of the various secondary processes.

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Laser–solid interaction in the femtosecond time regime

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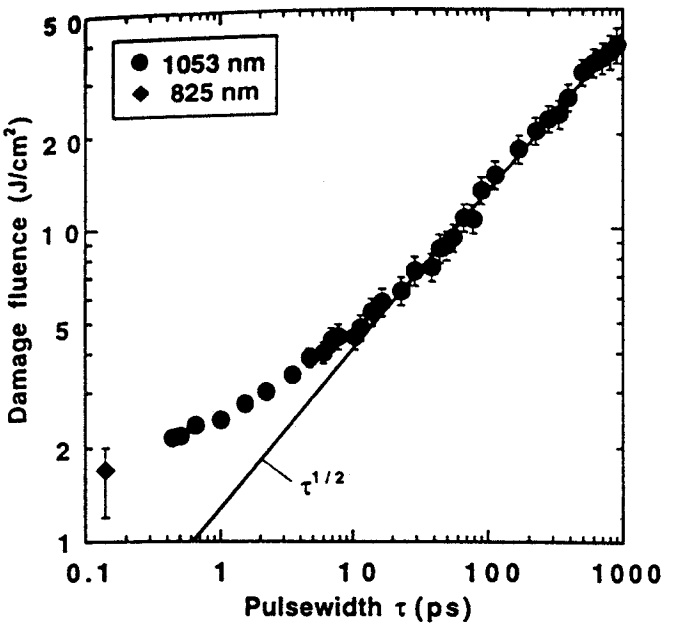

FIG. 3. Pulse width dependence of threshold damage fluence for fused silica.

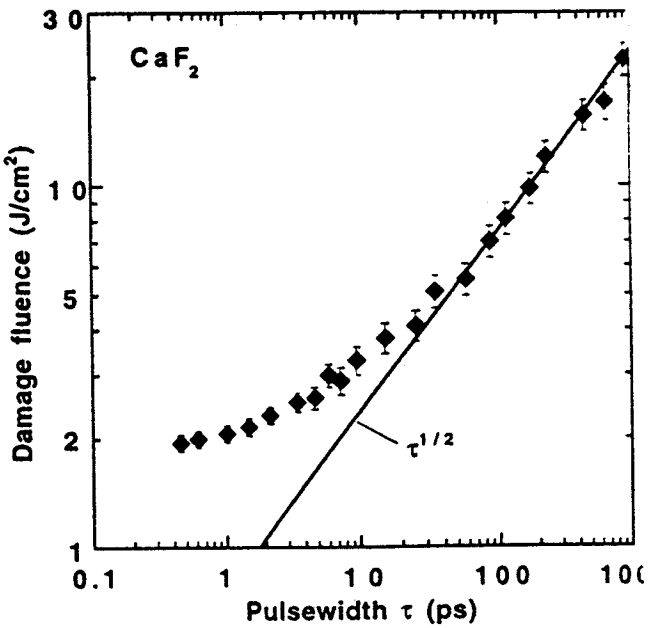

FIG. 7. Pulse width dependence of threshold damage flu calcium fluoride.

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ARTICLES

Nanosecond-to-femtosecond laser-induced breakdown in dielectrics

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If we define $N_{x\text{-}ray}$ as the number of x-rays absorbed per unit volume, then (using the relationship employed for visible light lasers):

$$N_{x\text{-}ray} = \alpha F(1-R)/E_{xray}$$

Where:
α is the absorption coefficient
F is the fluence (energy per unit area)
R is the reflectivity
E_{xray} is the energy of the x-ray

From the LCLS Design Study Report (December 1998), the FEL energy per pulse is *2.6 mJ*. Taking the source size and divergence at the end of the undulator to be *78 microns* and *1 microradian*, respectively, the fluence at 62 m from the ID is:

$$F = 2.6 \times 10^{-3}\ J/(.01cm)^2 = 26\ J/cm^2$$

For 8 keV x-rays:

$$E_{xray} = 1.3 \times 10^{-15}\ J$$

We will examine the effect of this fluence on silicon and diamond.

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Silicon	Diamond
Given:	Given:
$N_{\text{bonding electrons}} = 2 \times 10^{23}\ \text{cm}^{-3}$	$N_{\text{bonding electrons}} = 7 \times 10^{23}\ \text{cm}^{-3}$
$R = 0 \qquad \alpha = 146\ \text{cm}^{-1}$	$R = 0 \qquad \alpha = 14.1\ \text{cm}^{-1}$
Then:	Then:
$N_{\text{x-ray}} = 3 \times 10^{18}$ x-rays/cm^3	$N_{\text{x-ray}} = 3 \times 10^{17}$ x-rays/cm^3

From solid-state detector technology, it is known that it takes about 3.2 eV to form 1 e-h pair in silicon (it's at least 5.5 eV in diamond, probably more). If we use this value, the number of electrons/unit volume produced is:

$N_e = 7 \times 10^{21}/\text{cm}^3$	$N_e = 4 \times 10^{20}/\text{cm}^3$
(close to 10% $N_{\text{bonding electrons}}$)	(not so close to 10%)

So let's assume that neither crystal will experience non-thermal melting (a good assumption for diamond and perhaps not so good for silicon). Nonetheless, if this is the case then the question is:

Can the x-rays diffract from the crystal before significant (thermal) lattice distortion occurs?

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Continuing our "analysis"- assuming no nonthermal melting, we need to examine whether, given this power loading, we expect the crystal to (thermally) melt under the influence of one pulse. Again silicon and diamond will be considered.

To raise the temperature from room temperature (RT) to the melting point (Tm) you need to supply an energy per unit volume equal to:

$$\text{Energy/unit volume} = \Delta T\langle C\rangle$$

where <C> is the "average" value of the heat capacity over the temperature range and is equal to the "average" specific heat times the density.

Silicon	Diamond
Tm = 1685°K	Tm ≈ 4100°K
ρ= 2.3 gm/cm^3	ρ= 3.5 gm/cm^3
<c> = 0.8 J/gm °K	<c> = 0.6 J/gm °K
<C> = 1.84 J/cm^3 °K	<C> = 2.1 J/cm^3 °K
ΔH_f = 4200 J/cm^3	ΔH_f = N/A
$\Delta T\langle C\rangle$ = 2600 J/cm^3	$\Delta T\langle C\rangle$ = 8000 J/cm^3*
αF = 3700 J/cm^3	αF = 350 J/cm^3
(lattice may reach Tm but a phase change may not occur.)	(we are OK here)

* (At elevated temperatures graphitization can occur. If we want to keep the lattice temperature below 1000° K, then $\Delta T\langle C\rangle$ = 1500 J/cm^3.)

If we go 100 m away the beam size is about 130 microns and the fluence is reduced by a factor of 1.6. The energy deposited in silicon per unit volume then becomes:

$$\text{Energy/unit volume} = \alpha F = 2300 \text{ J/cm}^3$$

This may not even bring the crystal to the melting temperature (with one shot).

All does not look hopeless for optics for the LCLS!

What has not been considered in this estimate (or you might say overlooked) is:

(1) Nonlinear x-ray absorption coefficients, i.e. $\alpha(I)$
(2) Spontaneous SR hitting the optics and adding to the power deposited (especially low energy photons that are heavily absorbed on the optics surface.)

Possible Directions for Optics for the LCLS:

(1) Disposable Si optics (raster a Si wafer after every shot)
(2) Perhaps nondisposable Si optics
    no melting
    melting but regrowth from the unmelted portion
(3) Almost surely diamonds will survive

Comparison with femtosecond lasers

As a reality check, I wanted to see if a similar analysis for visible light lasers would predict the observed results.

Silicon:

For 625 nm lasers ($60 < \tau < 100$ fs) the measured melt threshold fluence, F_m, for Si is 170 mJ/cm^2. At fluences several times this threshold, the structural changes are fast (fs) but at or below threshold they occur on the ps timescale and are thought to be thermal in nature. *

In this case it is well known that, at these intensities in the visible region, the absorption coefficient is nonlinear (i.e. intensity dependent) and can be written as:

$$\alpha_{eff} = \alpha_{linear} + \alpha_{non\text{-}linear} = \alpha_{linear} + \beta(1-R)I_{max}$$

where $\beta \cong 55$ cm/GW, so

$$\alpha_{eff} = 3\text{-}5 \times 10^4 \text{ cm}^{-1}$$

At the melting threshold, the energy absorbed per unit volume is:

$$\alpha F_m(1-R) = 3300\text{-}5500 \text{ J/cm}^3 \quad \text{for } (R = 0.35)$$

This number seems to be consistent with the estimate that at least 2700 J/cm^3 need to be absorbed to get the lattice to the melt temp.

*Sokolowski-Tinten et al., Phys. Rev. B **51**, 14186, 1995.

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Graphite (since I could not find the data for diamond):

For 620 nm lasers (τ = 90 fs), the measured melt threshold fluence, F_m, for Si is 130 mJ/cm^2. *

For this wavelength in graphite, the linear absorption coefficient (apparently) dominates the nonlinear term so:

$$\alpha_{\text{eff}} = \alpha_{\text{linear}} + \alpha_{\text{non-linear}} = 3 \times 10^5 \text{ cm}^{-1}.$$

At the melting threshold, the energy absorbed per unit volume is:

$$\alpha F_m(1-R) = 27{,}000 \text{ J/cm}^3 \quad \text{for } (R = 0.3)$$

For graphite:
Tsub $\approx$ 4000°K
ρ = 2.3 gm/cm^3
<c> $\approx$ 1.7 J/gm °K (this is the value at 1000°K)
<C> $\approx$ 4 J/cm^3 °K

Therefore to raise temperature from RT to Tm requires:

$$\text{Energy/unit volume} \approx 15000 \text{ J/cm}^3$$

As in the case with silicon, the absorbed value of 27,000 J/cm^3 seems consistent with the possibility that the lattice temperature will be raised to the melting point.

*Reitze et al., Mat. Res. Soc. Symp. Proc. Vol 157, p425, 1990.

Part 2: Time Response of Bragg Reflection Monochromators for Free Electron Lasers

- Investigations of the temporal response of Bragg diffracting crystals have been made by Wark and He (and other groups) by explicitly including the time dependence in the solutions to Maxwell's equations in a medium with a periodic dielectric.

- The general results of these studies are that, when the x-ray pulse duration is on the order of the time to traverse an extinction length (for perfect crystals) or absorption length (for mosaic crystals), pulse broadening can occur.

- For the perfect crystal case, Wark and He define a dimensionless time as:

$$T = 2\ c\ t/l_{ext\ len} = c\ \pi\ \psi_H'\ t/\lambda$$

where c is the velocity of light, t the real time, $l_{ext\ len}$ the extinction length defined in the following diagram, ψ_H' the real part of the susceptibility, and λ the x-ray wavelength.

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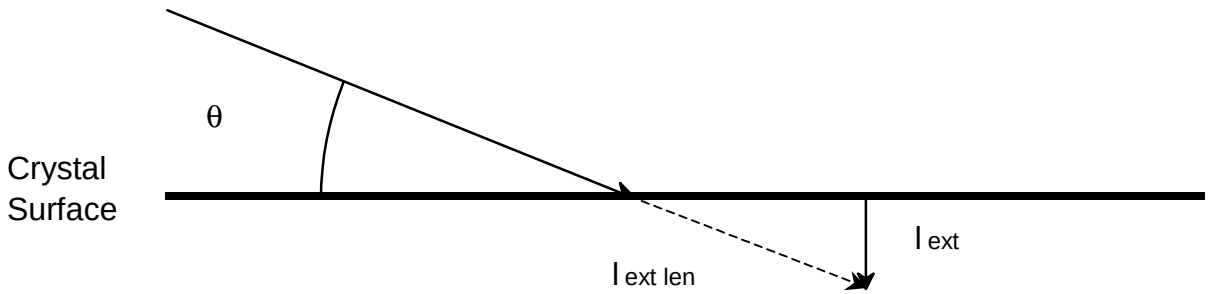
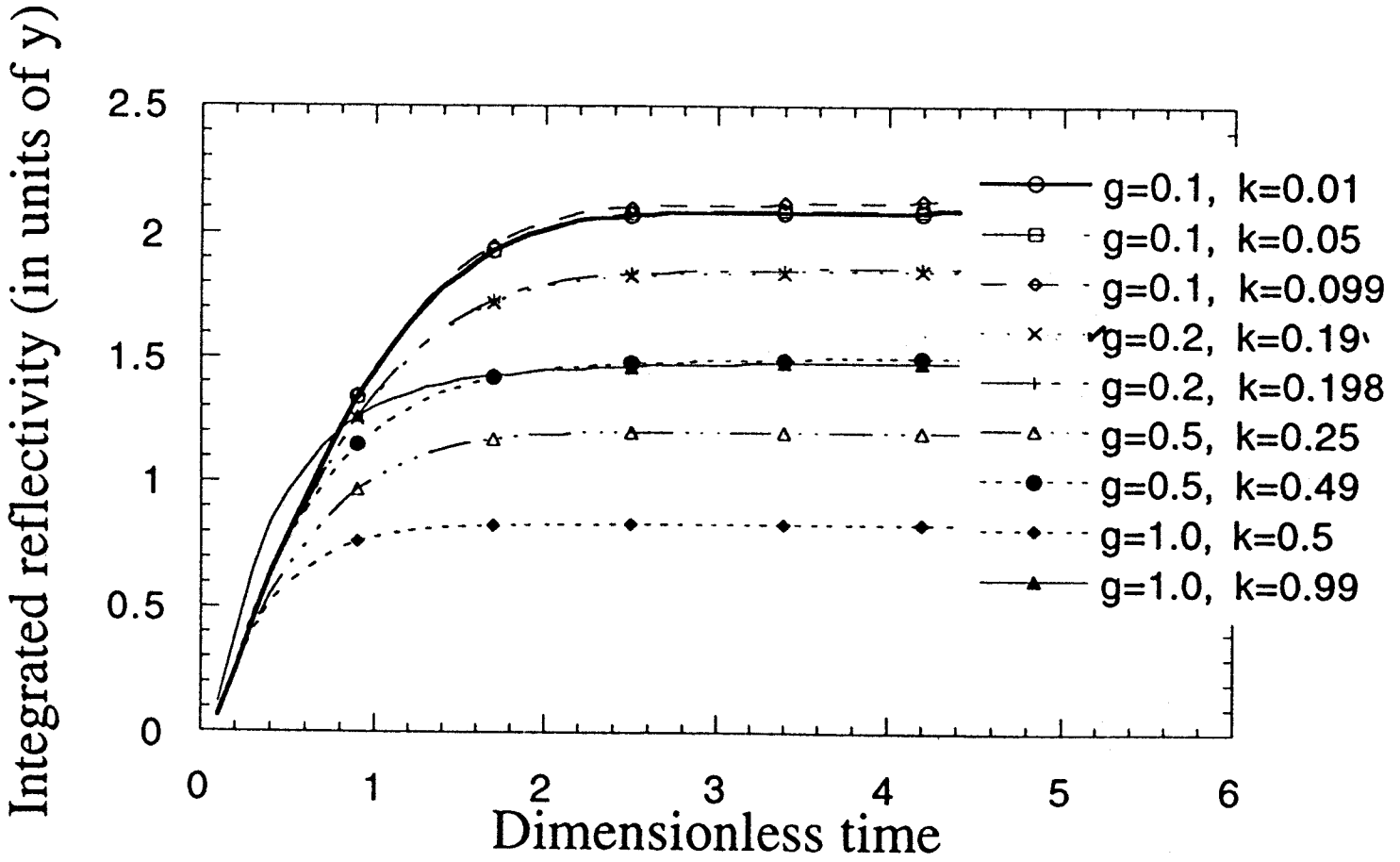


- A dimensionless time of T = 1 corresponds to the time required for an x-ray to penetrate to the extinction depth, l_{ext} , and get back out.

- The angle-integrated, instantaneous reflectivity of a perfect crystal subjected to an (semi-infinite) pulse of x-rays at time T = 0 is shown in the following figure for various values of the parameters g and k. (The g's and k's are the usual parameters for perfect crystals, where $k = \psi_H'' / \psi_H'$ and g is proportion to the ratio of the extinction depth to the absorption length.)

	λ(Å)	k	g	T = 1
Si (111)	1.54	$3\ 10^{-2}$	$4\ 10^{-2}$	20 fs
Si (111)	1.00	$1\ 10^{-2}$	$2\ 10^{-2}$	30 fs
C (111)	1.54	$3\ 10^{-3}$	$4\ 10^{-3}$	19 fs
C (111)	1.00	$1\ 10^{-3}$	$2\ 10^{-3}$	29 fs



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Subpicosecond X-ray diffraction

By J.S. WARK AND H. HE

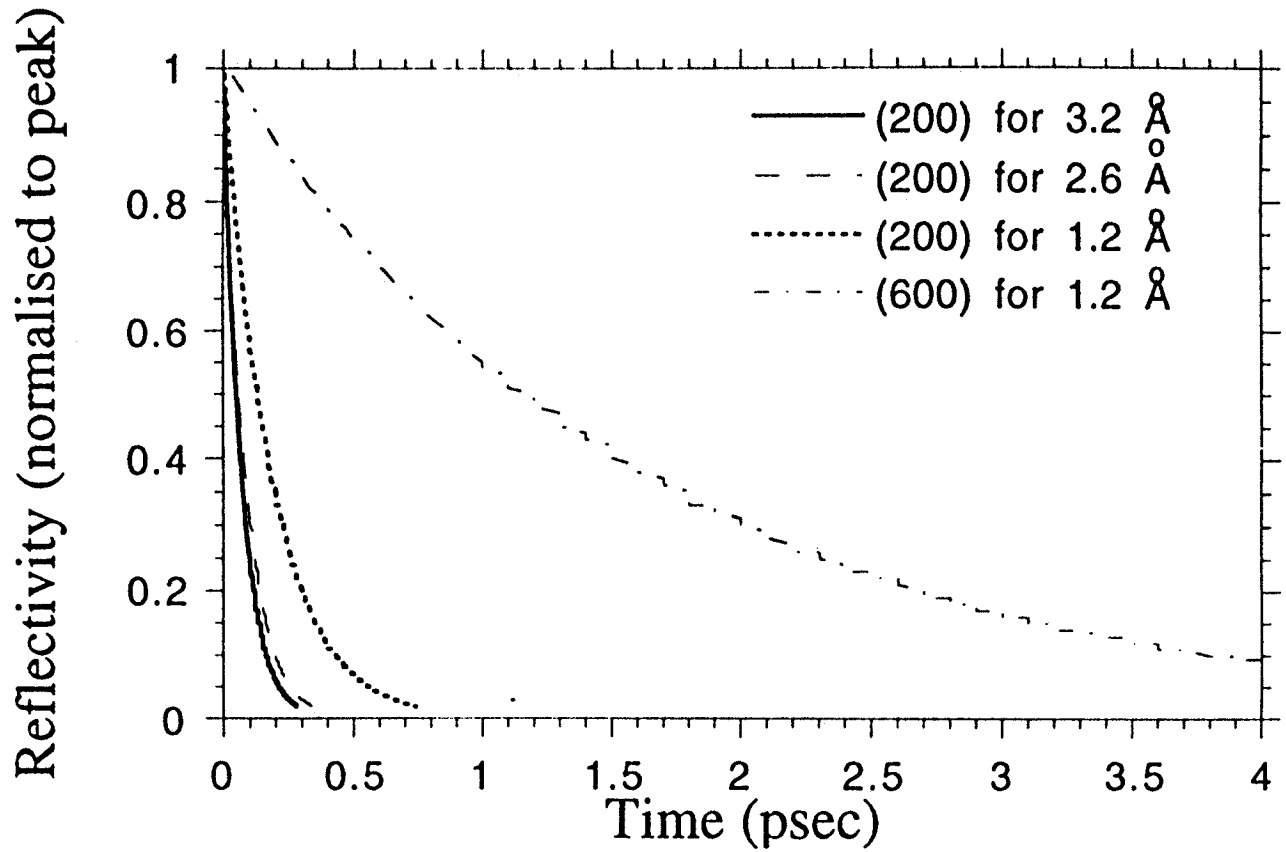

FIGURE 5. Time-dependent angle-integrated reflectivity for kinematic LiF subject to an X-ray pulse significantly shorter than the time taken to traverse an extinction depth.

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- If we consider the "response time" of the crystal to be one unit of dimensionless time, then the Bragg diffractors may act as a filter to smooth or homogenize the spikey temporal output from x-ray FELs.

- They may also ultimately limit the pulse duration of x-ray bursts.

- When mosaic crystals are considered, the response time is slower because the relevant length scale is not the extinction depth but the absorption length, which can be 100 times larger, stretching the crystal response time from 20 femtoseconds to several picoseconds.