Ultrafast transformations in matter induced by intense X-ray radiation

B. Ziaja[1,2]

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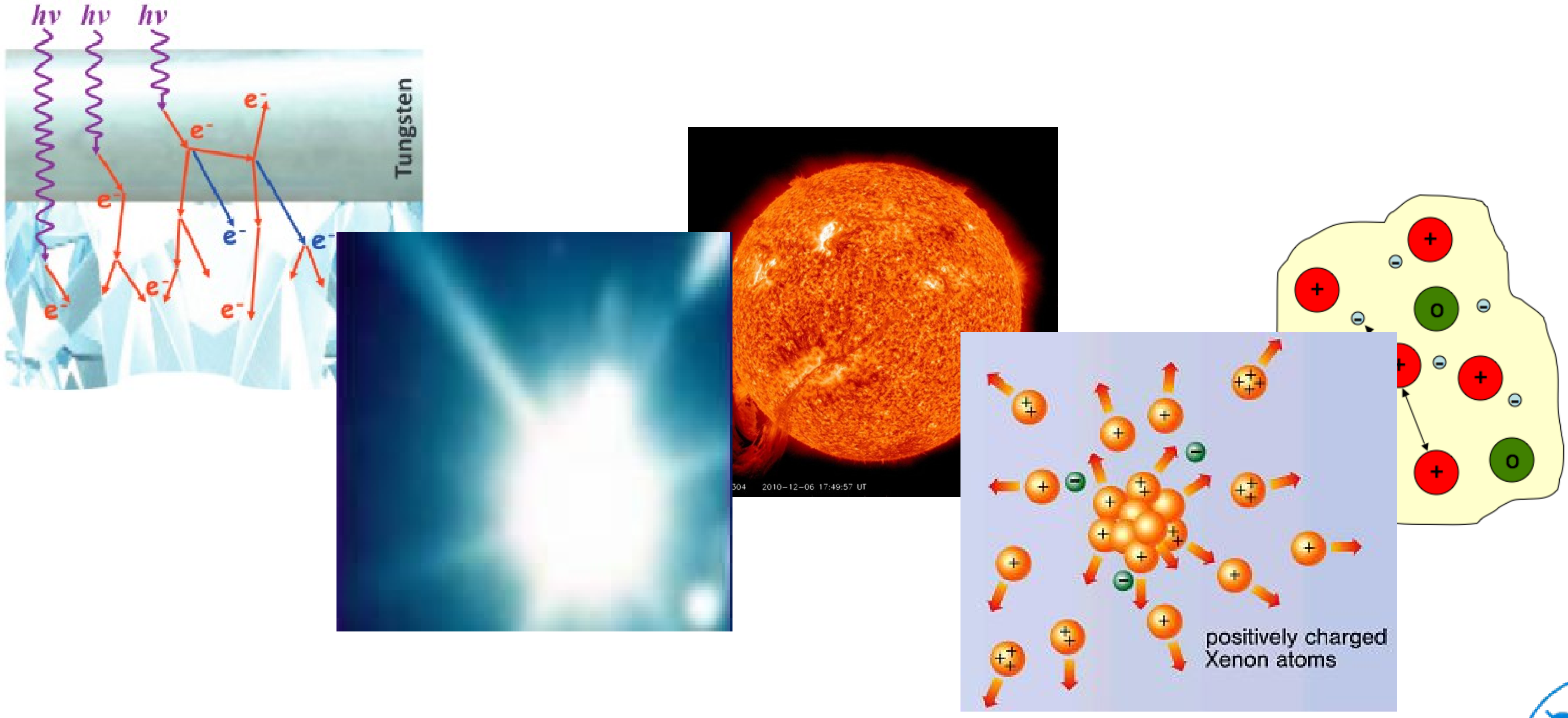

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CFEL-DESY Theory Group at the Center for Free-Electron Laser Science

The CFEL Theory Group develops theoretical and computational tools to predict the behavior of matter exposed to intense electromagnetic radiation. We employ quantum-mechanical and classical techniques to study ultrafast processes that take place on time scales ranging from 10^{-12} s to 10^{-18} s. Our research interests include the dynamics of excited many-electron systems; the motion of atoms during chemical reactions; and x-ray radiation damage in matter.

Members of the CFEL-DESY Theory Group:
C. Arnold, S. Bazzi, J. Bekx, Y.-J. Chen, O. Geffert, D. Gorelova, L. Inhester, Z. Jurek, A. Hanna, R. Kaur, D. Kolbasova, M. Krishna, Z. Li, V. Lipp, M. A. Malik, P. K. Mishra, R. Santra (Group Director), J. Schaefer, S.-K. Son, V. Tkachenko, K. Toyota, R.Welsch, B. Ziaja

3 subgroups:
'Ab-initio X-ray Physics' (S.-K.Son),
'Chemical Dynamics' (R.Welsch),
'Modeling of Complex Systems' (B. Ziaja)

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My excellent collaborators ...

V. Lipp

N. Medvedev

Now in Prague ...

V. Tkachenko

V. Saxena

Now in Delhi ...

J. Bekx

Outline

1. Transitions in matter triggered by X-rays

2. X-ray induced electronic and structural transitions in solids

3. Diagnostics of structural transitions

4. Amorphization of solids by intense X-ray pulse

5. Summary

Transitions in matter ...

Energy delivered to a thermodynamic system → transition into a different phase or state of matter

Examples:

Structural transition → leads to a change of a system structure
Magnetic transition → changes magnetic properties (e.g., demagnetization)
Superconductivity → superconducting phase
...

Or

Solid-to-solid → leads to a change of solid's structure
Solid-to-liquid → melting
Solid-to-plasma → ionization
...

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Structural transitions in solids induced by X-ray radiation

... Femtosecond intense pulses from X-ray free-electron laser ...

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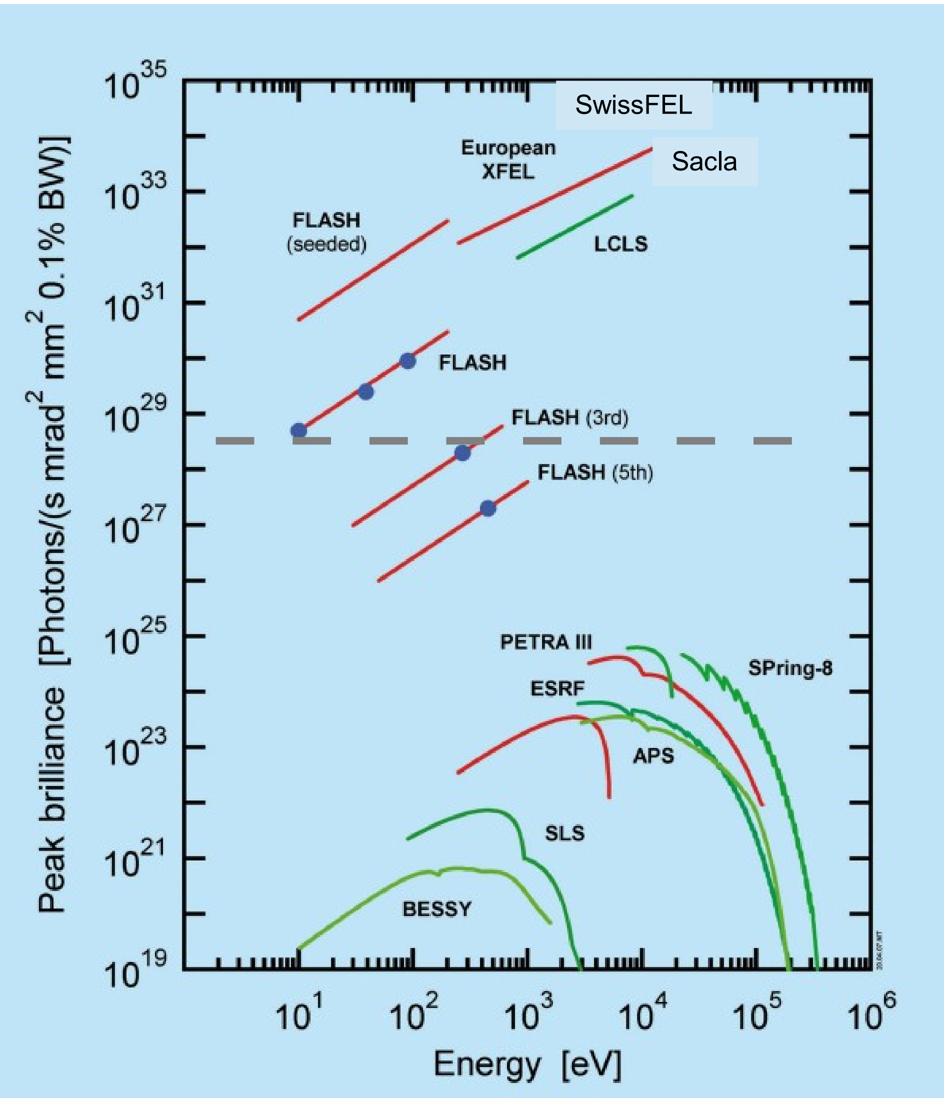
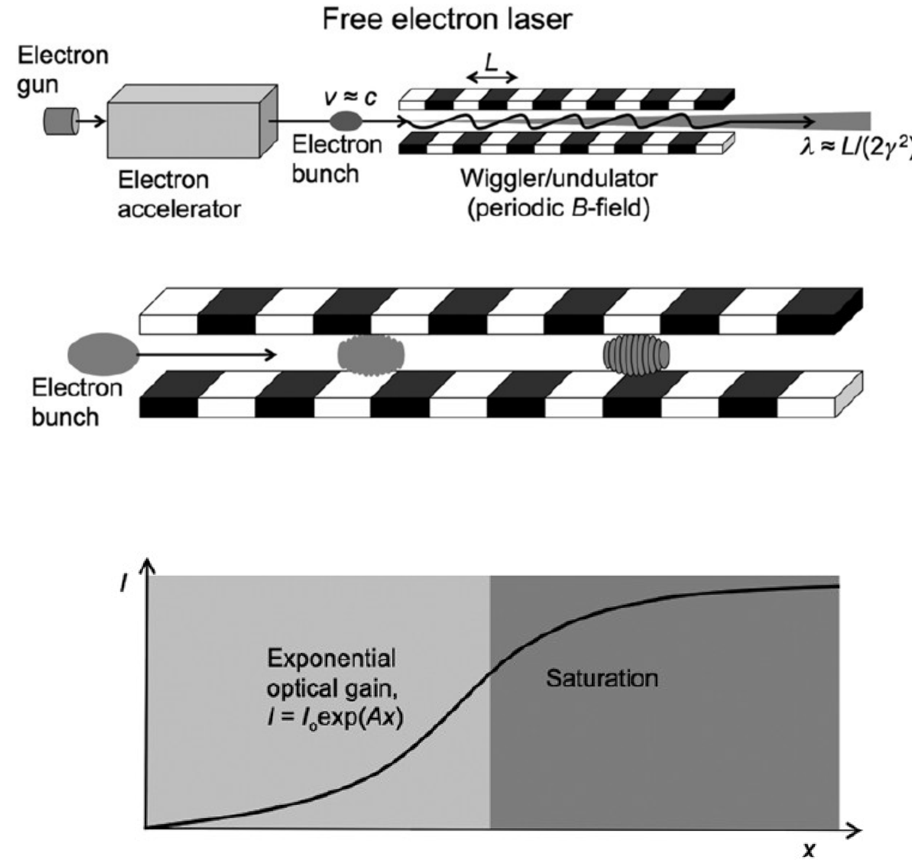
FELs: 4th generation light sources



photon-science.desy.de



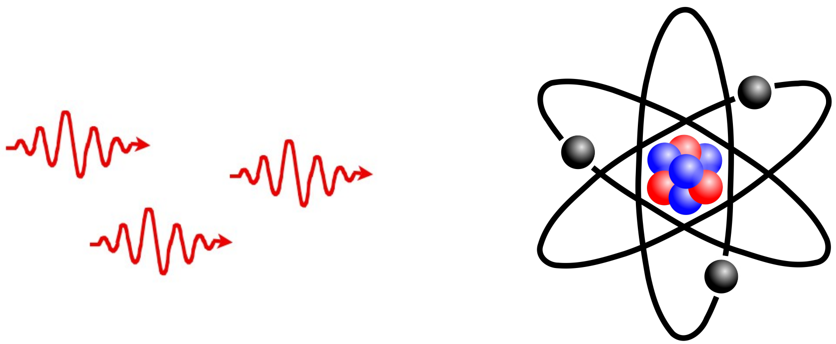
Ribic, Margaritondo, J. Phys. D **45** 213001 (2012)

Pulse duration ~ down to a few fs
Wavelength ~ VUV- hard X-ray

[This slide courtesy of Z. Jurek]

Structural transitions in solids induced by X-ray radiation

Transition depends on the average absorbed dose ....



egymbb.sk

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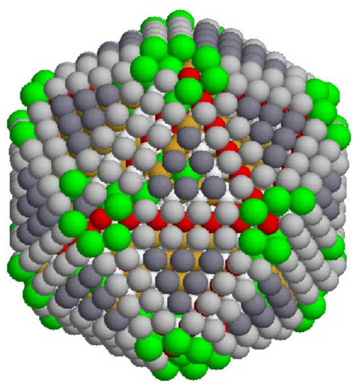
Main interactions:

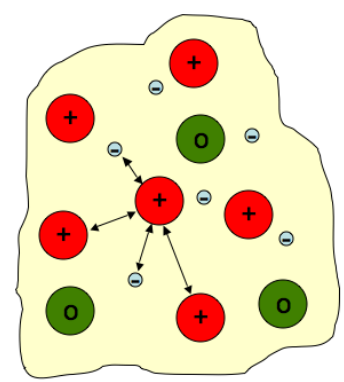
X-ray photons: elastic scattering, Compton scattering, photoionization (valence band, inner-shell), Auger & fluorescence decays

Electrons: collisional ionization and recombination from/to bands, thermalization → band modification

Ions: electrostatic repulsion → band modification → structural transition?



→



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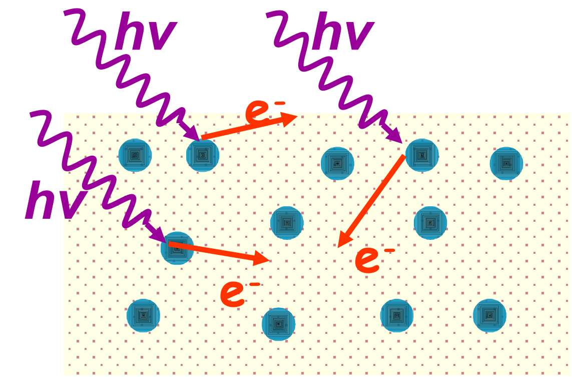
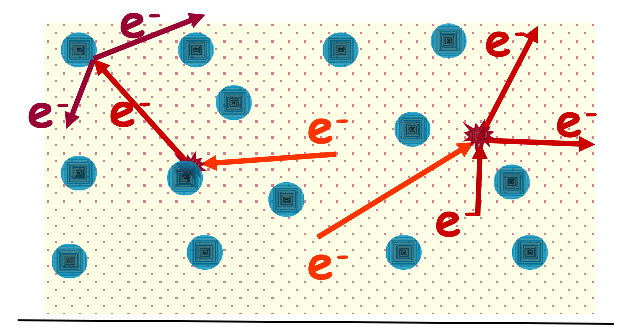
Electron kinetics after impact of low-fluence femtosecond X-ray pulse

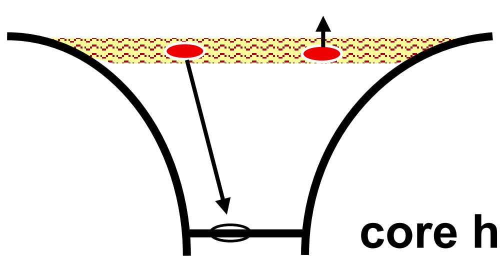
Low X-ray dose



Photoabsorption
during X-ray pulse



Electron kinetics:
impact ionization,
elastic scatterings



core hole

Damage Threshold

Auger decay of core holes → electron emission

[Medvedev et al., CPP 53 (2013) 347]

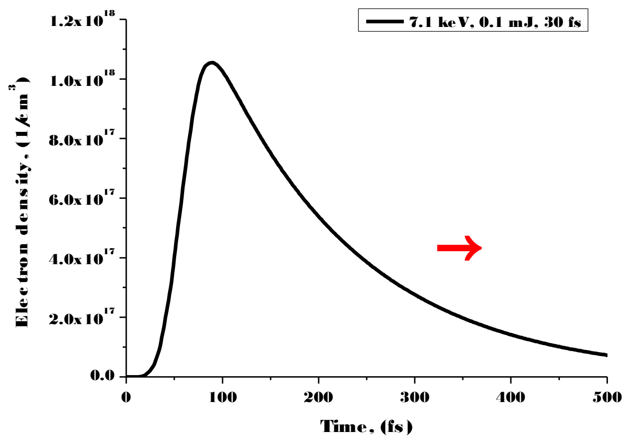
[Images courtesy of N. Medvedev]

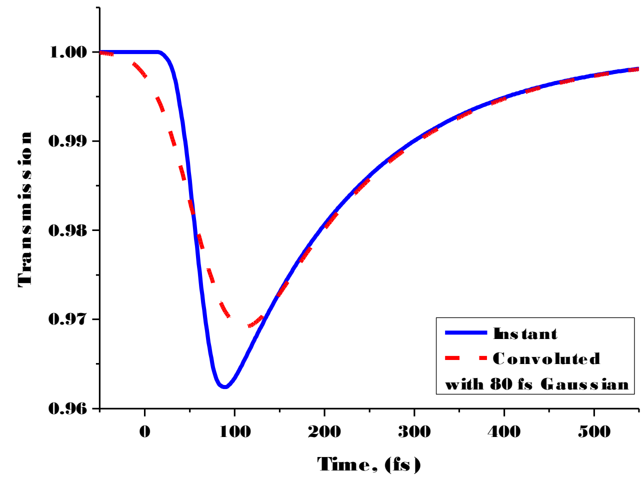
Interaction of solids with low-fluence femtosecond X-ray pulses: → **Electron Kinetics**

Low dose

Radiation excites free electrons within solids which induce transient change of solid's optical properties (reflectivity, transmission) but no structural changes.

Example:
SiO_2





Electron density translates into transient change of optical properties with **Drude model** (or ab-initio calculated dielectric function)
[Medvedev et al., CPP 53 (2013) 347]

→ application for a non-destructive high-resolution FEL pulse timing tool
[Harmand et al. (Medvedev, Ziaja), Nat. Phot. 7 (2013) 215]
[Riedel et al.(Medvedev,Ziaja), Nat. Commun. 4 (2013) 1731]
[Finetti et al. (Medvedev, Tkachenko, Ziaja), PRX (2017) accepted]

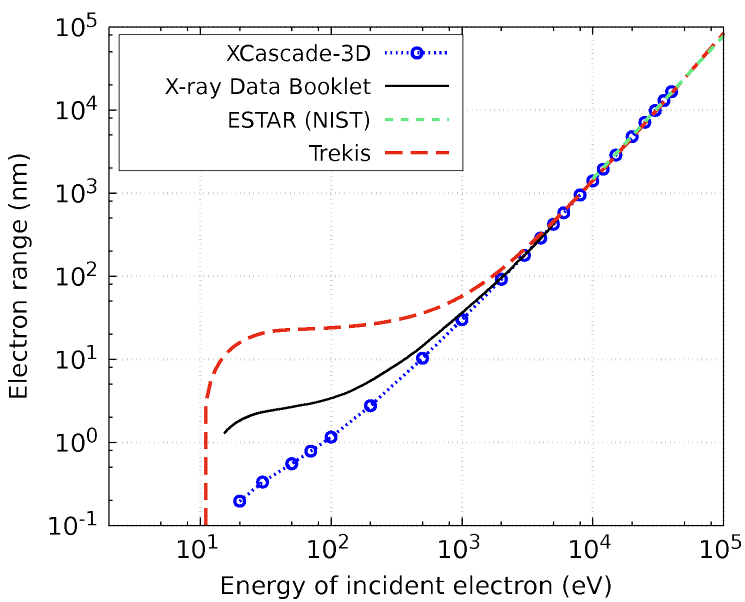
Damage Threshold

[Images courtesy of N. Medvedev]

Our efficient simulation tool: XCASCADE (3D) code

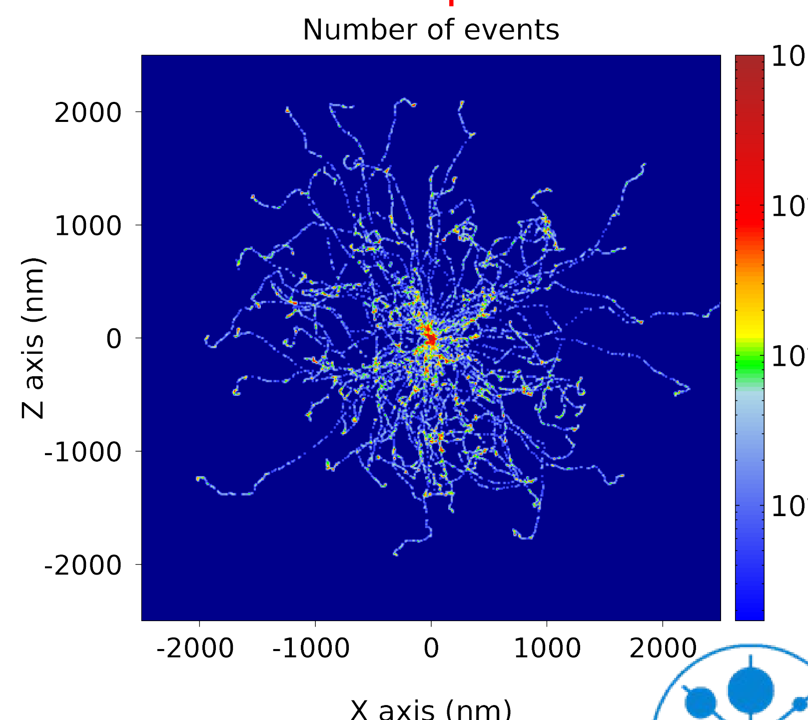
→ Resolves 3D spatio-temporal structure of electron cascades initiated by a primary (photo)electron impact

→ Efficient simulation scheme due to independent electron cascade approximation and low ionization degree of material in which electrons propagate



Predicted electron ranges in Si

100 cascades in LiF after 10 keV electron impact



[N. Medvedev, *Appl. Phys. B 118 (2015) 417*]
[V. Lipp, N. Medvedev, B. Ziaja, *SPIE Proc. 10236 (2017) 10236 H*]

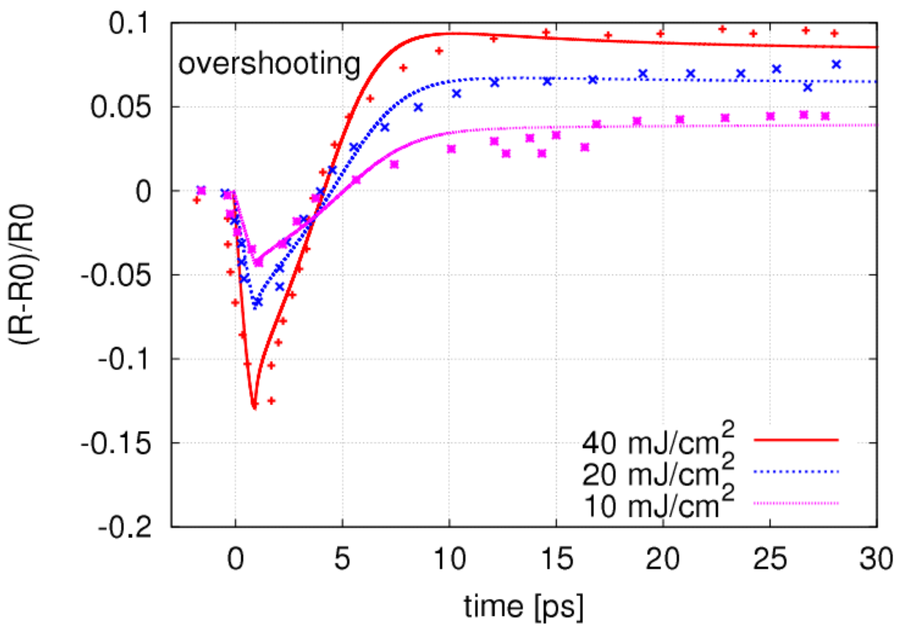
[Images courtesy of V. Lipp]

Interaction of solids with low-fluence femtosecond X-ray pulses →Electron Kinetics and Exchange with Lattice

Low dose

Reflectivity overshooting in GaAs

- **Reflectivity overshooting ← effect of band gap shrinking**
- **Timescale < 10 ps**
- **Observable at probe wavelength 800 nm (1.55 eV) ~ band gap width (1.43 eV) ← low absorption**



LCLS measurement (800 eV)

Damage Threshold

[B.Z., N. Medvedev, V. Tkachenko, T. Maltezopoulos, W. Wurth, *Sci. Rep*. **5**, 18068 (2015)]

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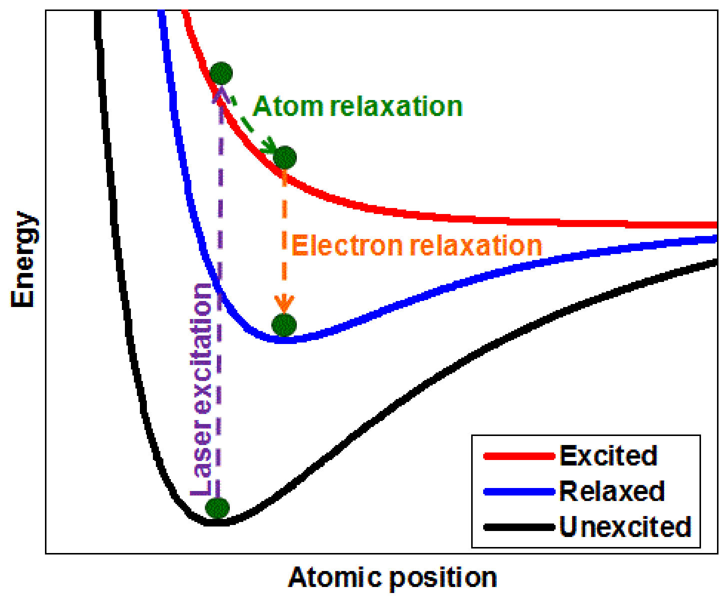
[Images courtesy of V. Tkachenko]

Interaction of solids with femtosecond X-ray pulses of fluence above the damage threshold

Damage threshold

Melting threshold

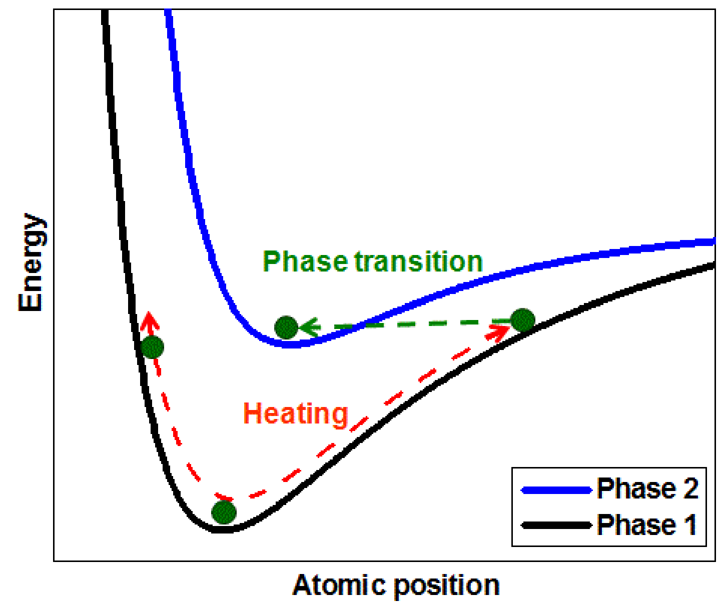
Non-thermal melting (~100 fs)



Change of interatomic potential

[Medvedev et al. (BZ): NJP 15 (2013) 015016;
PRB 88 (2013) 224304 & 060101;
PRB 91 (2015) 054113]

Thermal melting (~ ps)



Heating of atomic lattice due to el-ph coupling within the same potential

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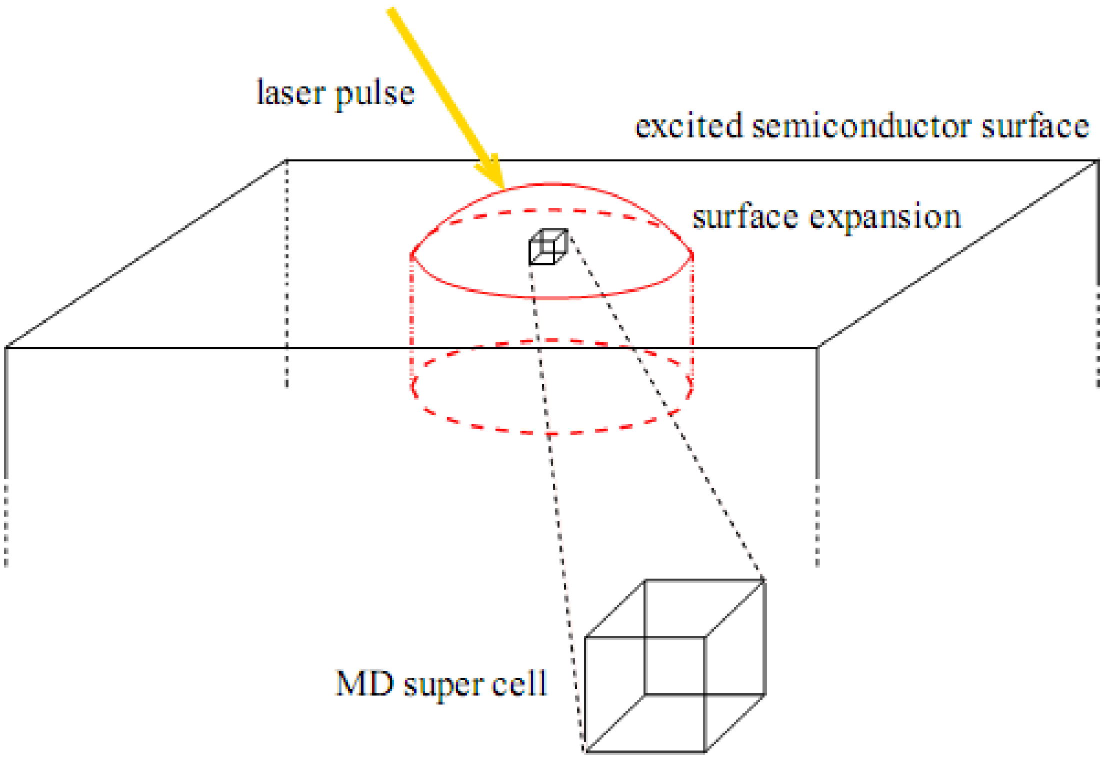
[Courtesy of N. Medvedev]

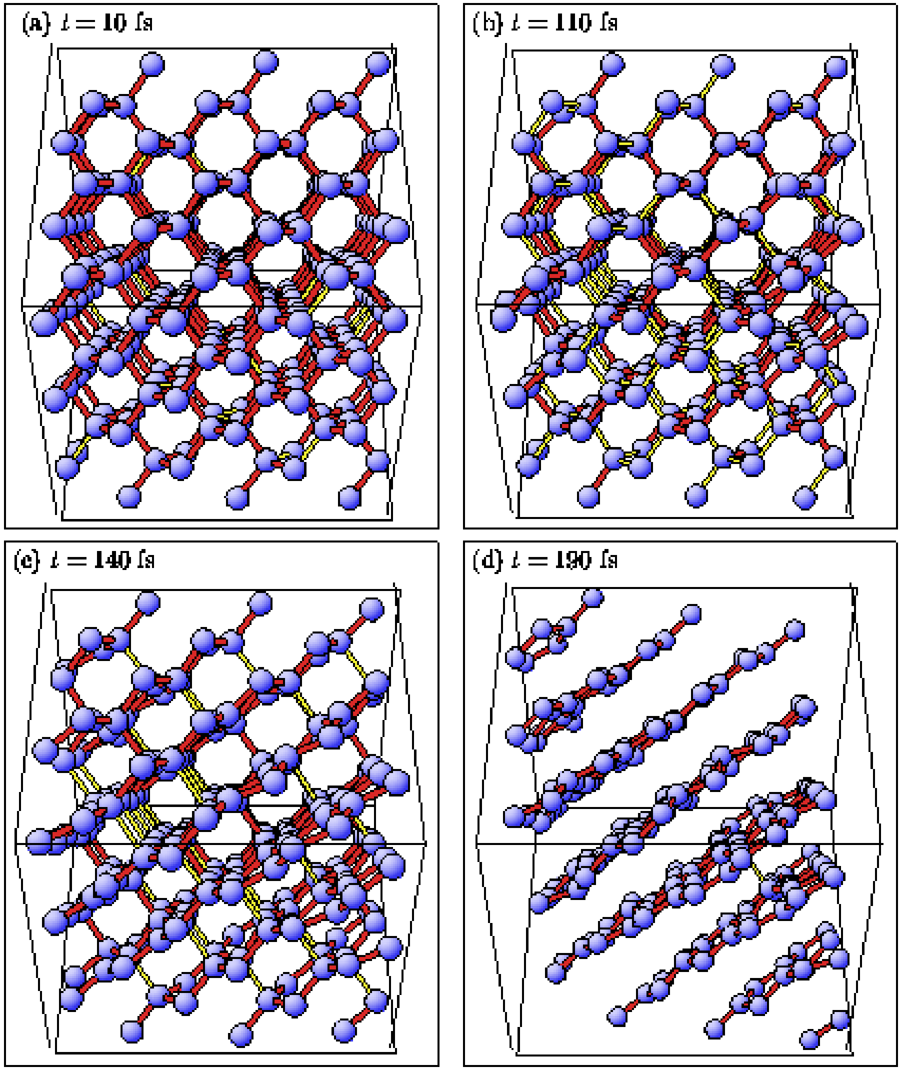
Our simulation tool XTANT: modular MD/MC/TB/Boltzmann approach

- MD (Parrinello-Rahman scheme) to describe dynamics of ions and atoms
- Boltzmann approach to describe dynamics of electrons within the valence and conduction bands
- Tight binding method/DFT to describe changes of band structure, potential energy surface
- MC approach to describe dynamics of high energy free electrons in conduction band and creation and relaxation of core holes
- Scattering/ionization rates calculated from complex dielectric function updated at each time step

[Medvedev et al. (BZ): NJP 15 (2013) 015016;
PRB 88 (2013) 224304 & 060101;
PRB 91 (2015) 054113]

XTANT:
modular MD/MC/TB/Boltzmann approach





Can be used to simulate both bulks as well as surfaces and thin layers

[H. Jeschke et al. PRL 2002]

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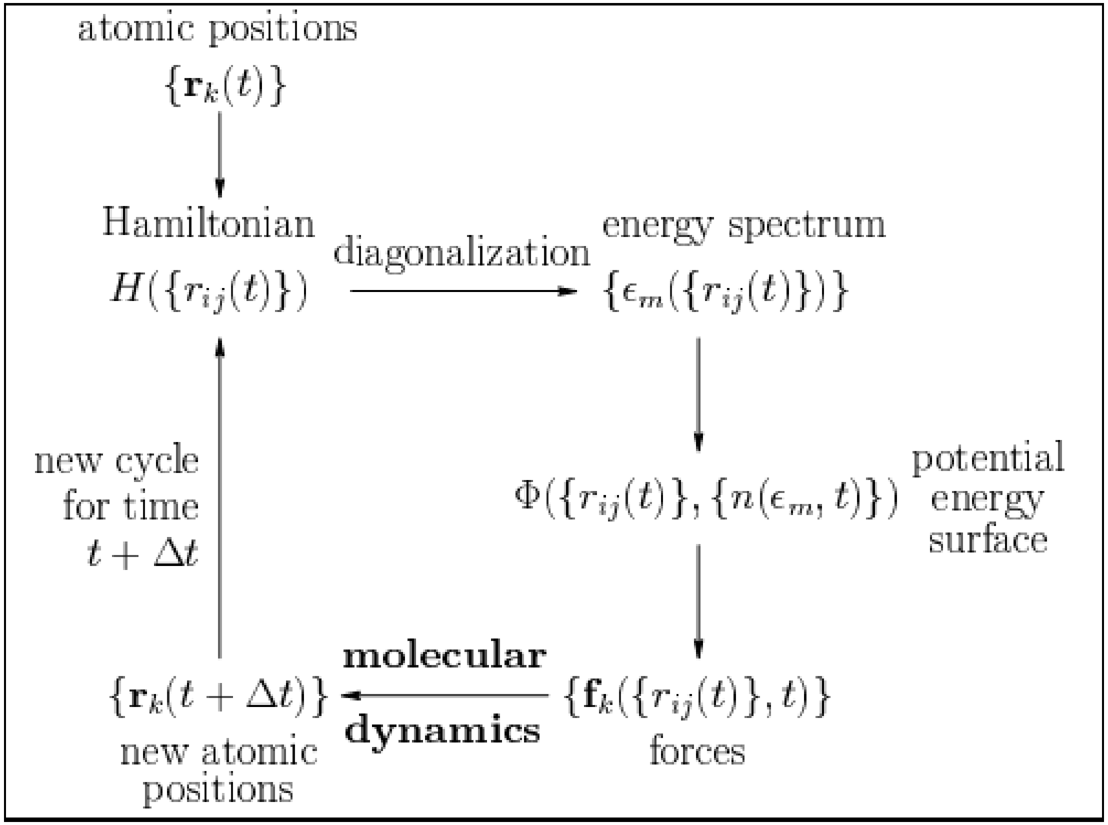
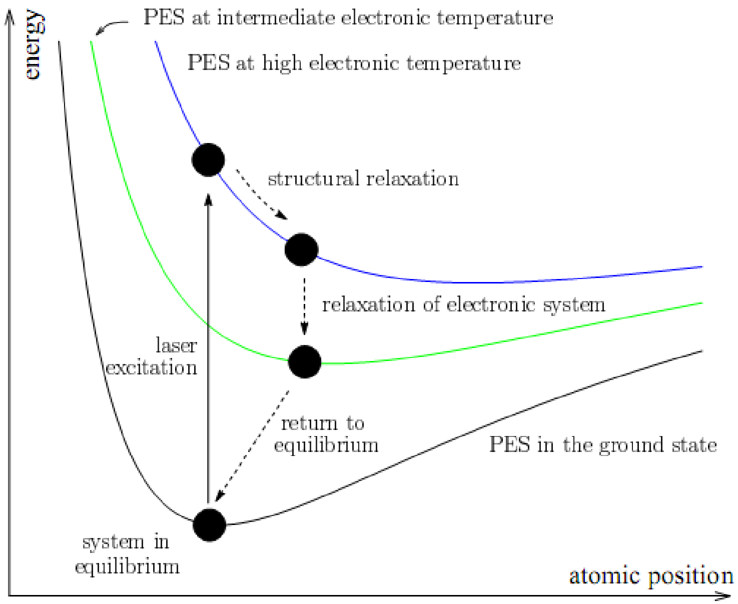
TB Method and molecular dynamics (TBMD)



[H. Jeschke et al. PRL 1999]

[This slide courtesy of N.Medvedev]

TB Method and molecular dynamics (TBMD)



$$m_k\,\ddot{\mathbf{r}}_k = -\frac{\partial \Phi(\{r_{ij}\},t)}{\partial \mathbf{r}_k}$$

Electrons

Core

$$\Phi(\{r_{ij}(t)\},t) = \sum_m f(\epsilon_m,t)\epsilon_m + \frac{1}{2}\sum_{\substack{ij\\ j\neq i}} E_{\mathrm{rep}}(r_{ij})$$

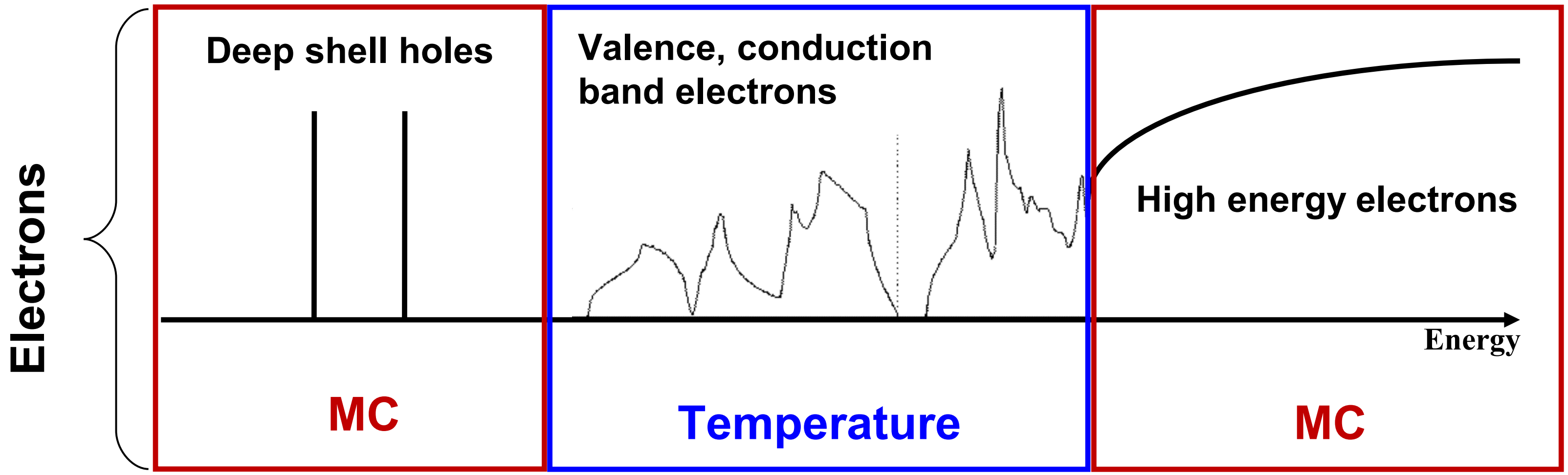
$f(\epsilon_m,t)$ **- transient electron distribution function**

$\epsilon_m(\{r_{ij}(t)\}) = \langle m|H_{\mathrm{TB}}(\{r_{ij}(t)\})|m\rangle$ **- transient band structure**

[This slide courtesy of N.Medvedev]

[H. Jeschke et al. PRL 1999]

Combined MC-TBMD



$$m_k\,\ddot{\mathbf{r}}_k = -\frac{\partial\Phi(\{r_{ij}\},t)}{\partial\mathbf{r}_k}$$

Electrons Core

$$\Phi(\{r_{ij}(t)\},t) = \sum_m n(\epsilon_m,t)\epsilon_m + \frac{1}{2}\sum_{\substack{ij\\ j\neq i}} 1f_{\_p}(r_{ij})$$

[This slide courtesy of N.Medvedev]

[B. Ziaja, N. Medvedev, HEDP 8, 18 (2012)]

Processes considered

1) Photoabsorbtion by deep shells and VB

2) Scattering of fast electrons:

- Deep shells ionization

•VB and CB scatterings

3) Auger-decays of deep holes

4) Thermalization in VB and CB

5) Lattice heating (e-phonon coupling)

6) Atomic dynamics

7) Changes of band structure

8) Changes of scattering rates (minor effect)

- MC (processes 1–3)

- Temperature & Boltzmann equation (processes 4–5)

- TBMD (processes 6–8)

[This slide courtesy of N.Medvedev]

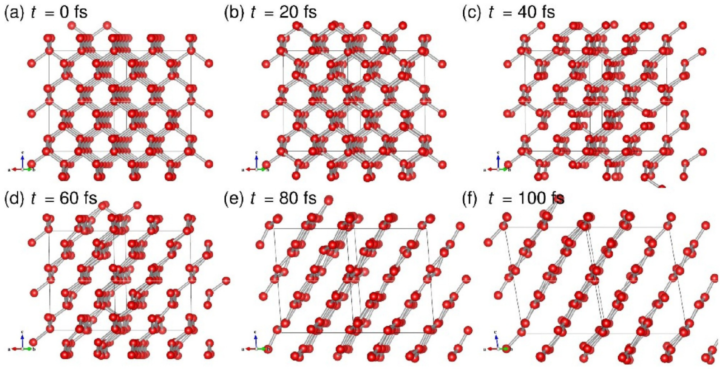
Interaction of solids with femtosecond X-ray pulses of fluence above the damage threshold:
→Electron Kinetics + Atomic Relocations

Damage threshold

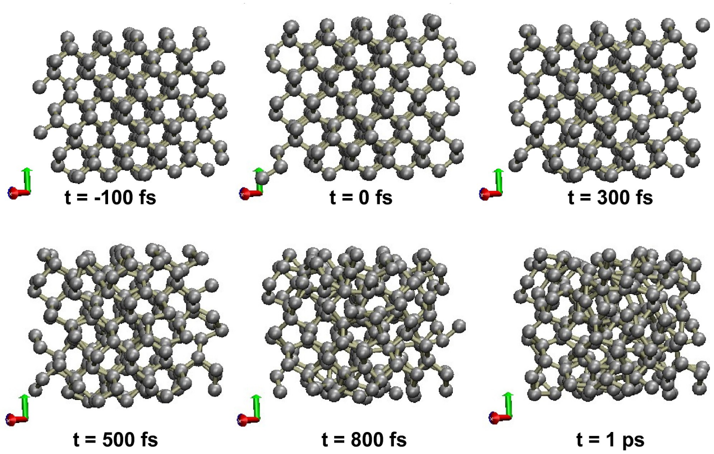
Structural transitions in solids:

→ graphitization of diamond
ultrafast non-thermal process modeled within Born-Oppenheimer scheme

Photon energy 92 eV, FWHM = 10 fs



→ amorphization of silicon
contribution of non-thermal and thermal melting (due to electron-phonon coupling); extended Born-Oppenheimer scheme



Melting threshold

[Medvedev et al. (BZ): NJP 15 (2013) 015016; PRB 88 (2013) 224304 & 060101; PRB 91 (2015) 054113]

Damage thresholds in good agreement with experiments!

[Images courtesy of N. Medvedev]

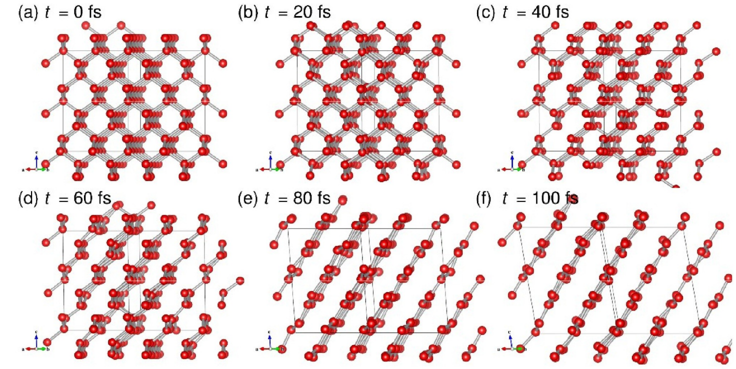
Interaction of solids with femtosecond X-ray pulses of fluence above the damage threshold:
→Electron Kinetics + Atomic Relocations

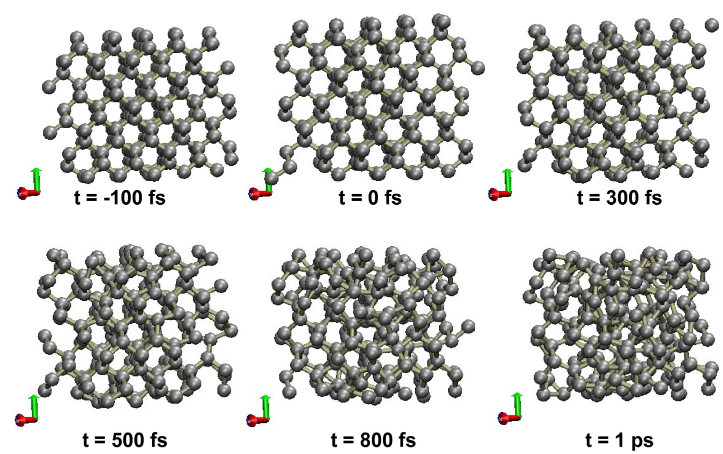
Damage threshold

Simulations with dedicated code XTANT: X-ray induced Thermal and Non-Thermal Transitions [Medvedev et al.] →

→

Photon energy 92 eV, FWHM = 10 fs





Melting threshold

[Medvedev et al. (BZ): NJP 15 (2013) 015016;
PRB 88 (2013) 224304 & 060101;
PRB 91 (2015) 054113]

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Damage thresholds in good agreement with experiments!

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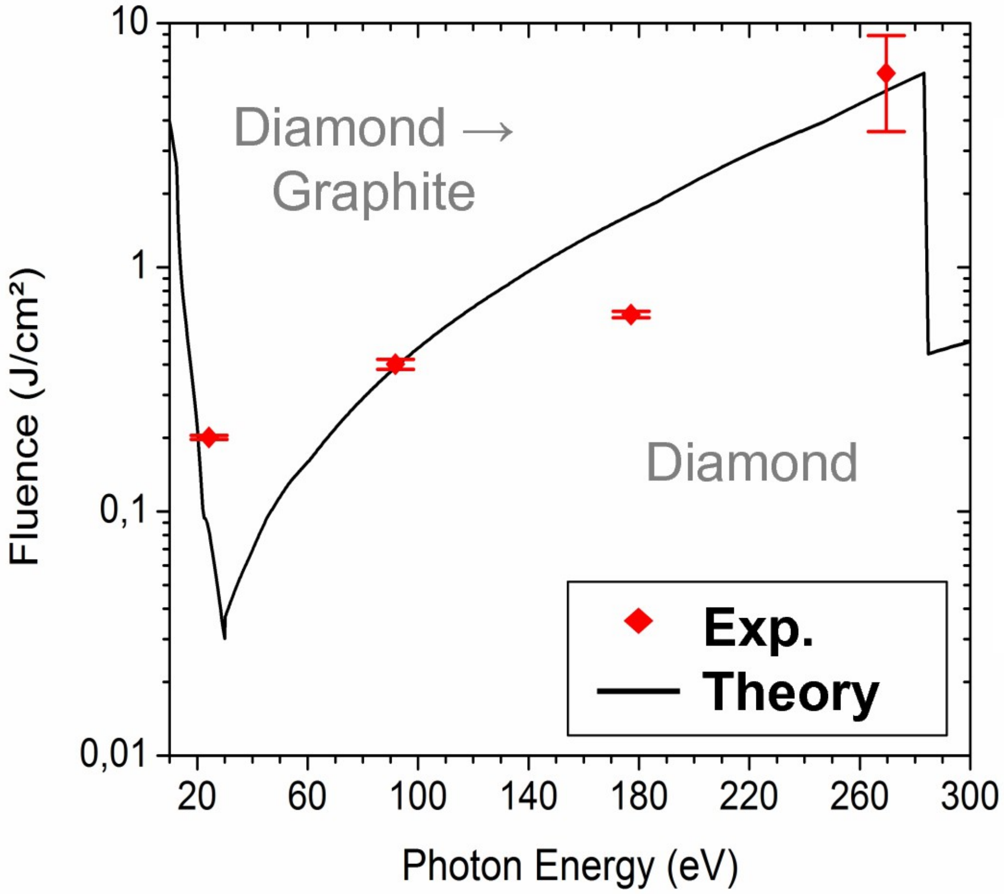
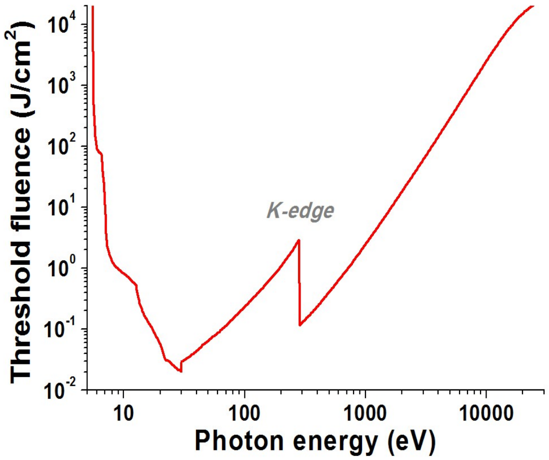
[Images courtesy of N. Medvedev]

Graphitization Damage threshold

Irradiated diamond turns into graphite if the fluence is high:





Extrapolation to hard X-rays

Damage threshold is in a good agreement with the experiments by J. Gaudin *et al.* (FLASH)

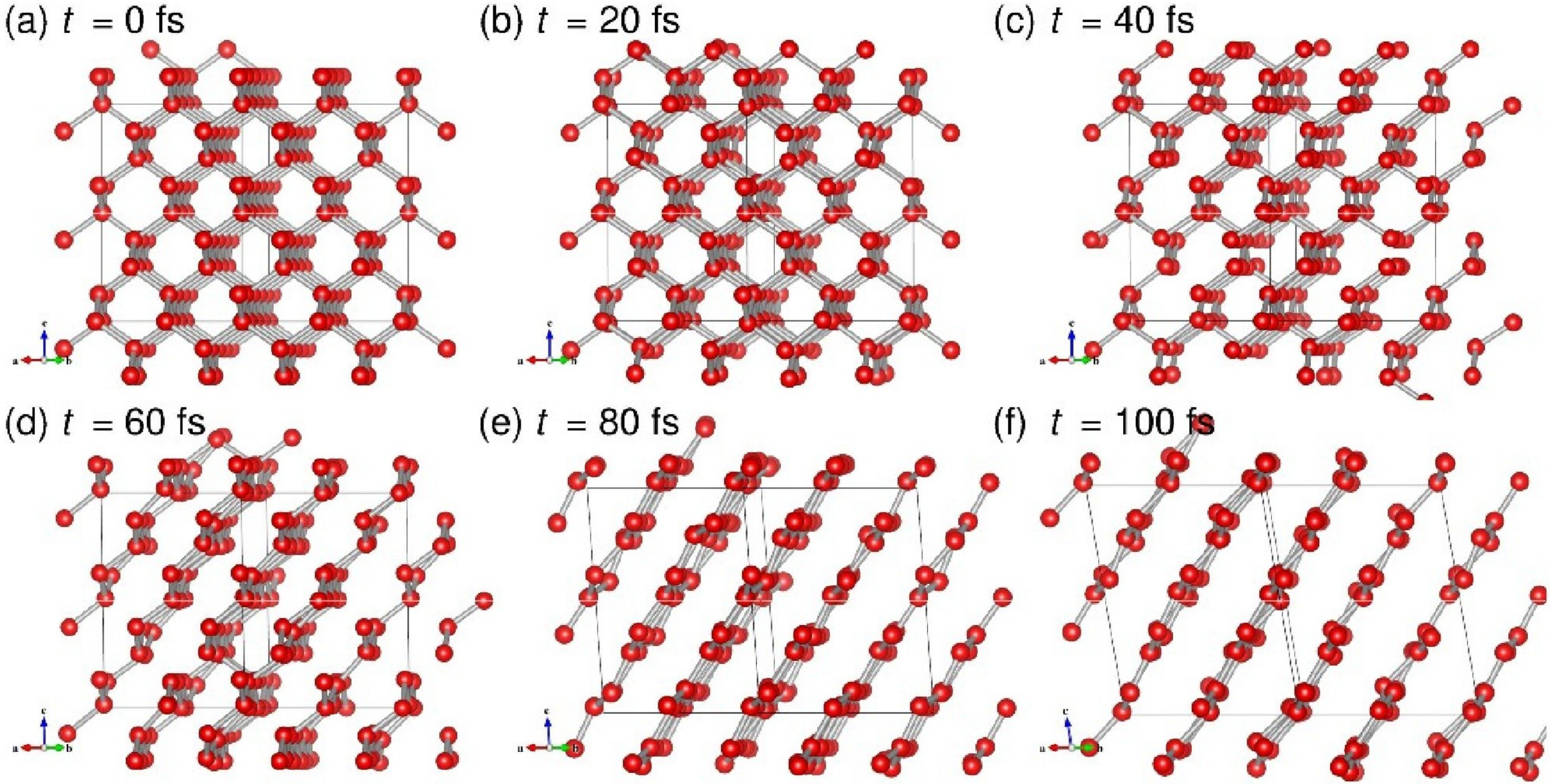
[J. Gaudin et al., PRB, Rapid Comm. 88 (2013) 060101 (R)]

[N. Medvedev , H. Jeschke, BZ, PRB 88 (2013) 224304]

[This slide courtesy of N.Medvedev]

Graphitization : Atomic snapshots

Photon energy 92 eV, FWHM = 10 fs



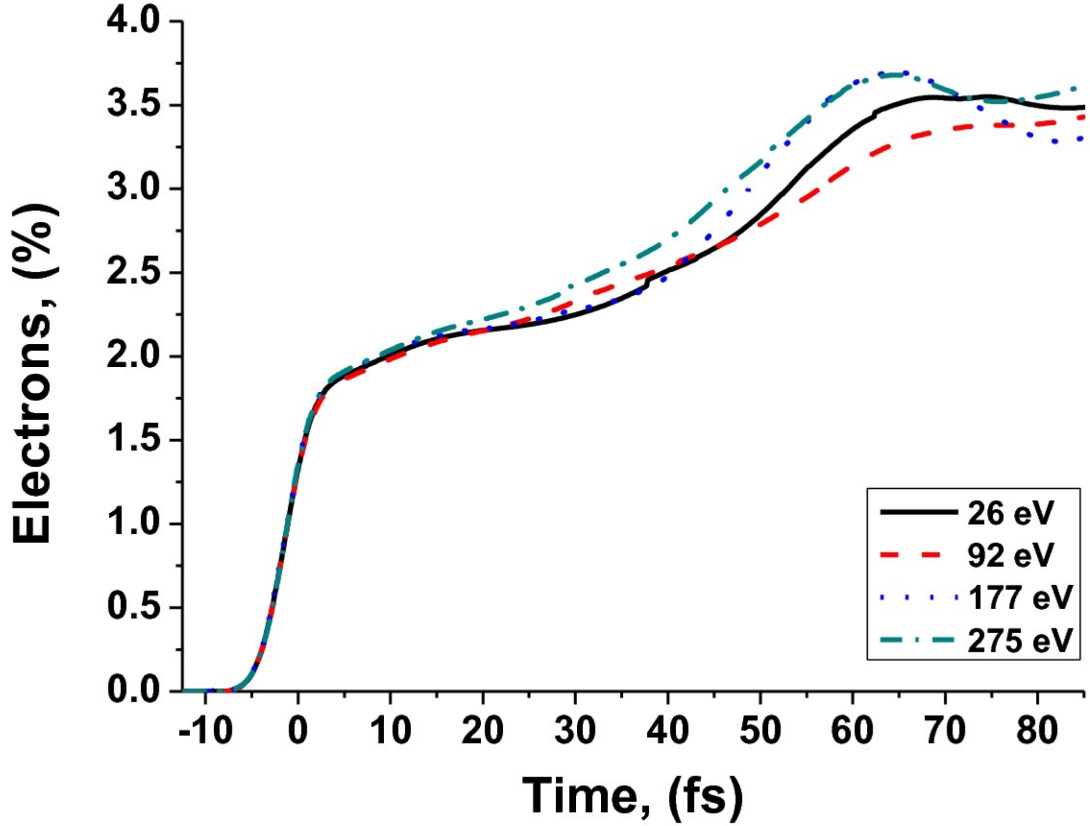
Ultrafast graphitization of diamond

[N. Medvedev, H. Jeschke, B. Ziaja, NJP 15 (2013) 015016]

[This slide courtesy of N.Medvedev] **Increase of electronic density → band gap collapse**

Results: Conduction band electrons

Different photon energies: 26 eV, 92 eV, 177 eV, 275 eV

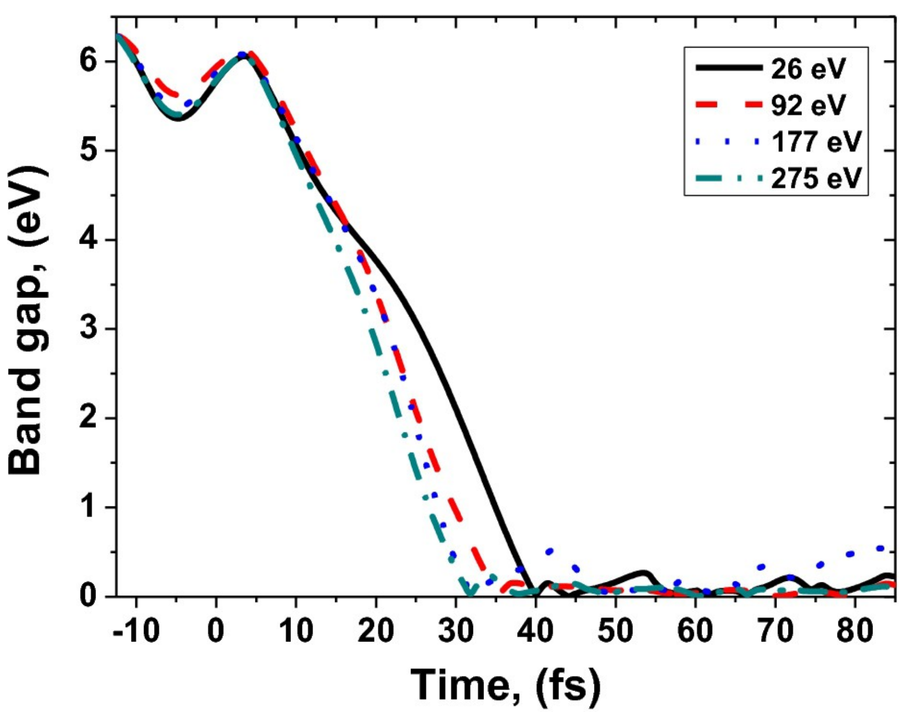


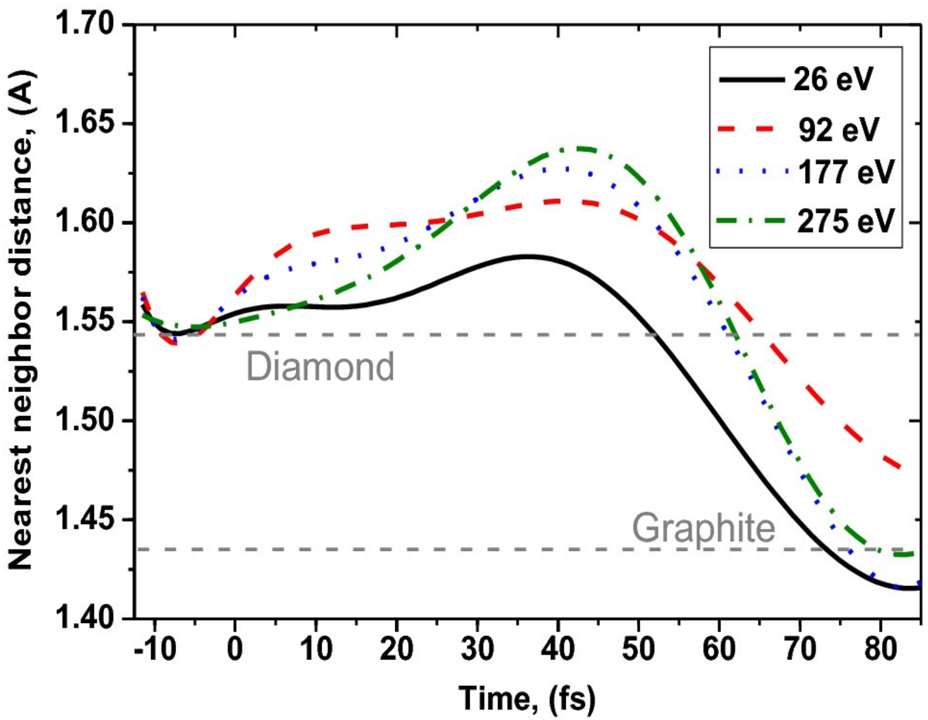
When electron density overcomes threshold value of 1.5 %, phase transition occurs

[This slide courtesy of N.Medvedev]

Results: Bandgap collapse

Different photon energies: 26 eV, 92 eV, 177 eV, 275 eV

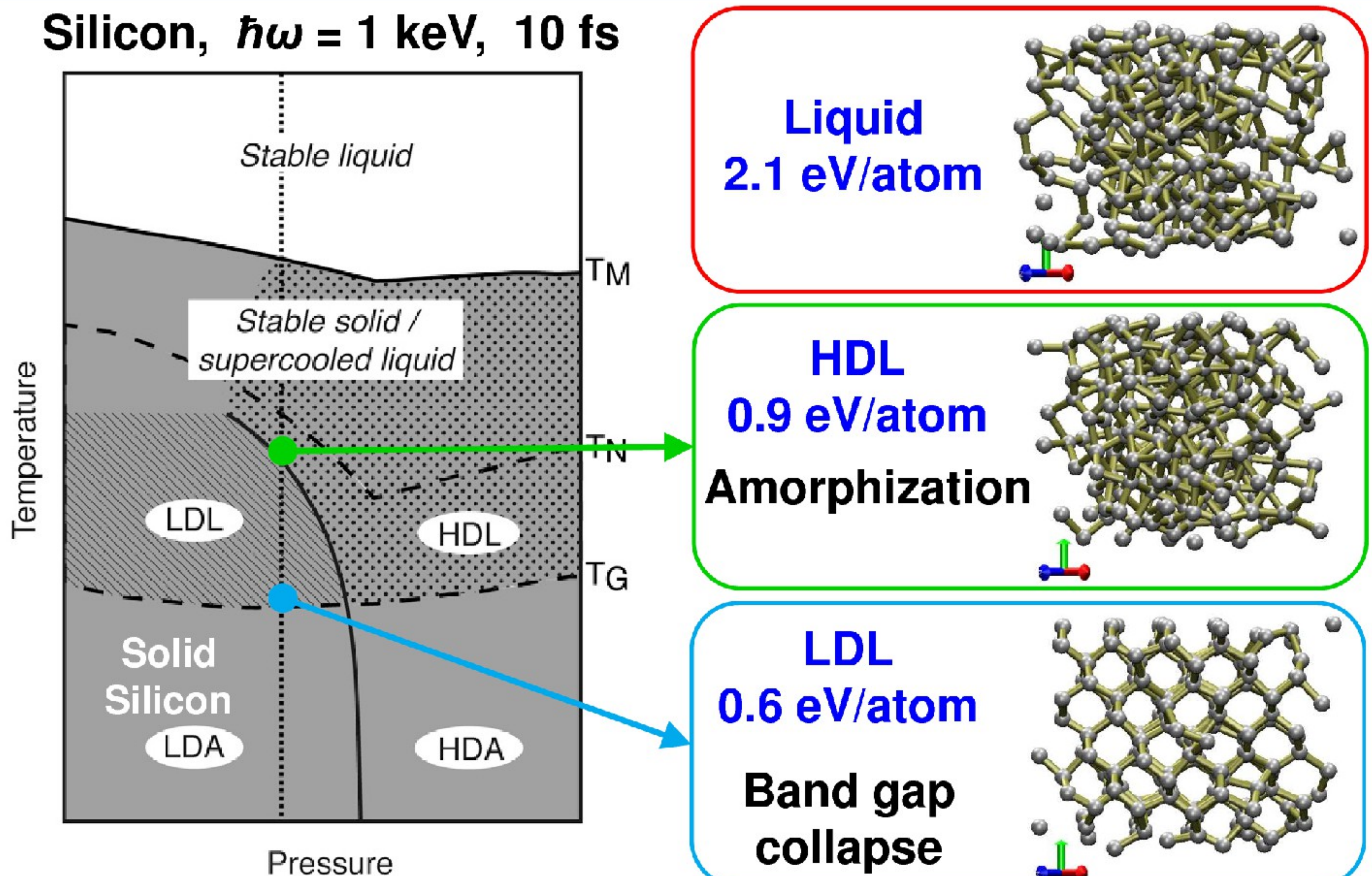




Bandgap collapse induces ultrafast phase transition

[This slide courtesy of N.Medvedev]

Structural transition in Si: interplay of thermal and non-thermal processes



M. Beye, *et al.*, *J. of El. Spectr.* 188 (2013) 172

N. Medvedev, Z. Li, B. Ziaja, PRB 91 (2015) 054113

[This slide courtesy of N.Medvedev]

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Diagnostics of transitions?

Damage thresholds → post mortem measurements on samples

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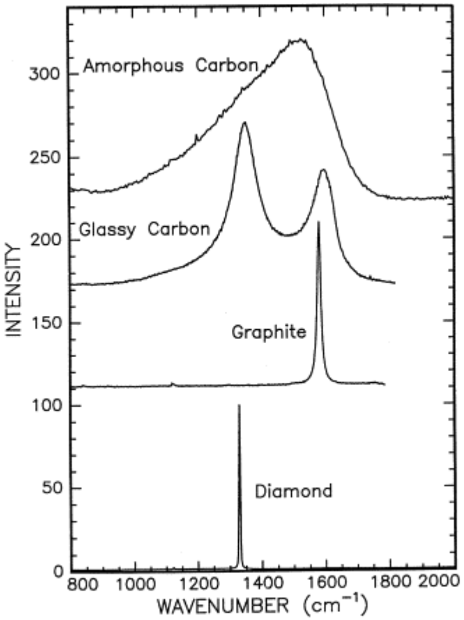

matsci4uwi.wordpress.com

Diagnostics of transitions?

Damage thresholds → post mortem measurements on samples

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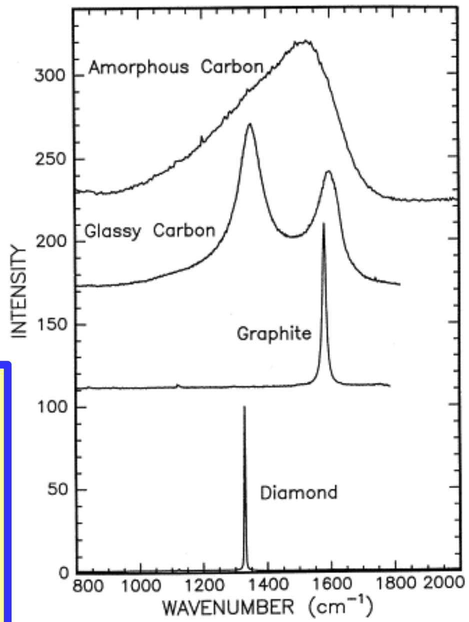

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Challenge: long-time large-scale simulations needed for comparison to post-mortem measurements

←

long time-span between ultrafast excitation and final relaxation of the material: lattice heating, diffusion, recrystallization ...

Time-resolved diagnostics of transitions:

Pump-probe experiments:

- pump pulse initiates transition ...

- probe pulse probes it at varying time delay ...

Transient optical properties as diagnostics of X-ray induced transitions

Low material excitation below and around damage threshold → band structure evolution accurately described with transferable tight binding method

Long-wavelength limit (q → 0), **Tight-binding (TB) model**

Optical **dielectric function** within the random-phase approximation (Lindhard formula) [3]:

$$\epsilon^{\alpha\beta}(E) = \delta_{\alpha,\beta} + \frac{4\pi e^2\hbar^2}{m\Omega}\sum_{n,n'}(\eta_{n'} - \eta_n)\frac{F^{\alpha\beta}_{n,n'}}{E_{n,n'}}\left[\frac{1}{E - E_{n,n'} + i\gamma}\right]$$

$$F^{\alpha\beta}_{n,n'} = \frac{2\langle n|\hat{p}_\alpha|n'\rangle\langle n'|\hat{p}_\beta|n\rangle}{mE_{n,n'}}$$ - the oscillator strength [3]

Calculated within tight-binding model by F. Trani et al, as: $\mathbf{P}(\mathbf{R},\mathbf{R}') = \frac{m}{i\hbar}[\mathbf{R} - \mathbf{R}']H(\mathbf{R},\mathbf{R}')$

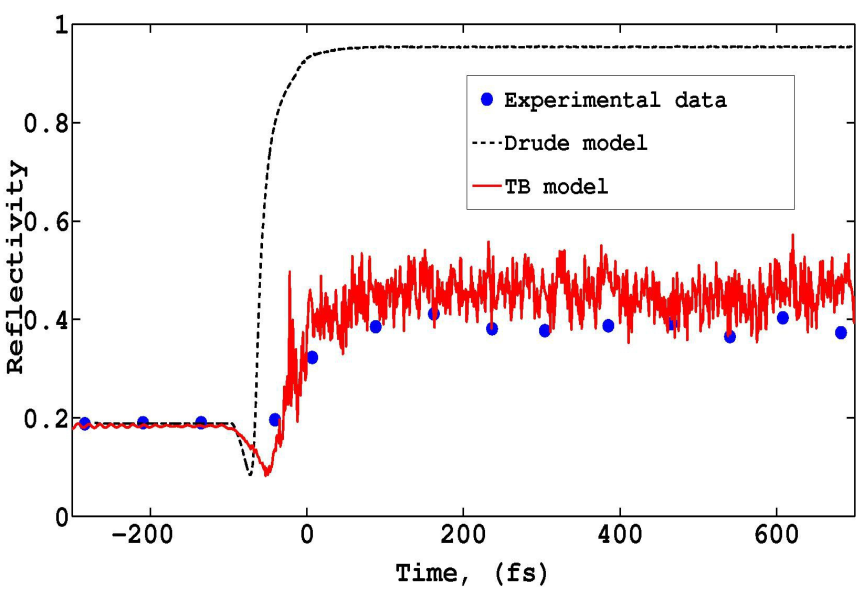
Dielectric function → refractive indices n, k

[Courtesy of V. Tkachenko] [V. Tkachenko, N. Medvedev et al. (BZ), *Phys. Rev. B* 93 (2016) 144101]

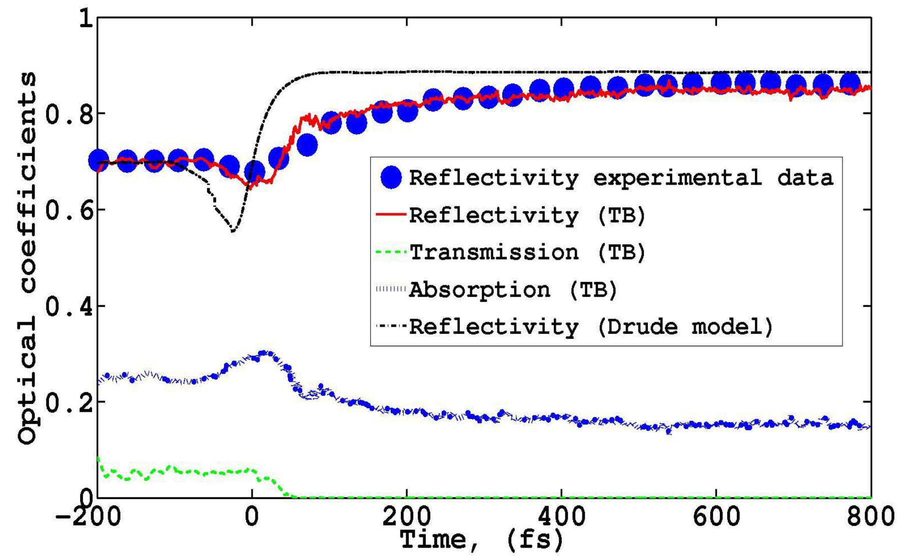
Transient optical properties as diagnostics of X-ray induced transitions

Low material excitation below and around damage threshold → band structure evolution accurately described with transferable tight binding method

-Diamond and silicon are excited with a laser pulse ...
-Transient optical properties are probed with the optical laser pulse ...
-Complex dielectric function calculated from an ab-initio scheme ...



Diamond



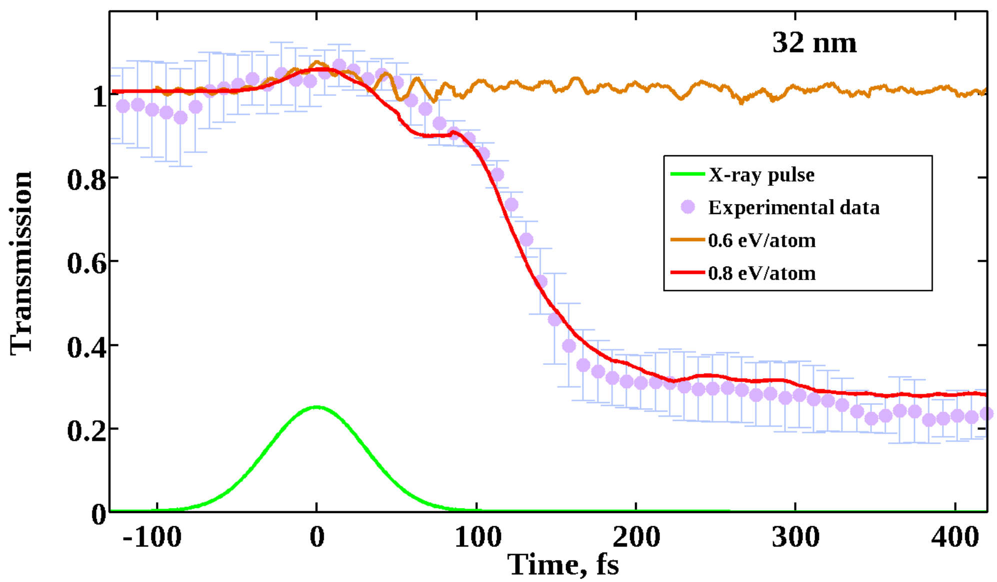
Silicon

[Courtesy of V. Tkachenko] [V. Tkachenko, N. Medvedev et al. (BZ), *Phys. Rev. B* 93 (2016) 144101]

Transient optical properties as diagnostics of X-ray induced transitions

Damage threshold

First observation of time-resolved graphitization



Absorbed dose = 0.8 eV/atom

FEL pulse duration = 51 fs

FEL photon energy = 47.4 eV

Probe pulse duration = 32.8 fs

Probe wavelength = 630 nm

Angle of X-ray pulse incidence = 20°

Experiment performed by Sven Toleikis, Franz Tavella, Hauke Hoeppner, Mark Prandolini et al. at FERMI facility

-- Characteristic drop of transmission is observed during the experiment on fs time-scale

-- Evidence of phase transition within ~150 fs.

-- Very good agreement with our theoretical predictions for the absorbed dose of 0.8 eV/atom (above graphitization threshold)

Melting threshold

[F. Tavella et al. (V.Tkachenko, N. Medvedev, BZ), HEDP 24 (2017) 22] → DESY Press Release

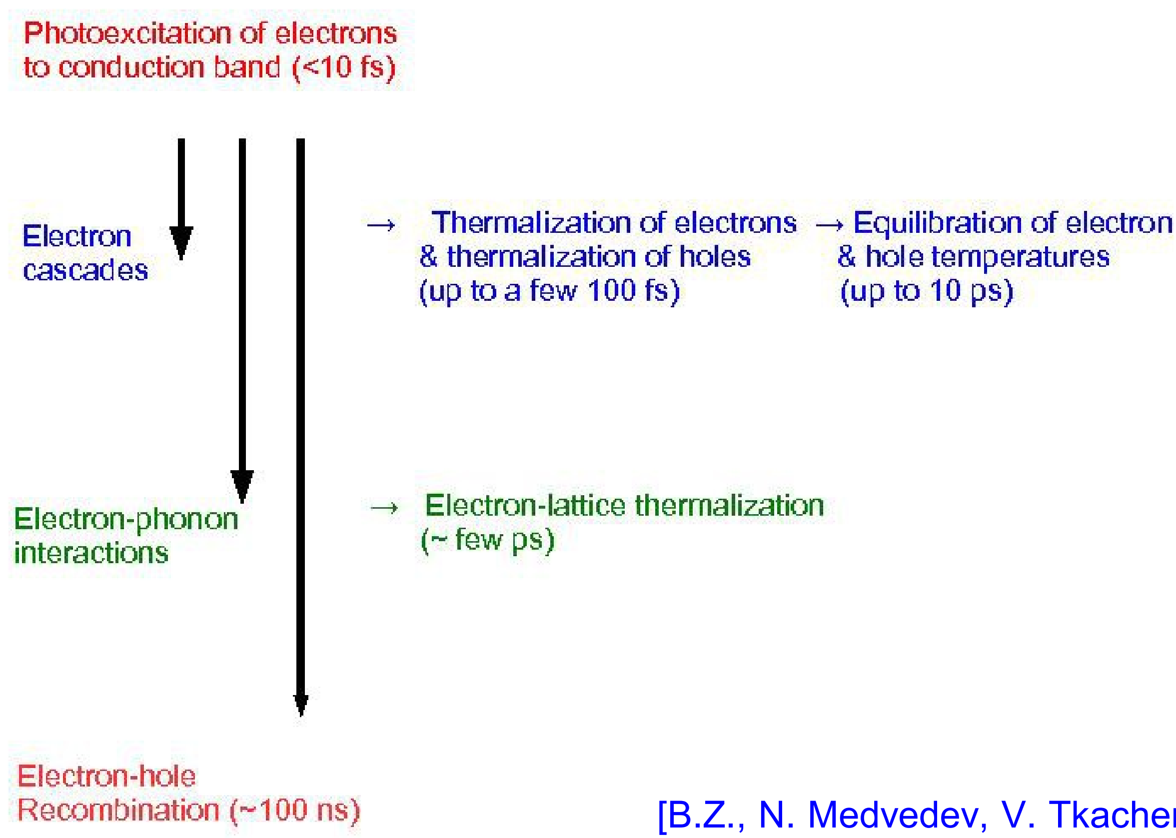
[Courtesy of V. Tkachenko]

Transient optical properties as diagnostics of picosecond transitions within irradiated systems

Low dose

Reflectivity overshooting in GaAs ← effect of band gap shrinking

Timescales of relaxation and excitation processes.



Damage Threshold

[B.Z., N. Medvedev, V. Tkachenko, T. Maltezopoulos, W. Wurth, *Sci. Rep*. **5**, 18068 (2015)]

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

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[Courtesy of V. Tkachenko]

Transient optical properties as diagnostics of picosecond transitions within irradiated systems

Low dose

Damage Threshold

Reflectivity overshooting in GaAs

- Rate equations → the evolution of free-carrier densities as a function of time [5];

$$d\,n_{e-h}(t)/dt = \gamma_{e-h}(t)$$ ←Before ΔR/R minimum

$$d\,n_{e-h}(t)/dt = -\gamma_{rec}\cdot n_{e-h}(t)$$ ←After ΔR/R minimum

- Two-temperature model → electron-lattice equilibration [5];

$$d\,T_{latt}(t)/dt = +G_{latt}(T_{e-h}(t) - T_{latt}(t))$$

$$d\,T_{e-h}(t)/dt = -G_{e-h}(T_{e-h}(t) - T_{latt}(t))$$

- Drude model → follows the transient reflectivity (extended for interband transitions) [5].

[B.Z., N. Medvedev, V. Tkachenko, T. Maltezopoulos, W. Wurth, *Sci. Rep.* **5**, 18068 (2015)]

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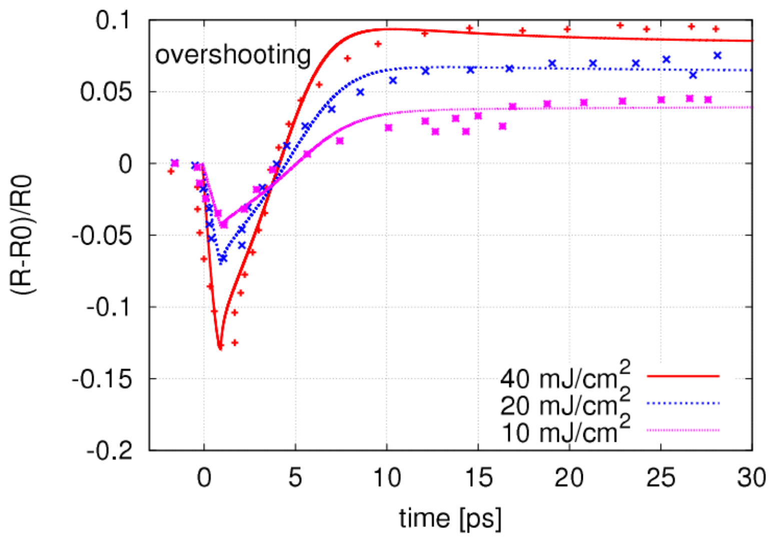
[Courtesy of V. Tkachenko]

Transient optical properties as diagnostics of picosecond transitions within irradiated systems

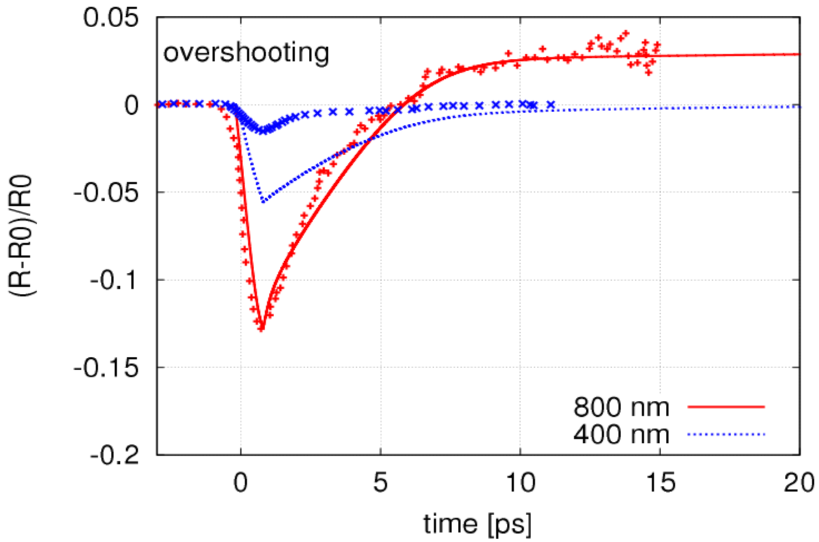
Reflectivity overshooting in GaAs ← effect of band gap shrinking

Low dose

- Timescale of a few ps
- Observable at probe wavelength ~ band gap width (low absorption)
- Measurement of electron-phonon coupling with femtosecond resolution ($\tau_{el\text{-}latt}$~ 2-3 ps) and transient electronic temperatures (~ 2-3 eV)
- Expected for other narrow band-gap semiconductors



LCLS measurement (800 eV)



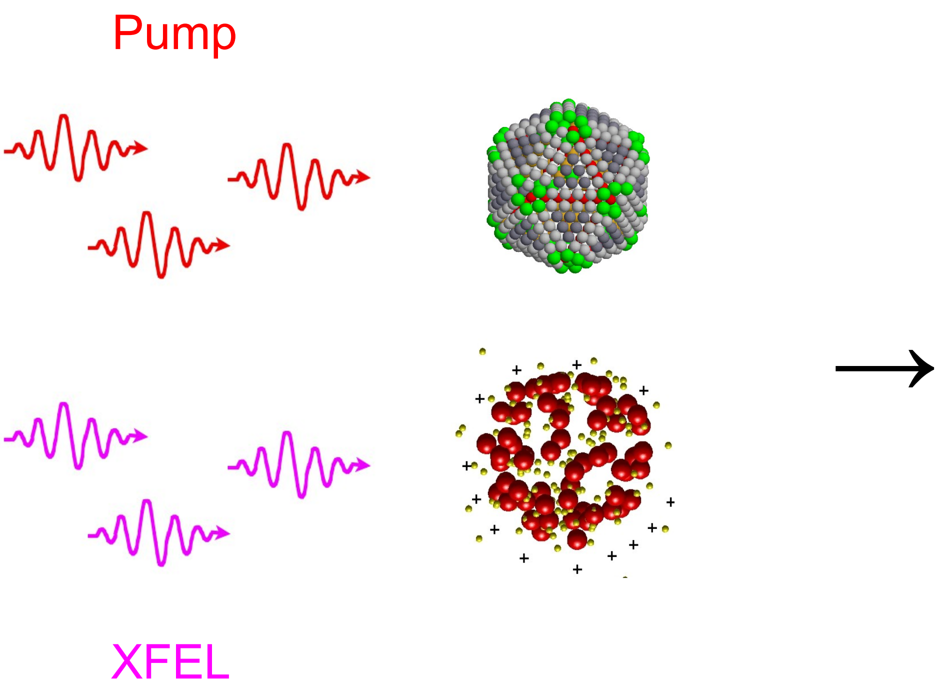
FLASH measurement (40 eV)

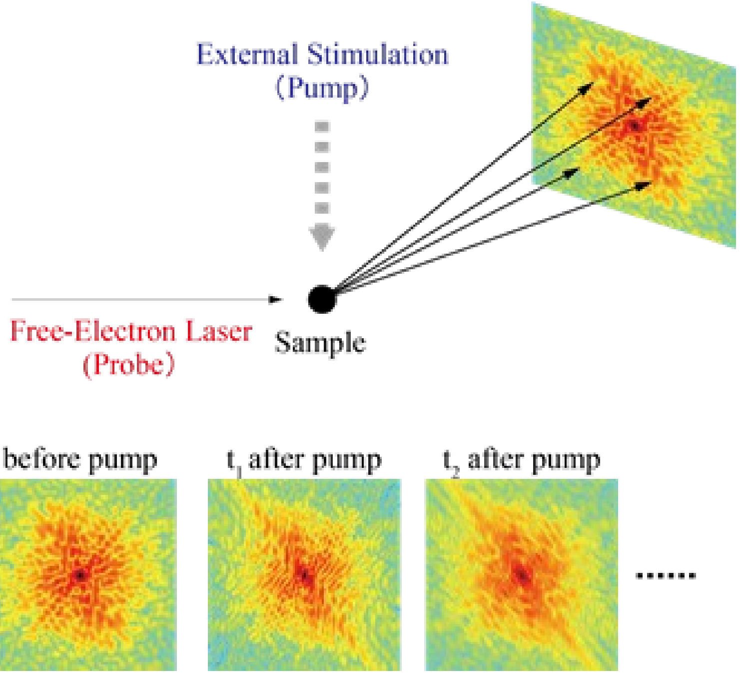
Damage Threshold

[B.Z., N. Medvedev, V. Tkachenko, T. Maltezopoulos, W. Wurth, *Sci. Rep*. **5**, 18068 (2015)]

[Courtesy of V. Tkachenko]

X-ray diffraction as diagnostics of structural transitions?





[cxo-www.es.hokudai.ac.jp]

Outline

1. Transitions in matter triggered by X-rays

2. X-ray induced electronic and structural transitions in solids modeled with our in-house codes XCASCADE and XTANT

3. Diagnostics of structural transitions

4. Amorphization of solids by intense X-ray pulse → plasma creation

5. Summary

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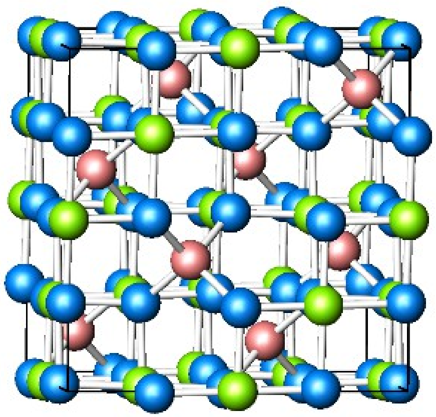
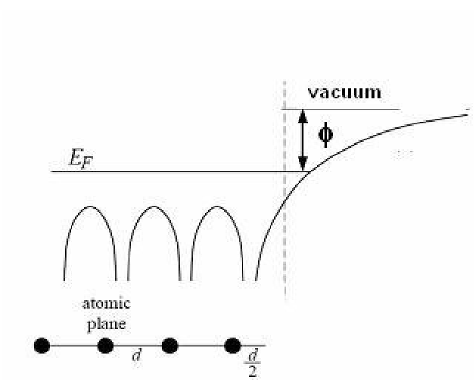
Impact of high-fluence fs X-ray pulses:
→Transition to Warm Dense Matter or Plasma

Melting threshold

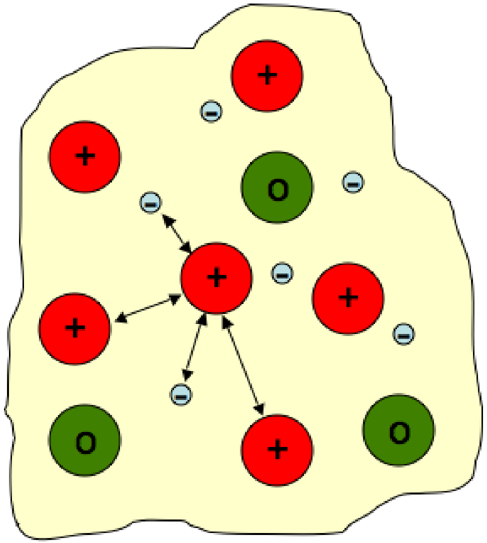
'Ensemble' of bonded atoms





→

'Gas' of free ions and electrons



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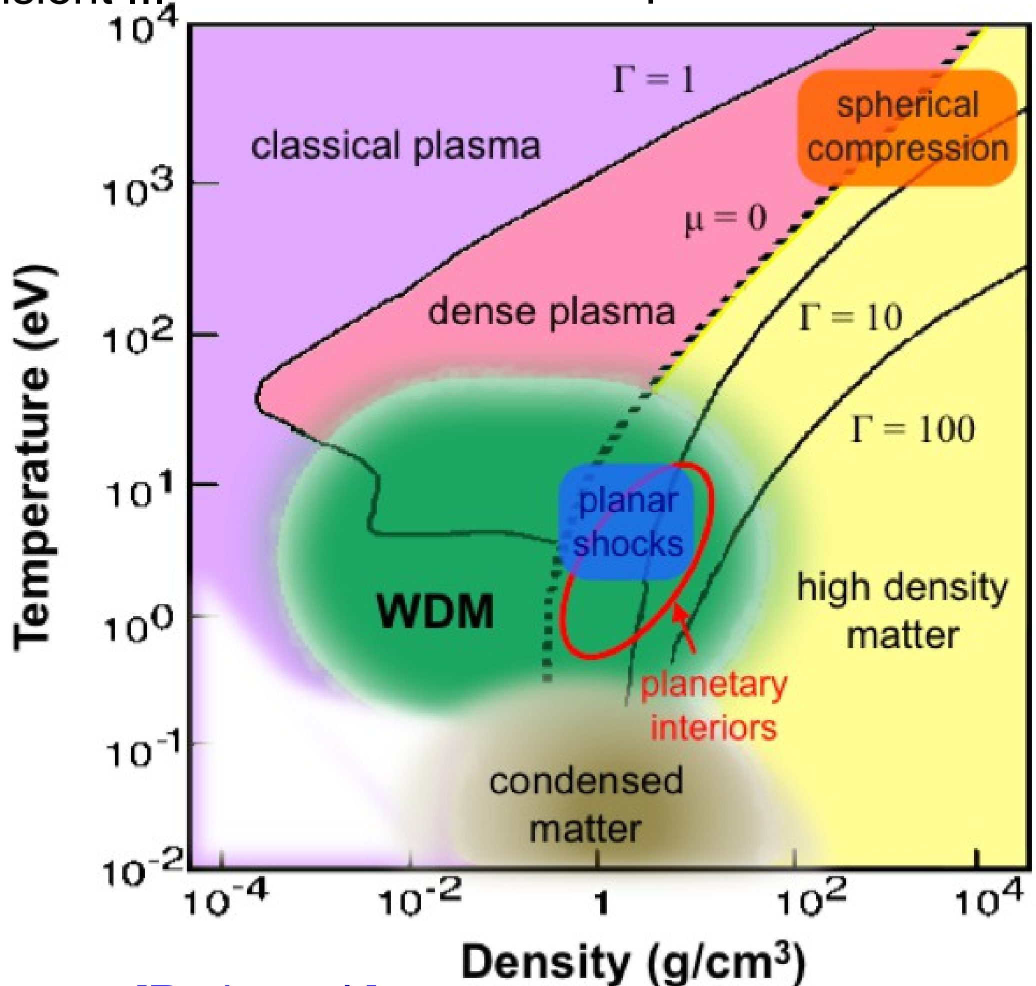
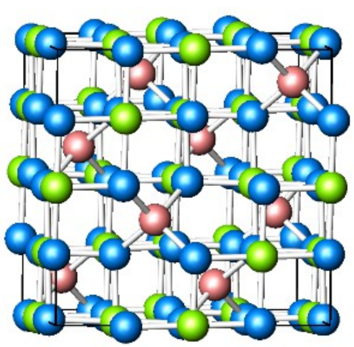
Matter in warm dense matter (WDM) state

Located between solid state and plasma state. Because of its extreme temperatures and pressures, WDM tends to be drastically transient ...

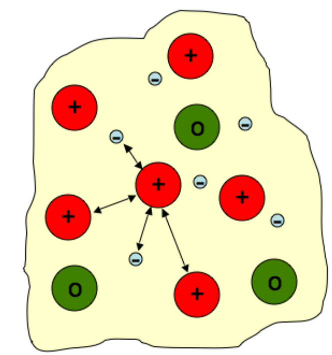
Y





[Roth et al.]

WDM defined by Γ, Y ≈ 1.



Γ – Coulomb coupling parameter =

potential energy/
kinetic energy

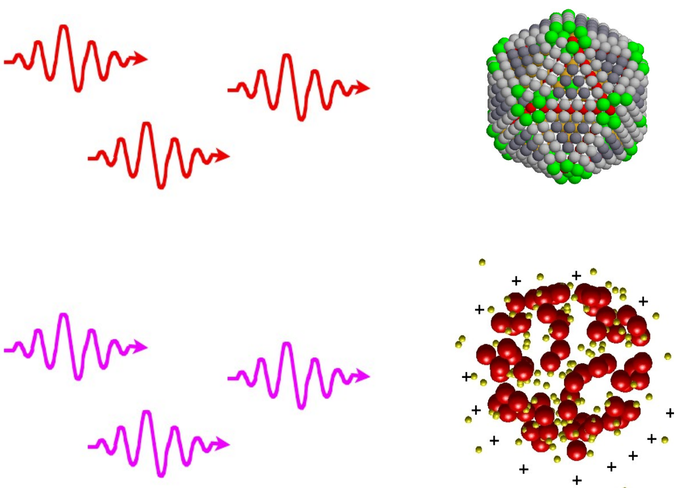
Y – degeneracy parameter =

Fermi energy/
kinetic energy

X-ray diffraction as diagnostics of structural transitions

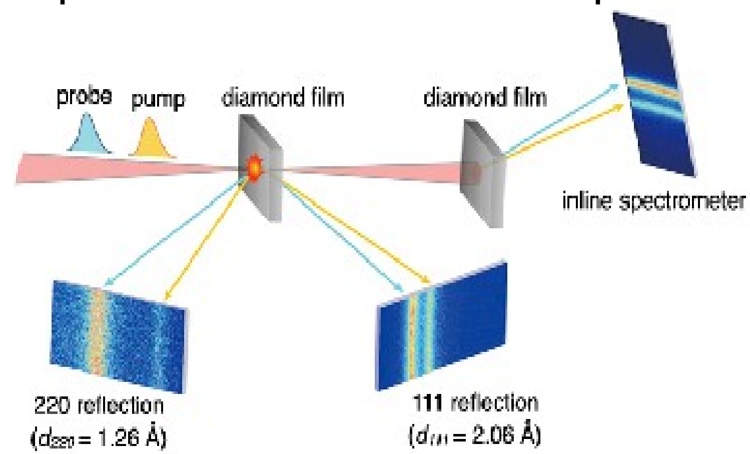
Example: diamond melted into plasma ...

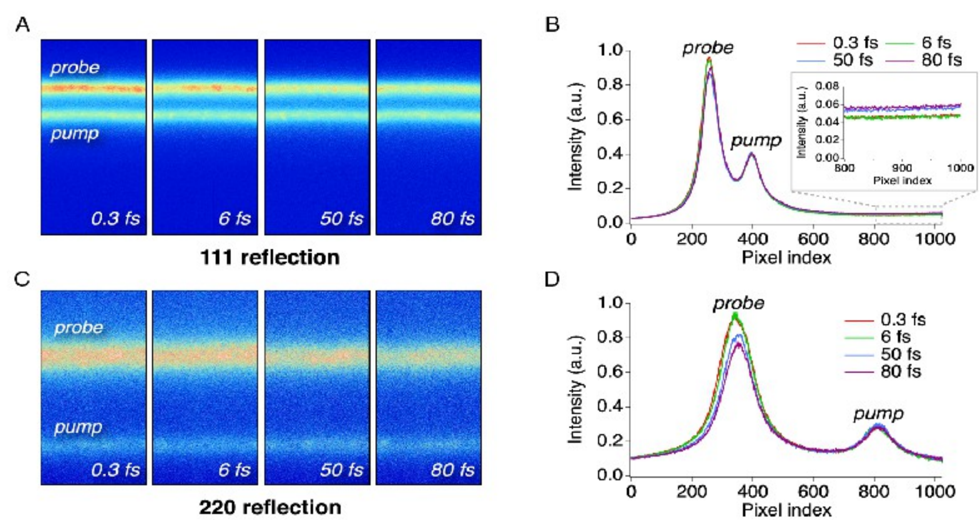
Pump



XFEL

→





[I. Inoue et al., PNAS 113 (2016) 1492]

SACLA pump/probe scheme:

3 / 7 J/cm^2

5 / 5 fs

6.1/ 5.9 keV

Amorphisation of diamond: atomic snapshots

Irradiation of diamond crystal
with 5 fs-long pump pulse:

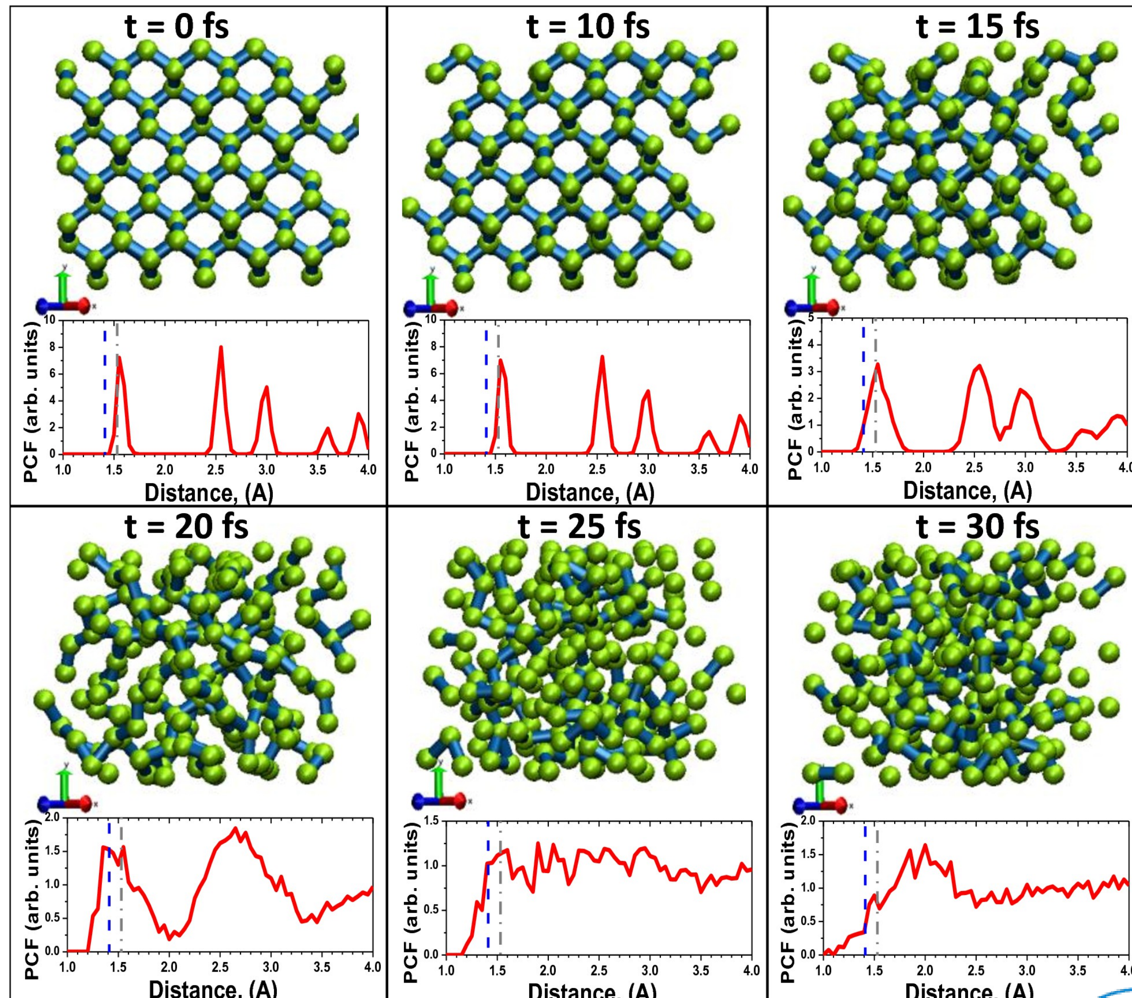
X-ray photons: 6.1 keV energy
Fluences: 2.3 - 3.1 · 10^4 J/cm^2

↓

Average absorbed dose/atom:
19-25 eV/atom

↓

Intermediate graphitization phase
at ~ 20 fs -
with overdense graphite ...

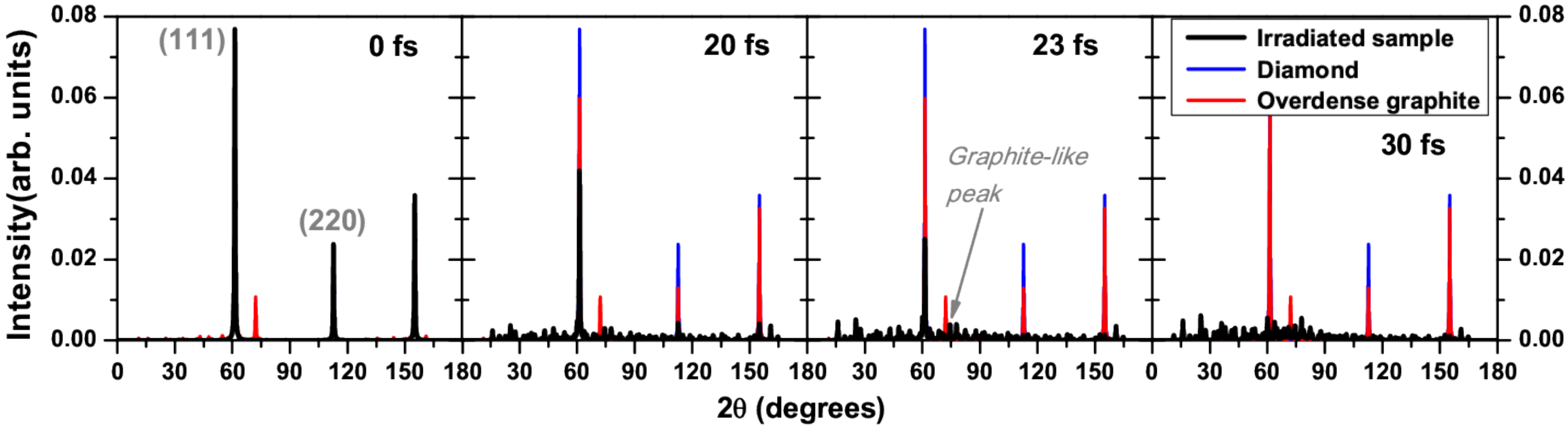


[N. Medvedev, B. Ziaja, Sci. Rep. 8 (2018) 5284]

XTANT simulations by N. Medvedev

Amorphisation of diamond: transient graphitization phase?

Intermediate few-fs long graphitization phase:
simulated powder diffraction peaks



Powder diffraction patterns in diamond irradiated with an X-ray pulse of 6.1 keV photon energy, 5 fs FWHM duration, at the average absorbed dose of 24.9 eV/atom at different time instants after the pump pulse maximum.

[N. Medvedev, B. Ziaja, Sci. Rep. 8 (2018) 5284]

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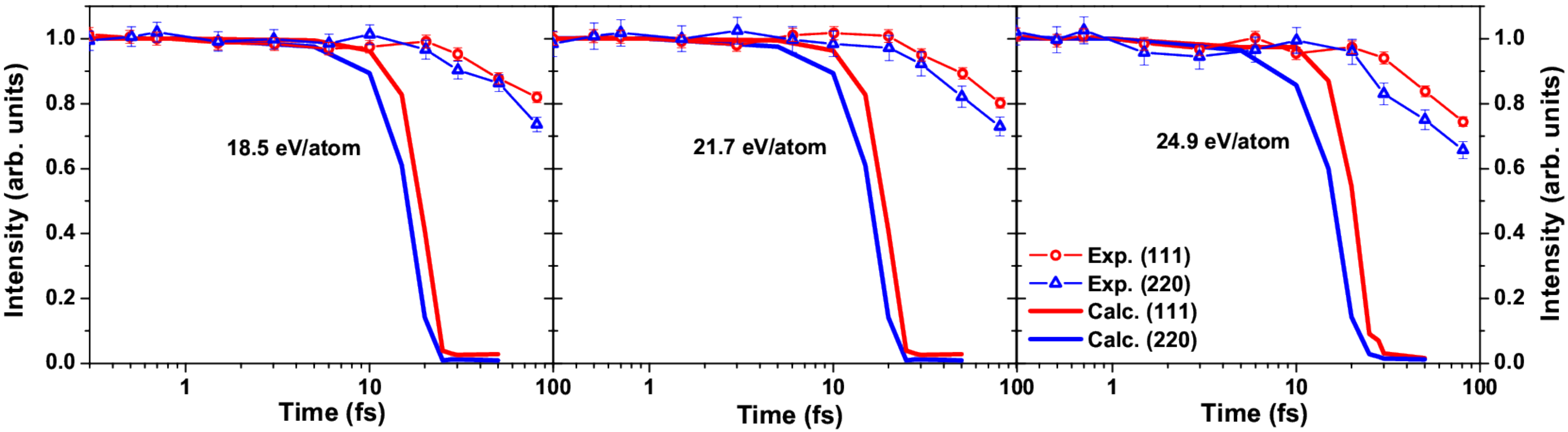
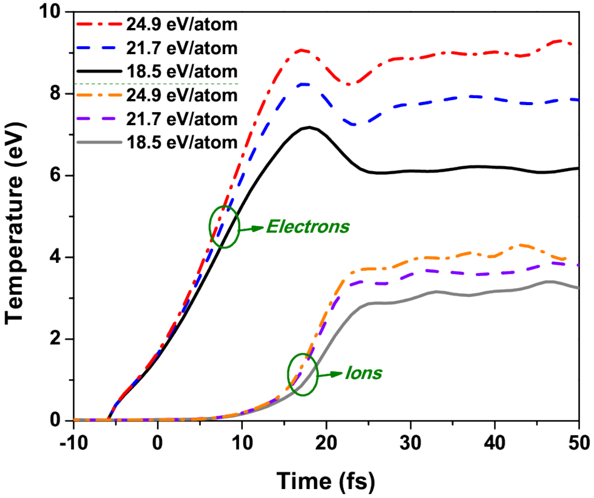
Comparison with experiment



↑

Integrated diffraction peak intensities (111) and (220) in X-ray irradiated diamond →
Too fast intensity decrease predicted

Temperatures of electrons and ions in X-ray irradiated diamond → Timescales of the T_i increase in agreement with DW fit from experiment



[N. Medvedev, B. Ziaja, Sci. Rep. 8 (2018) 5284]

Necessary model improvements

Currently, no fully ab-initio model exists to describe accurately WDM formation after solid's irradiation with X-rays!

XTANT could be a possible hybrid solution if some current shortcomings are addressed:

- correct description of atomic orbitals and impact ionization cross sections in dense plasmas

- impact of K-shell holes

- band structure description underway to dense plasma → tight-binding model we use breaks down at high densitites of excited electrons (i.e., times > 20 fs)

- effect of probe pulse (5 fs FWHM)

[N. Medvedev, B. Ziaja, Sci. Rep. 8 (2018) 5284]

DESY

Necessary model improvements

Currently, no fully ab-initio model exists to describe accurately WDM formation after solid's irradiation with X-rays!

XTANT could be a possible hybrid solution if some current shortcomings are overcome:

- correct description of atomic orbitals and impact ionization cross sections in dense plasmas → work on-going (J.Bekx, S.-K. Son, R. Santra, BZ)

- impact of K-shell holes→turns out to be not critical in this case

- band structure description underway to dense plasma → tight-binding model we use breaks down at high densitites of excited electrons (i.e., times > 20 fs) → ab-initio model under construction (J.Bekx, V. Lipp, N. Medvedev, R. Santra, S.-K. Son, V. Tkachenko, BZ)

- effect of probe pulse (5 fs FWHM) → negligible here

[N. Medvedev, B. Ziaja, Sci. Rep. 8 (2018) 5284]

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Summary

Transitions in solids induced by X-ray radiation depend on material properties and pulse parameters:

-below damage threshold – non-equilibrium electron kinetics →XTANT

-below melting threshold – also rearrangement of atomic structure ↑

-above melting threshold – amorphization; plasma, warm-dense matter formation →model developments on-going!

Diagnostics of transitions:

- transient optical properties ← time-resolved

- X-ray diffraction ← time-resolved

- post mortem measurements

Summary

Transitions in solids induced by X-ray radiation depend ... erial properties and pulse parameters:

-below damage threshold – non-equ... →XTANT

-below melting thresh... atomic structure ↑

-above m... ...ization; plasma, warm-dense matter

... ormation →model developments on-going!

Diag... ...ons:

- trans... optical properties ← time-resolved

- X-ray diffraction ← time-resolved

- post mortem measurements

Bottleneck: lack of universal ab-initio description of transient electronic structure in response to nuclear dynamics → Remedy: DFTB + method

Applications so far ...

Low fluence material excitation below and around damage threshold.
Transient optical properties can follow:

[V. Tkachenko, N. Medvedev et al. (BZ), *Phys. Rev. B* 93 (2016) 144101]

- Electron kinetics ~ 100 fs →application for FEL pulse diagnostics

[M.Harmand et al. (Medvedev, BZ), *Nat. Phot.* 7 (2013) 215;
R. Riedel et al.(Medvedev,BZ), *Nat. Commun*. 4 (2013) 1731,
P. Finetti et al. (Medvedev, Tkachenko, BZ), *Phys. Rev. X* (2017) accepted]

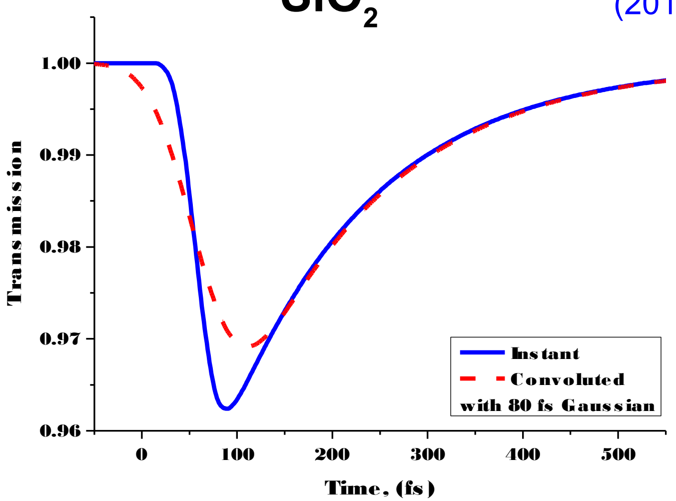
- Structural transitions ~ 100 fs - ps→application for damage studies in FEL optics

[N.Medvedev et al. (BZ): NJP 15 (2013) 015016; PRB 88 (2013) 224304 & 060101]

- Lattice heating ~ few ps → application for material studies

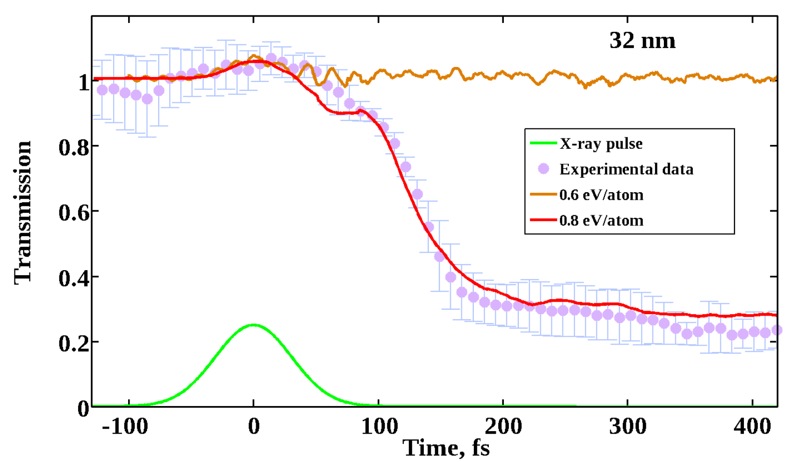
[B.Z., N. Medvedev, V. Tkachenko, T. Maltezopoulos, W. Wurth, *Sci. Rep*. 5, 18068 (2015)]

SiO_2



Electron kinetics follows temporal pulse profile ...

Diamond



Time-resolved non-thermal graphitization ...

[F. Tavella et al. (V.Tkachenko, N. Medvedev, BZ), 2016 submitted]

Thanking my collaborators and the CFEL-DESY Theory Group

V. Lipp

N. Medvedev

V. Saxena

V. Tkachenko

\+ J. Bekx

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Thanking our external collaborators...

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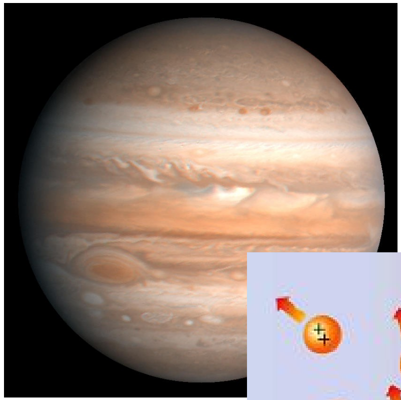
H. Jeschke (U. Frankfurt), Z. Li (LCLS), P. Piekarz (INP, Kraków)

L. Juha, M. Stransky (FZU, Prague), R. Sobierajski (IF PAN, Warszawa)

H.-K. Chung (IAEA, Vienna), R. W. Lee (LBNL, Berkley)



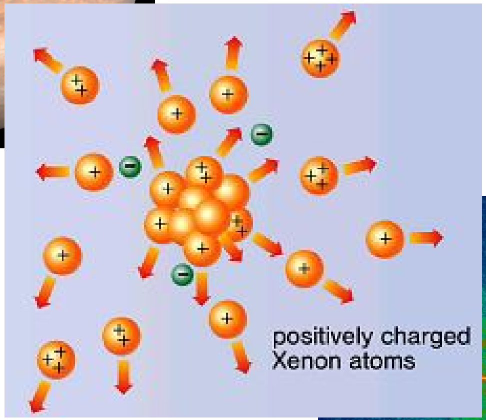
M. Harmand (LULI,CNRS), M. Cammarata (U. Rennes)

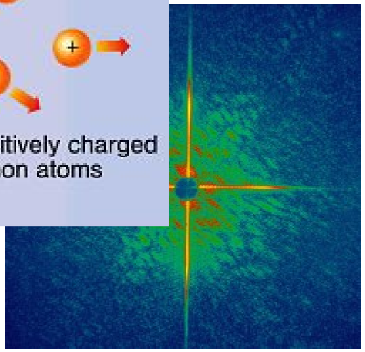
A. Ng (U. British Columbia), Z.Chen, Y.Y. Tsui (U. Alberta), V. Recoules (CEA, DAM)

F. Tavella (LCLS), U. Teubner (U. Oldenburg) and FERMI team

S. Toleikis, H. Hoeppner, M. Prandolini, T. Takanori (DESY)

and ...





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XTOOLs of the CFEL-DESY Theory Group

- **XATOM**[1]: an ab-initio integrated toolkit for x-ray atomic physics
- **XMOLECULE**[2]: an ab-initio integrated toolkit for x-ray molecular physics
- **XMDYN**[3]: an MD/MC tool for modeling matter irradiated with high intensity x-rays
- **XHYDRO**[4]: a hydrodynamic tool for simulating plasma in local thermodynamic equilibrium
- **XSINC**[5]: a tool for calculating x-ray diffraction patterns for nanocrystals
- **XTANT**[6]: a hybrid tight-binding/MD/MC tool to study phase transitions
- **XCASCADE**[7]: MC tool to follow electron cascades induced by low x-ray excitation
- **XCALIB**[8]: an XFEL pulse profile calibration tool based on ion yields

R. Santra	B. Ziaja	S.-K. Son	Z. Jurek	N. Medvedev	V. Saxena	L. Inhester	K. Toyota	V. Lipp	M.M. Abdullah	V. Tkachenko
1-5, 8	3,4,6,7, Boltzmann-code	1,2,3,8	3,5,8	6,7 (now in Prague)	4 (now in India)	1,2	1,2,8	6,7	3,5	6,7

Released versions of XATOM and XMDYN available at http://www.desy.de/~xraypac

[Slide courtesy of Z. Jurek]

Thank you for your attention !

Radiative Properties of Hot Dense Matter 2018

Hamburg, 21-26 October 2018

Organizers: DESY & European XFEL

MD: Parrinello – Rahman method

$$L=\sum_{i=1}^{N}\frac{m_i}{2}\dot{\mathbf{s}}_i^{\mathrm{T}}h^{\mathrm{T}}h\,\dot{\mathbf{s}}_i+K_{\mathrm{cell}}-\Phi(\{r_{ij}\},t)-U_{\mathrm{cell}}$$

$$K_{\mathrm{PR}}=\frac{w_{\mathrm{PR}}}{2}\,\mathrm{Tr}(\dot{h}^{\mathrm{T}}\dot{h})$$

$$U_{\mathrm{cell}}=p_{\mathrm{ext}}\Omega$$

$$\Omega\;=\;\det(h)$$

$$\ddot{\mathbf{s}}_i=-\frac{1}{m_i}\sum_{j\neq i}\frac{\partial\Phi(r_{ij})}{\partial r_{ij}}\frac{\mathbf{s}_i-\mathbf{s}_j}{r_{ij}}-g^{-1}\dot{g}\dot{\mathbf{s}}_i$$

$$\ddot{h}=\;(\Pi-p_{\mathrm{ext}})\frac{\sigma}{w_{\mathrm{PR}}}$$

$$\Pi=\frac{1}{\Omega}\sum_{i=1}^{N}m_i\mathbf{v}_i\mathbf{v}_i^{\mathrm{T}}-\frac{1}{\Omega}\sum_{i=1}^{N}\sum_{j>i}\frac{\partial\Phi(\{r_{ij}\},t)}{\partial r_{ij}}\frac{\mathbf{r}_{ij}\mathbf{r}^{\mathrm{T}}}{r_{ijij}}$$

Size and shape of the super-cell are changing

$$g=h^{\mathrm{T}}h,\;\mathbf{v}_i=h\dot{\mathbf{s}}_i\qquad\sigma_{\alpha\beta}=\partial\Omega/\partial h_{\alpha\beta}.$$

[This slide courtesy of N.Medvedev]