Computational approaches to nuclear many-body problems
and related quantum systems
Feb. 12-16, 2013, RIKEN, Wako, Japan

Time-dependent density functional theory for ultrafast electron dynamics in solid

First-principles computational approach for Frontiers of Laser Sciences

Kazuhiro YABANA

Center for Computational Sciences, University of Tsukuba

TDDFT: First-principles tool for electron dynamics simulation

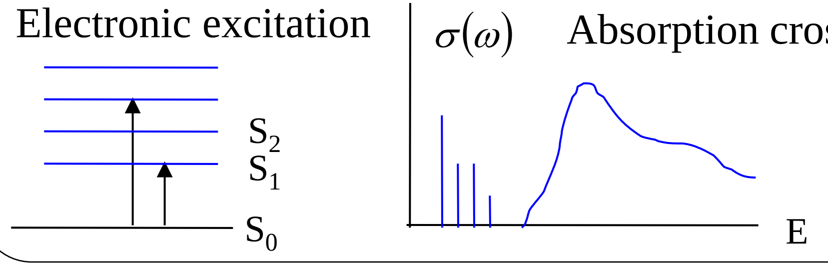
$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)=\{h_{KS}[\rho(\vec{r},t)]+V_{ext}(\vec{r},t)\}\psi_i(\vec{r},t)$$

$$\rho(\vec{r},t)=\sum_i|\psi_i(\vec{r},t)|^2$$

Linear response regime
(Perturbation theory)

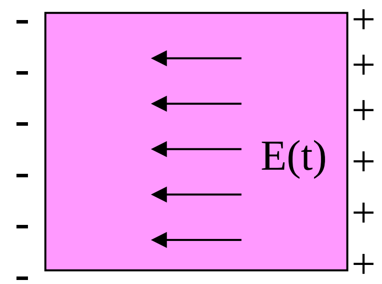
Electronic excitation

Absorption cross section

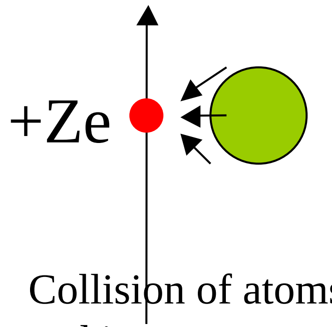


Laser-solid interaction

Dielectric function

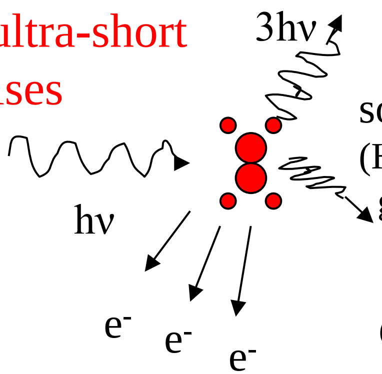


Coherent phonon
Electron-hole plasma
Optical breakdown



Collision of atoms and ions

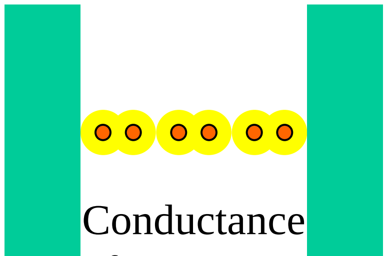
Intense, ultra-short Laser pulses



soft X ray (High harmonic generation)

Coulomb explosion

Multiple ionization



Conductance of nano-wire

Nonlinear, nonperturbative regime
(Initial value problem)

Theoretical description of light-matter interactions

A standard description

Electromagnetism:
Maxwell equation for macroscopic fields,
E, D, B, H

Constitution relation

$$D = D[E] = \varepsilon(\omega)E$$

Quantum Mechanics:
Perturbation theory to calculate linear susceptibilities,
$\varepsilon(\omega)$

In current frontiers of optical sciences,

Nanosized material requires nonlocal description in space

$$D(\vec{r},t) = \int^t dt' \varepsilon(\vec{r},\vec{r}',t-t')E(\vec{r}',t')$$

Ultra-short laser pulses require real-time description

$$D(\vec{r},t) = \int^t dt' \varepsilon(t-t')E(\vec{r},t')$$

Strong electric field induces nonlinear electron dynamics

$$D(\vec{r},t) = \int^t dt' \varepsilon(t-t')E(\vec{r},t') + 4\pi \int^t dt' \int^t dt'' \chi^{(2)}(t-t',t-t'')E(\vec{r},t')E(\vec{r},t'') + \cdots$$

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   - time-dependent band calculation, treatment of boundaries. -

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   - Dielectric function and optical breakdown, … -

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   - First-principles simulation for macroscopic electromagnetic field in intense regime,
   Dense electron-hole plasma induced by intense laser pulses -

Frontiers in Optical Sciences: Intense field

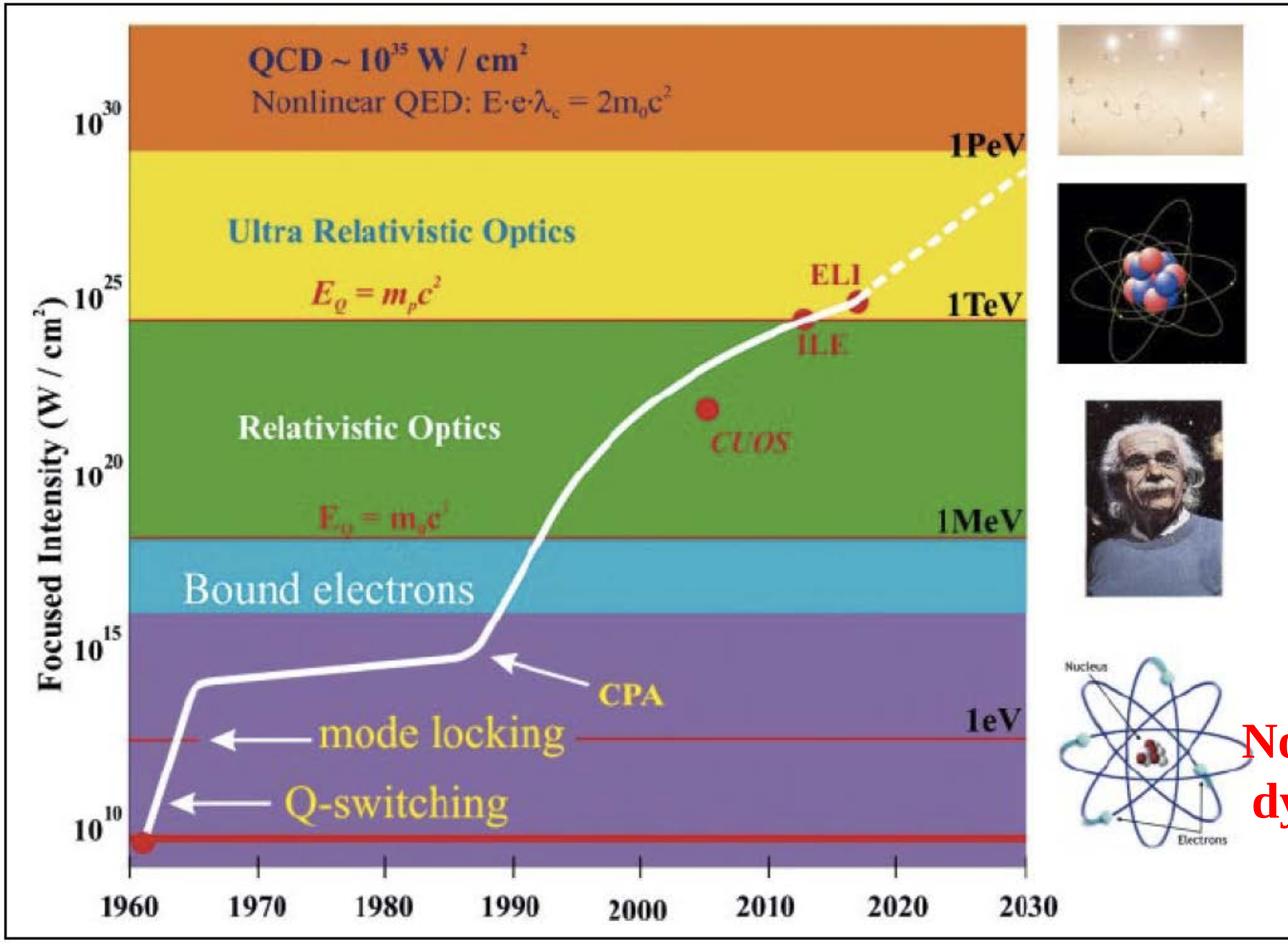


FIG. 1: **Maximum laser intensity as a function of time and fields of research accessible with these intensities.**

QED Vacuum breakdown

Nuclear reaction, Particle Acceleration

Relativistic Classical

Nonlinear electron dynamics

Nonrelativistic Quantum

G. Mourou Optik & Photonik December 2010 No. 4

Phenomena in intense laser pulses irradiated on bulk materials

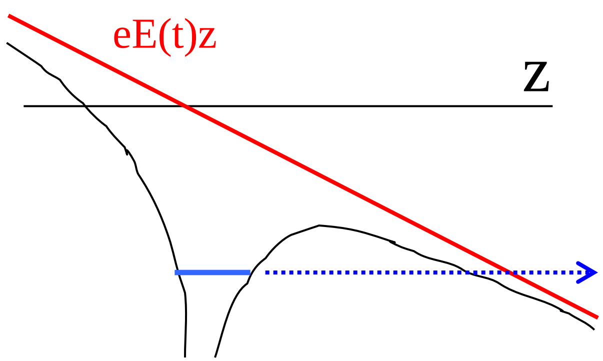
Laser intensity

$10^{13} - 10^{15}\,\mathrm{W/cm^2}$

Nonlinear optics	Coherent phonon	HHG	Electron-hole plasma Optical breakdown Laser machining	Laser acceleration	Vacuum breakdown

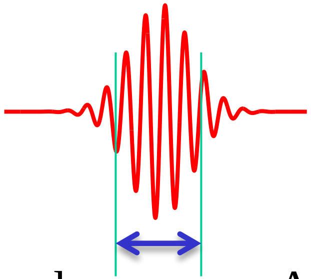
Nonrelativistic
Quamtum mechanics

Relativistic
Classical mechanics



External electric field by laser pulse
≈ Internal electric field by nuclei

Frontiers in Optical Sciences: Ultrafast dynamics



Picosecond 10^{-12}s

Femtosecond 10^{-15}s

Attosecond 10^{-18}s

10^{-23}s Time

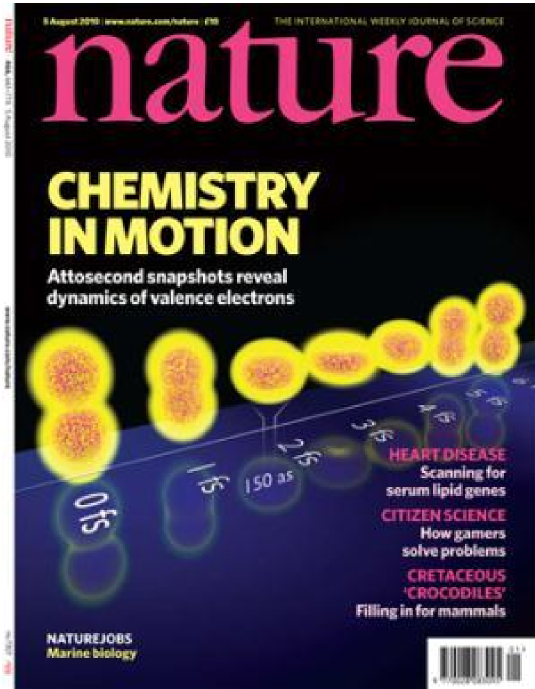
Period of Optical phonon (Si, 64 fs)

Period of electron orbital in Hydrogen, 150as

Period of Ti-sapphire laser pulse

Shortest laser pulse 80 as (2008)

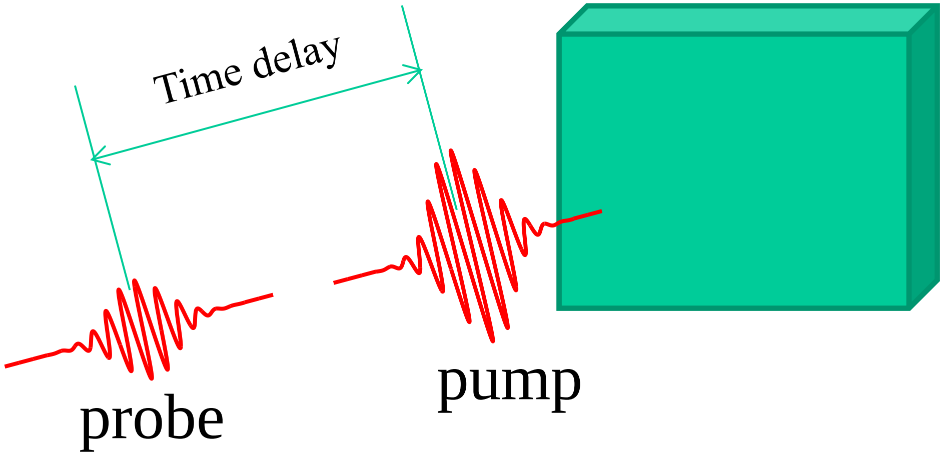
Nucleon motion in nucleus

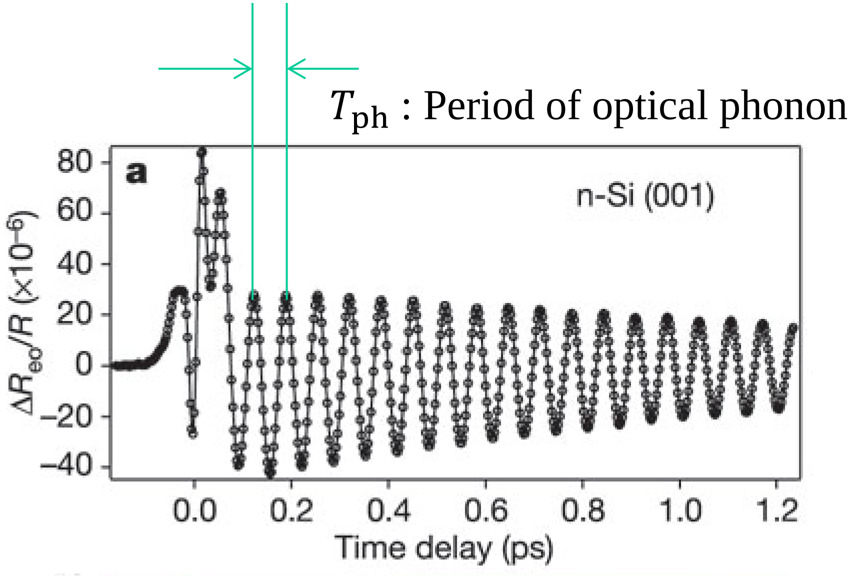


Real-time observation of valence electron motion
E. Goulielmakis et.al, Nature 466, 739 (2010).

Pump-Probe Measurement: Coherent Phonon

Intense 1st pulse excites electrons and atoms.
Weak 2nd pulse measure change of reflectivity.





M. Hase, et al. Nature (London) 426, 51 (2003)

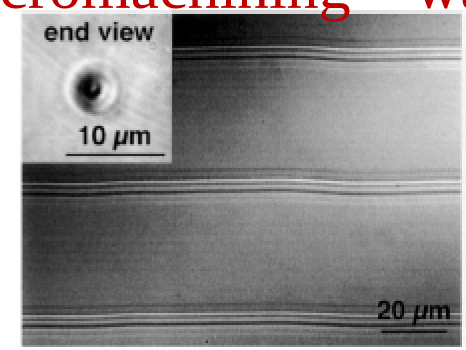
$$\frac{\Delta R(t)}{R} \propto e^{-\Gamma t} \sin(\Omega_{\rm ph} t + \phi)$$

Femto-technology: nonthermal machining by femtosecond laser pulses

Figure B1 Femtosecond laser micromaching process. **a**, Schematic of the laser incident on a transparent material. **b**, Diagram of the excitation of electrons to the conduction band. **c**, Microscope images showing the large variation in the feature characteristics depending on the experimental conditions. Left: single 10-nJ pulse and right: 25,000 5-nJ pulses at a frequency of 25 MHz (both with the same focal spot).

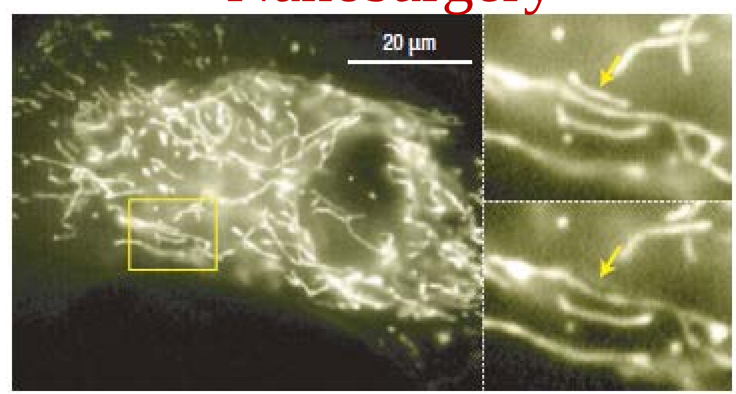
R.R. Gattass, E. Mazur, Nature Photonics 2, 220 (2008).

Micromachining – waveguide-



Optical microscope image of waveguides written inside bulk glass by a 25-MHz train of 5-nJ sub-100-fs pulses, C.B. Schaffer et.al, OPTICS LETTERS 26, 93 (2001)

Nanosurgery



Ablation of a single mitochondrion in a living cell.
N. Shen et.al, Mech. Chem. Biosystems, 2, 17 (2005).

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Calculation in real-time and real-space

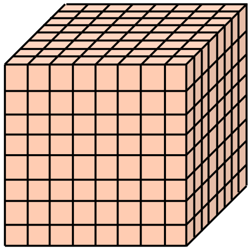
Time-dependent Kohn-Sham equation

$$i\hbar\frac{\partial}{\partial t}\psi_i(\vec{r},t)=h_{KS}[n(\vec{r},t)]\psi_i(\vec{r},t) \qquad n(\vec{r},t)=\sum_i|\psi_i(\vec{r},t)|^2$$

$$h_{KS}[n(\vec{r},t)]=-\frac{\hbar^2}{2m}\nabla^2+V_{ion}(\vec{r})+\int d\vec{r}'\frac{e^2}{|\vec{r}-\vec{r}'|}+\mu_{xc}[n(\vec{r},t)]+V_{ext}(\vec{r},t)$$

Norm-conserving pseudopotential

3D real-space grid representation, high order finite difference



$$-\frac{\hbar^2}{2m}\left[\sum_{n_1=-N}^{N}C_{n_1}\psi(x_i+n_1h,y_j,z_k)+\sum_{n_2=-N}^{N}C_{n_2}\psi(x_i,y_j+n_2h,z_k)+\sum_{n_3=-N}^{N}C_{n_3}\psi(x_i,y_j,z_k+n_3h)\right]$$

$$+[V_{\text{ion}}(x_i,y_j,z_k)+V_H(x_i,y_j,z_k)+V_{\text{xc}}(x_i,y_j,z_k)]\psi(x_i,y_j,z_k)=E\psi(x_i,y_j,z_k)\ .$$

Time evolution: 4-th order Taylor expansion

$$\psi_i(t+\Delta t)=\exp\left[\frac{h_{KS}(t)\Delta t}{i\hbar}\right]\psi_i(t)\approx\sum_{k=0}^{N}\frac{1}{k!}\left(\frac{h_{KS}(t)\Delta t}{i\hbar}\right)\psi_i(t), \qquad N=4$$

Treatment of optical electric field

We assume a long wavelength limit, lattice const. << light wavelength

↓

Electron dynamics in a unit cell under time-dependent, spatially uniform field

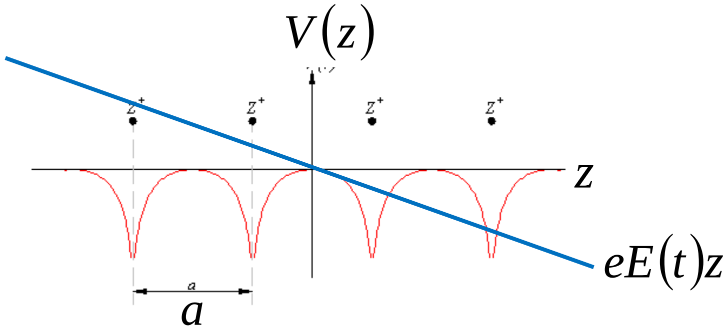
Two key issues

Use (spatially uniform) vector potential instead of (spatially linear) scalar potential to express macroscopic electric field.

Boundary effect (macroscopic shape effect) needs to be considered from outside of the theory.

We can manage them by the appropriate choice of gauge.

Electron dynamics in crystalline solid under spatially uniform field



Scalar potential $eE(t)z$ spoils spatial periodicity of the Hamiltonian

$$h(\vec{r}+\vec{a}) \neq h(\vec{r})$$

Employing a vector potential replacing the scalar potential, one may recover the periodicity of the Hamiltonian

Time-dependent, spatially uniform electric field

$$\vec{E} = -\vec{\nabla}\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$$

$$\phi = E(t)z \quad \Leftrightarrow \quad \vec{A}(t) = c\int^{t} dt' E(t')\hat{z}$$

$$i\hbar\frac{\partial}{\partial t}\psi(t) = \left[\frac{1}{2m}\left(\vec{p}-\frac{e}{c}\vec{A}(t)\right)^2 + V(\vec{r},t)\right]\psi(t)$$

$$h(\vec{r}+\vec{a},t) = h(\vec{r},t) \qquad \psi_{nk}(\vec{r}+\vec{a},t) = e^{i\vec{k}\vec{a}}\psi_{nk}(\vec{r},t)$$

Time-dependent Bloch function

Equation for time-dependent Bloch function

$$i\hbar \frac{\partial}{\partial t} u_{n\vec{k}}(\vec{r},t) = \left[\frac{1}{2m} \left(\vec{p} + i\vec{k} - \frac{e}{c}\vec{A}(t) \right)^2 + V(\vec{r},t) \right] u_{n\vec{k}}(\vec{r},t)$$

$$n(\vec{r},t) = \sum_{nk} \left| u_{n\vec{k}}(\vec{r},t) \right|^2$$

$$\psi_{nk}(\vec{r},t) = e^{i\vec{k}\vec{r}} u_{nk}(\vec{r},t)$$

$$u_{nk}(\vec{r}+\vec{a},t) = u_{nk}(\vec{r},t)$$

Treatment of Polarization (Macroscopic Shape of Sample)

- We solve electron dynamics in a unit cell inside a crystalline solid.

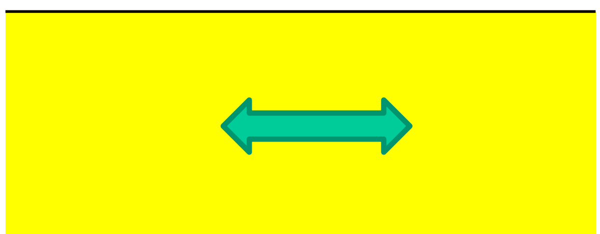
- The electric field in the unit cell depends on macroscopic geometry of the sample.

- We need to specify the ‘macroscopic geometry’ in the calculation.

$$i\hbar \frac{\partial}{\partial t} \psi_{nk}(t) = \left[\frac{1}{2m} \left(\vec{p} - \frac{e}{c} \vec{A}(t) \right)^2 + V(\vec{r}, t) \right] \psi_{nk}(t)$$

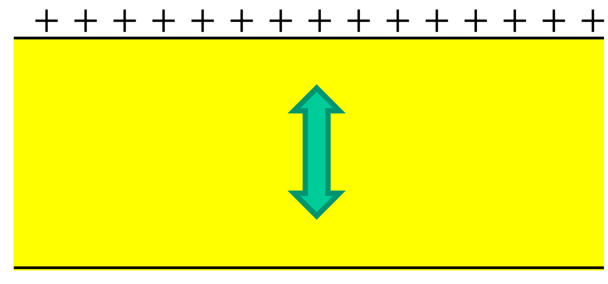
$$\vec{E} = -\frac{1}{c} \frac{\partial \vec{A}}{\partial t} \qquad \vec{A}(t) = c \int^{t} dt' E(t') \hat{z}$$

Optical response of thin film



Transverse

$$A(t) = A_{ext}(t)$$



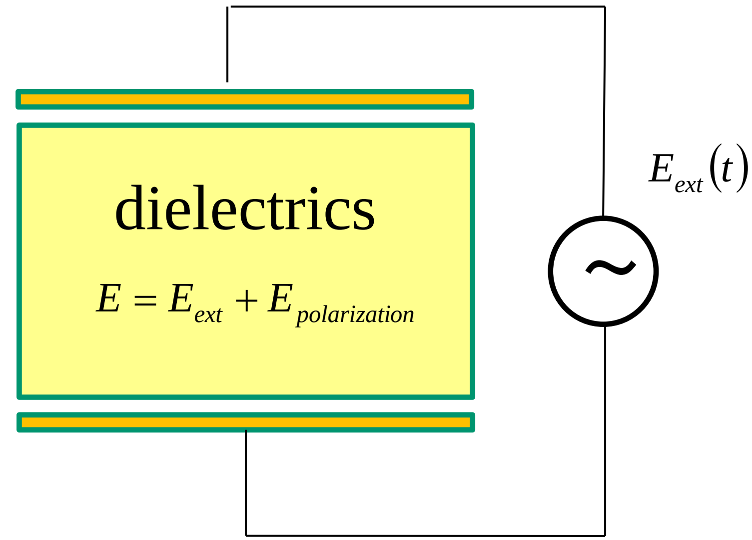
Longitudinal

$$A(t) = A_{ext}(t) + A_{polarization}(t)$$

Case of longitudinal geometry: Treatment of induced polarization

Bertsch, Iwata, Rubio, Yabana, Phys. Rev. B62(2000)7998.

"parallel-plate-capacitor with dielectrics".



$$A(t) = A_{extr}(t) + A_{polarization}(t)$$

$$E(t) = -\frac{1}{c}\frac{\partial A(t)}{\partial t}$$

$$A(t) = -c\int^{t} E(t')dt'$$

Equation for polarization

$$\frac{d^2 \vec{A}_{polarization}(t)}{dt^2} = \frac{4\pi}{\Omega}\int_{\Omega(cell)} d\vec{r}\; \vec{j}(\vec{r},t)$$

$\vec{A}(t)$ ↓ ↑ $\vec{j}(\vec{r},t)$

Time-dependent Kohn-Sham equation

$$i\hbar\frac{\partial}{\partial t}\psi_i = \frac{1}{2m}\left(-i\hbar\vec{\nabla} + \frac{e}{c}\vec{A}\right)^2\psi_i - e\phi\psi_i + \frac{\delta E_{xc}}{\delta n}\psi_i$$

$$n = \sum_i |\psi_i|^2 \qquad \vec{j} = \frac{1}{2m}\sum_i\left(\psi_i^*\left(\vec{p} + \frac{e}{c}\vec{A}\right)\psi_i - c.c.\right)$$

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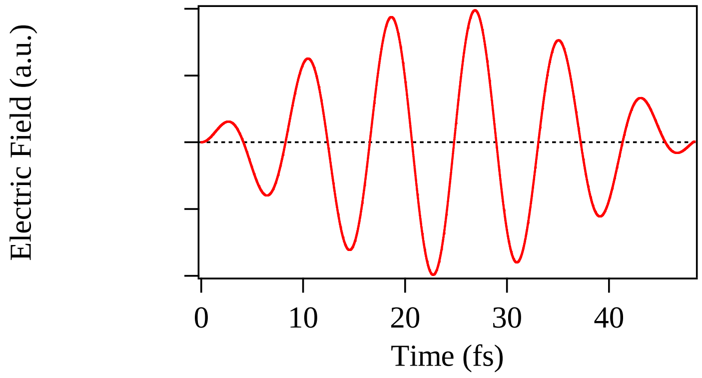
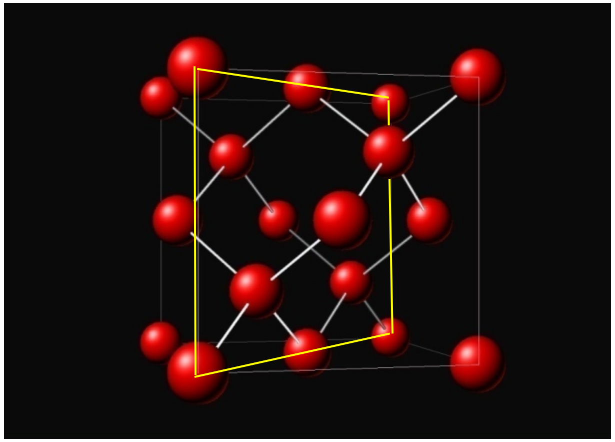
Electron dynamics in bulk silicon under pulse light

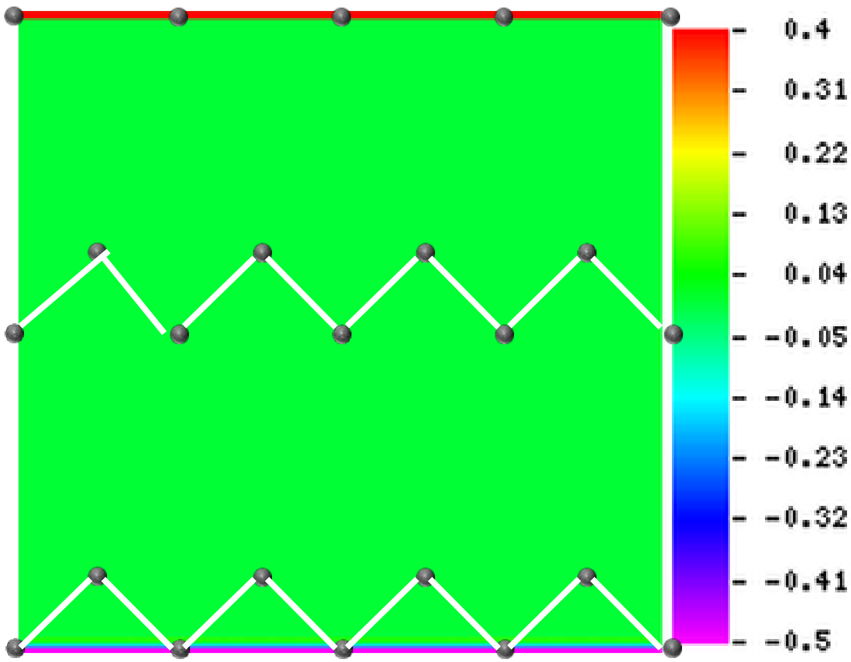
I= 3.5×10^{14} W/cm^2, T=50 fs, $\hbar\omega$=0.5 eV

Laser photon energy is much lower than direct bandgap.

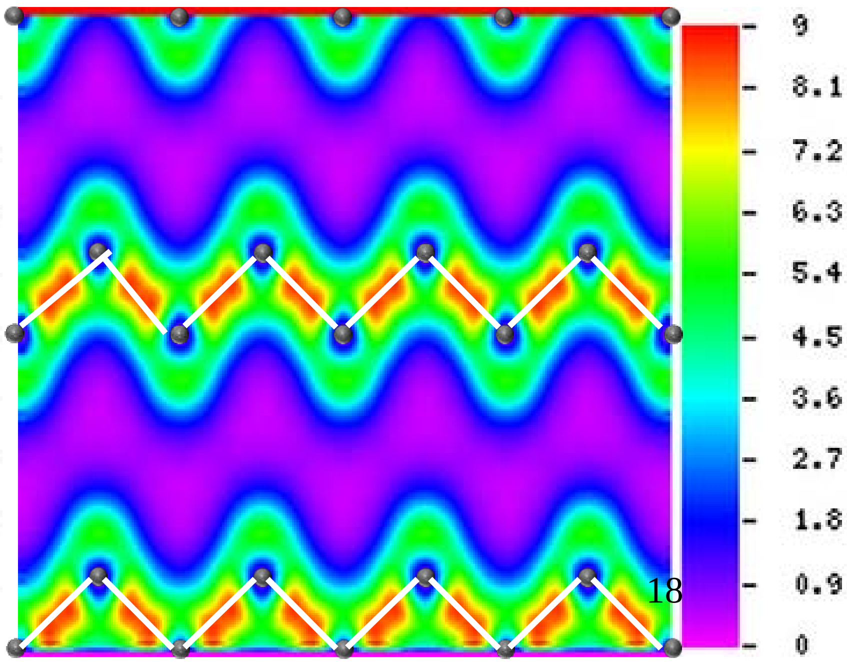




Density change from the ground state (110)



Ground state density (110)



Red +
Green 0
Blue -

Linear response:

Two methods to calculate dielectric function from real-time electron dynamics

Transverse geometry

$$J(t) = \int^{t} dt' \sigma(t-t')\left(-\frac{1}{c}\frac{dA}{dt}\right)$$

$$\sigma(\omega) = \int dt e^{i\omega t}\sigma(t)$$

$$\varepsilon(\omega) = 1 + \frac{4\pi i \sigma(\omega)}{\omega}$$

Longitudinal geometry

$$A_{tot}(t) = A_{ext}(t) + A_{pol}(t)$$

$$\frac{d^2 A_{pol}(t)}{dt^2} = 4\pi J(t)$$

$$A_{tot}(t) = \int^{t} dt' \varepsilon^{-1}(t-t') A_{ext}(t')$$

$$\frac{1}{\varepsilon(\omega)} = \frac{\int dt\, e^{i\omega t} A_{tot}(t)}{\int dt\, e^{i\omega t} A_{ext}(t)}$$

For an impulsive external field,

$$E(t) = k\delta(t), \quad A(t) = -kc\theta(t)$$

$$J(t) = k\sigma(t)$$

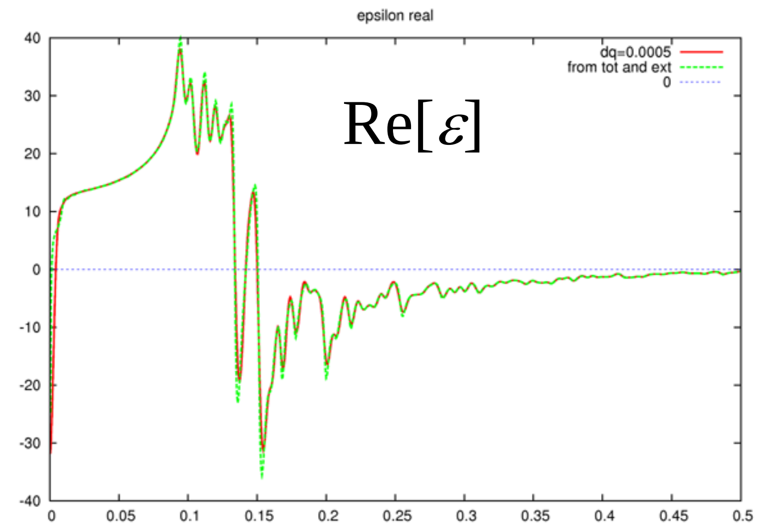
$$E_{tot}(t) = -\frac{1}{c}\frac{dA_{tot}}{dt} = k\varepsilon^{-1}(t)$$

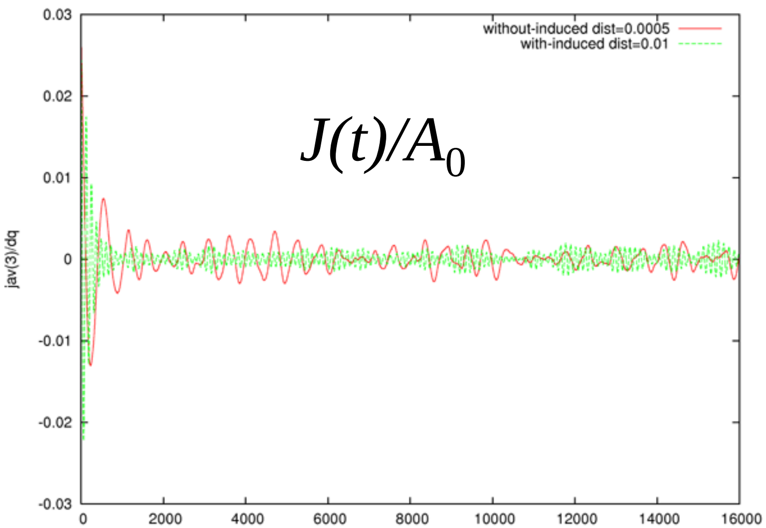
Comparison of numerical results for dielectric function of Si by two methods

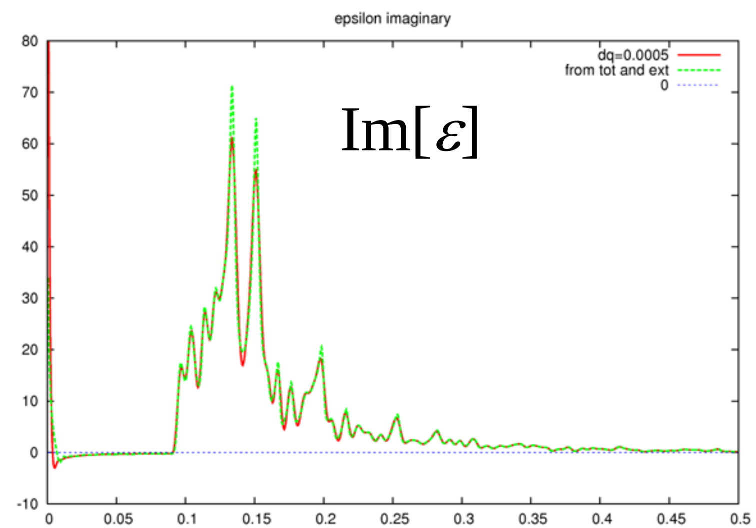
- Green : longitudinal
- Red : transverse

Spatial grid: 16^3
k-points : 8^3

Distortion strength:
A_0 = 0.01 (longitudinal)
0.0005 (transverse)

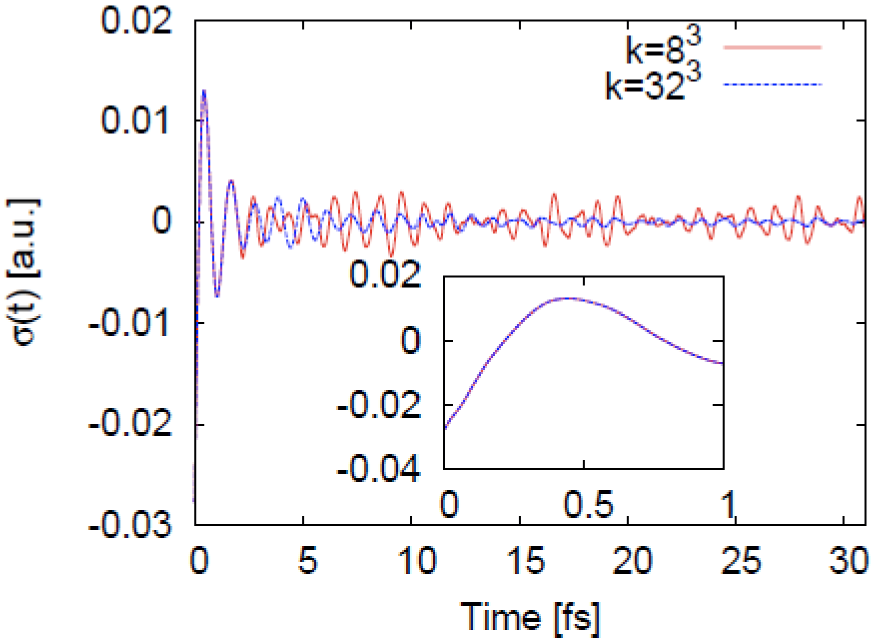


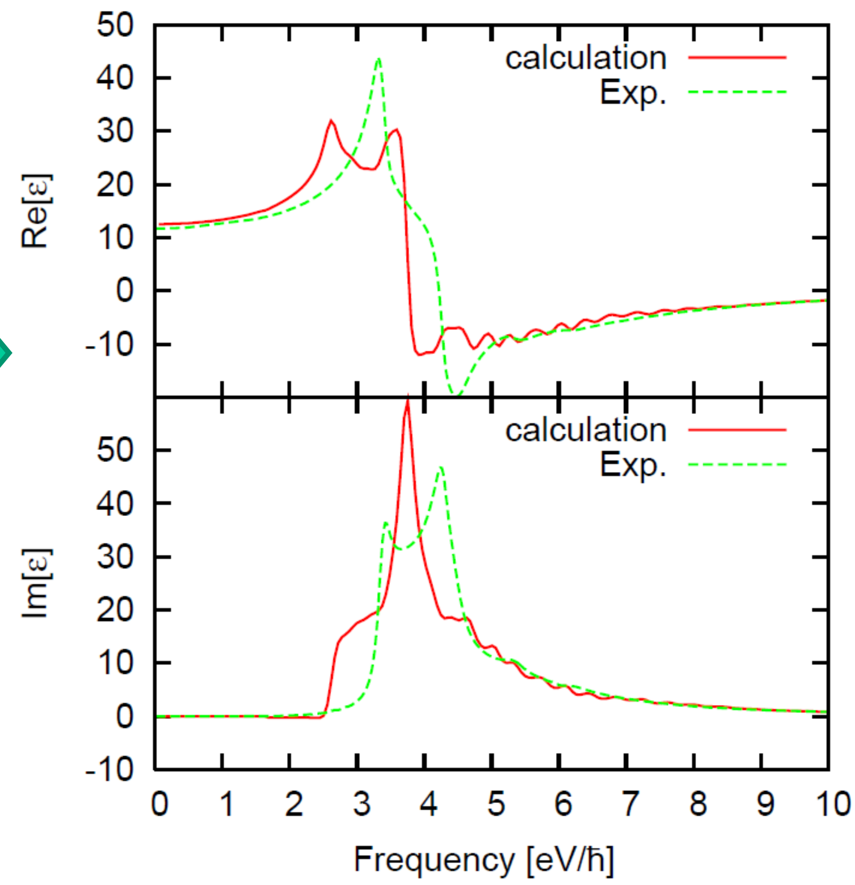




Dielectric function of Si in TDDFT (ALDA)
Transverse calculation

Instantaneous pulse field is applied at t=0,
the induced current as a function of time.





Dielectric function by TDDFT (ALDA) is not accurate enough.

GW approx. + Bethe-Salpeter

Most successful but
Beyond Kohn-Sham
framework

Dots: experiment
Dash-dotted: RPA
Solid: Bethe-Salpeter

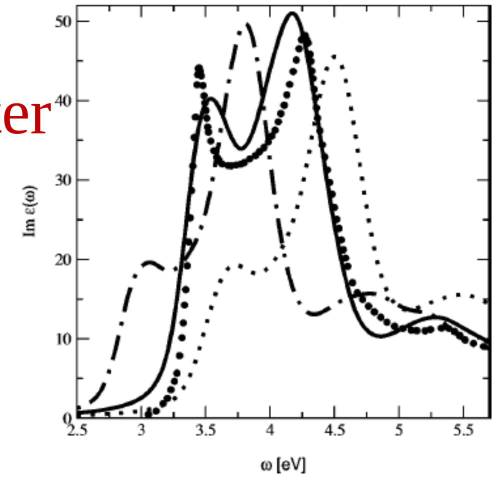
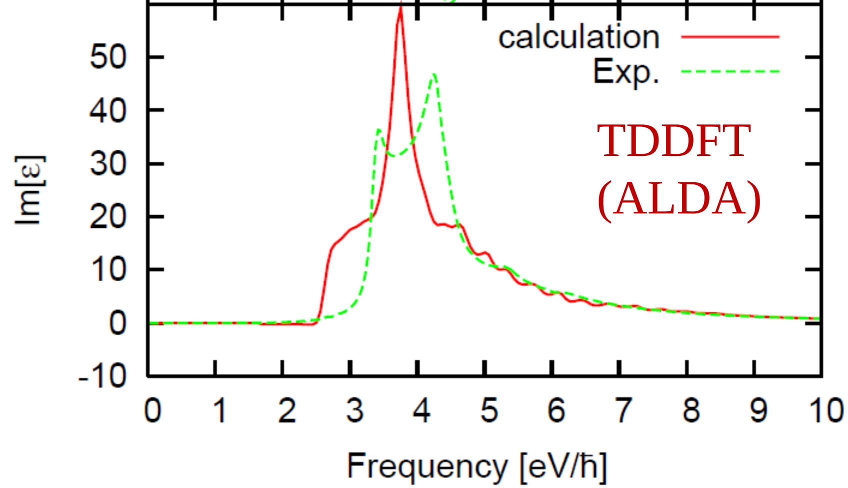
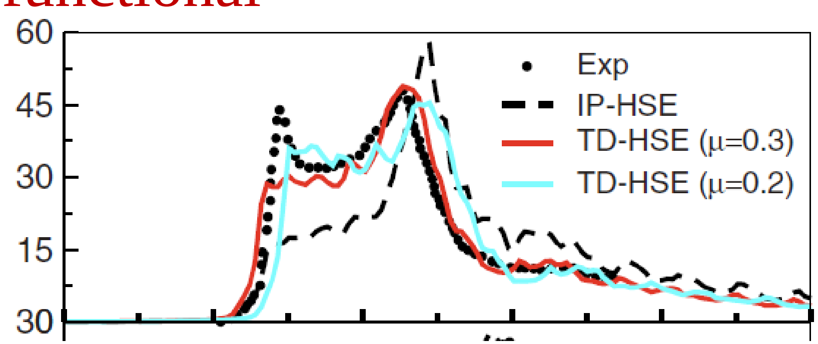


FIG. 5. Silicon absorption spectrum [Im(ε_M)]: ●, experiment (Lautenschlager *et al.*, 1987); dash-dotted curve, RPA, including local field effects; dotted curve, *GW*-RPA; solid curve, Bethe-Salpeter equation.

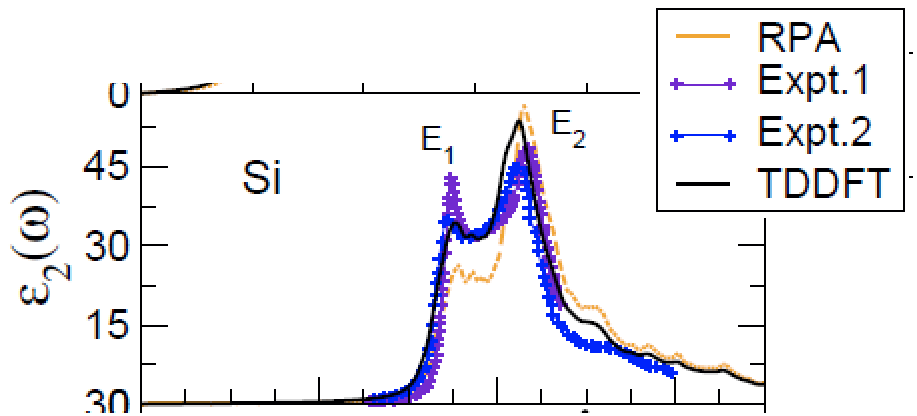
G. Onida, L. Reining, A. Rubio,
Rev. Mod. Phys. 74(2002)601.



TDDFT with hybrid (nonlocal) functional



Good results for small gap materials,
Less satisfactory for large gap materials.
J. Paier, M. Marsman, G. Kresse,
Phys. Rev. B78,121201 (2008)



PRL107, 186401 (2011)
S. Sharma, J.K. Dewhurst, A. Sanna, E.K.U. Gross,
Bootstrap approx. for the exchange-correlation kernel
of time-dependent density functional theory

Limited to linear response regime.

Intense laser pulse on solid

Laser intensity

$10^{13} - 10^{15}\,\mathrm{W/cm^2}$

Nonlinear optics

Coherent phonon

HHG

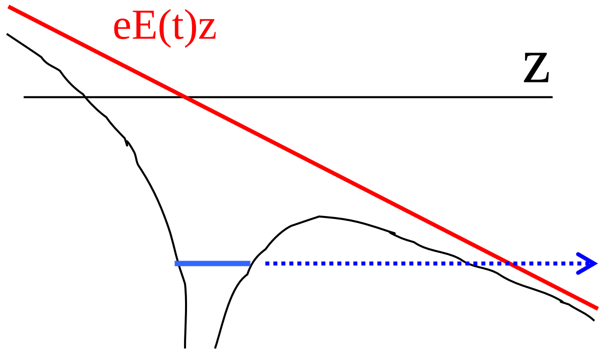
Electron-hole plasma
Optical breakdown
Laser machining

Laser acceleration

Vacuum breakdown

Nonrelativistic
Quamtum mechanics

Relativistic
Classical mechanics



External electric field by laser pulse

≈ Internal electric field by nuclei

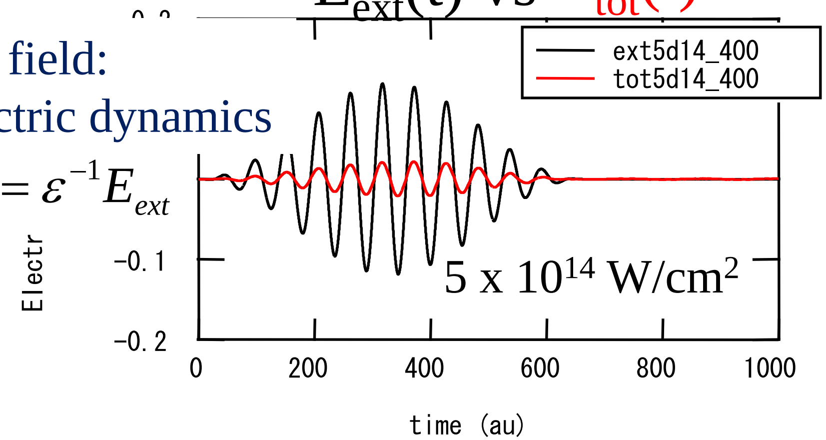
As the laser intensity increases,

Calculation for diamond
laser frequency: 3.1eV,
below bandgap (4.8 eV)

$E_{ext}(t)$ vs $E_{tot}(t)$

Weak field:
Dielectric dynamics

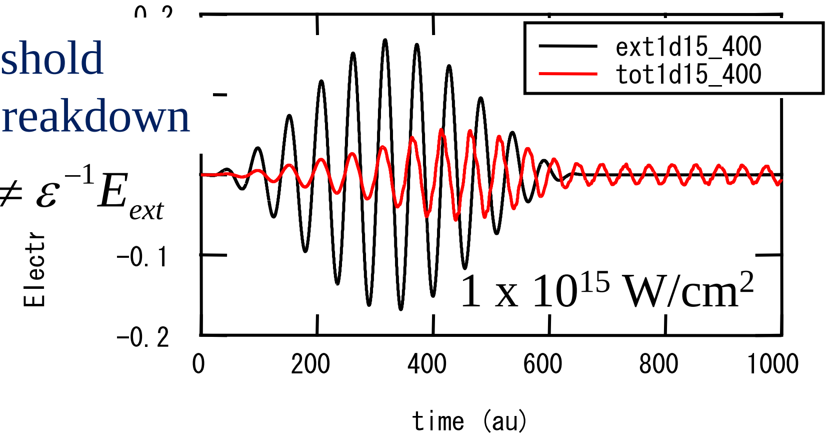
$$E_{tot} = \varepsilon^{-1} E_{ext}$$



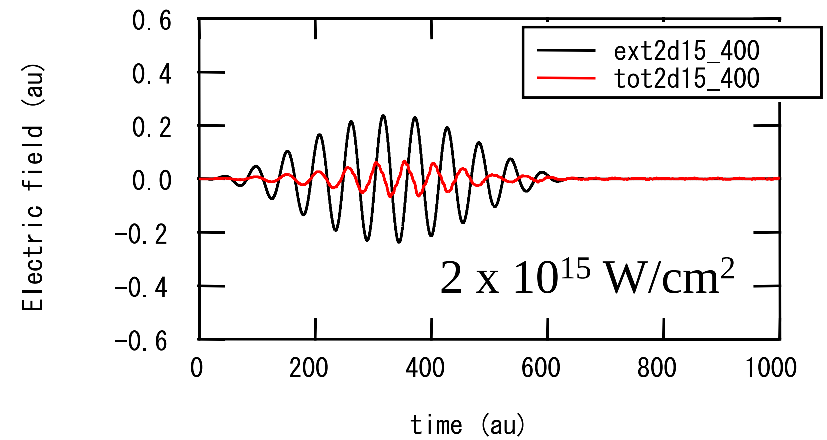
At a certain intensity, resonant energy transfer is observed.

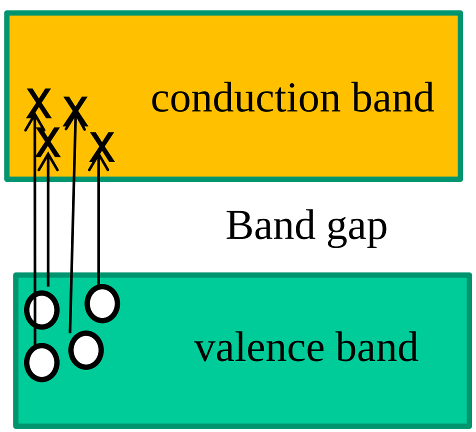
Threshold
for breakdown

$$E_{tot} \neq \varepsilon^{-1} E_{ext}$$



T. Otobe, M. Yamagiwa, J.-I. Iwata, K.Y. T. Nakatsukasa, G.F. Bertsch, Phys. Rev. B77, 165104 (2008)





Resonant energy transfer
(1×10^{15} W/cm^2, 3.1eV, 40fs)

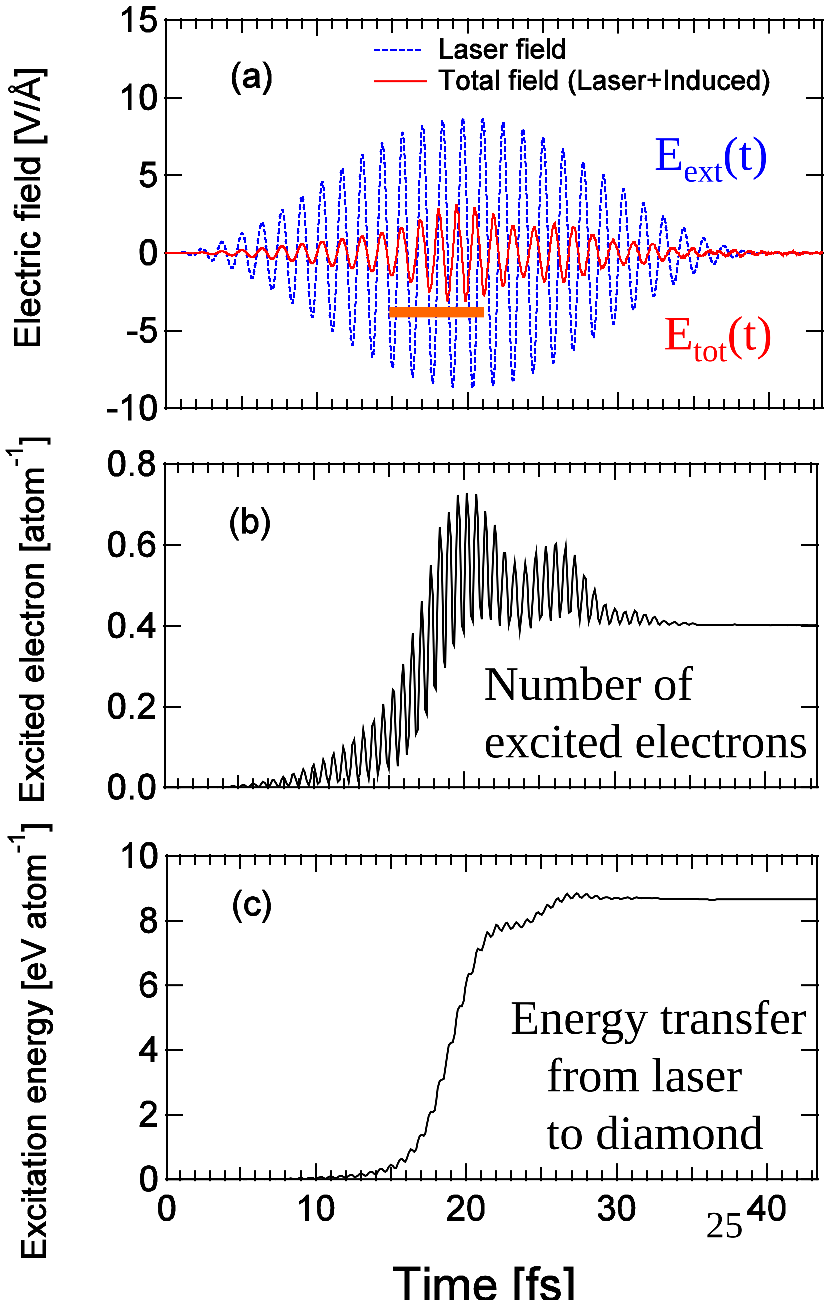
Incident laser frequency
= plasma frequency of excited electrons

Plasma frequency for 0.4/atom

$$\omega_p = \left(\frac{4\pi n_{ex}}{m\varepsilon(0)} \right) \approx 4\text{eV}$$

exceeds the frequency of laser pulse, 3.1eV

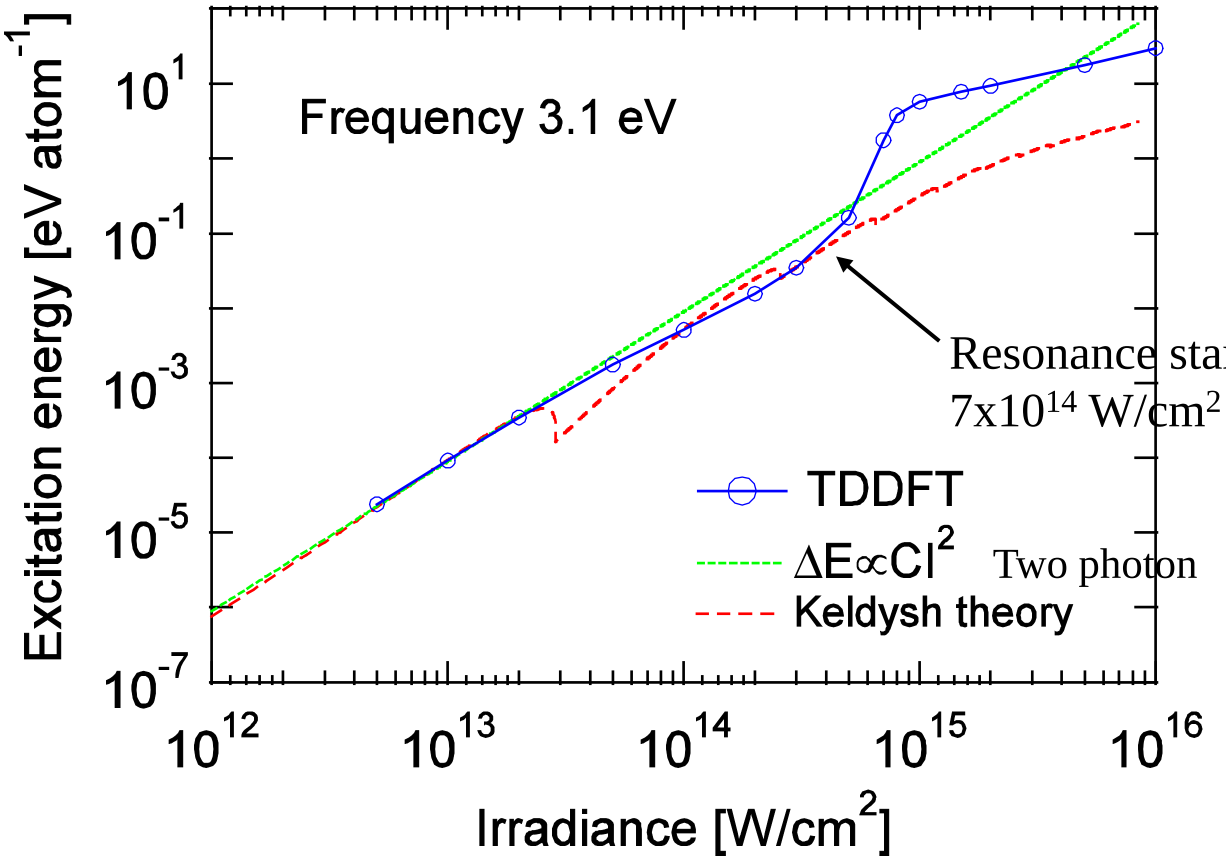
diamond



Resonant intensity is higher than measured optical breakdown threshold

Calculated threshold: 6J/cm^2
Measured threshold: 0.63±0.15 J/cm^2

D.H. Reitze et.al, Phys. Rev. B45, 2677(1992)



Resonance starts
7x10^{14} W/cm^2 (16fs)

Two photon

When nonlinear effects are important,
neither longitudinal or transverse calculation is sufficient.

Up to now , we considered electron dynamics under a given field

Next step is to consider dynamics of
both electrons and electromagnetic fields simultaneously.

CONTENTS

1. A frontier in light - matter interaction : intense and ultrafast
   - Theories and computations required in current optical sciences -

2. Real-time and real-space calculation for electron dynamics in solid
   - time-dependent band calculation, treatment of boundaries. -

3. Electron dynamics in solid for a given electric field
   - Dielectric function and optical breakdown, … -

4. Coupled Maxwell + TDDFT multiscale simulation
   - First-principles simulation for macroscopic electromagnetic field in intense regime,
     Dense electron-hole plasma induced by intense laser pulses -

Usually, light-matter interaction is described by

Electromagnetism:

Maxwell equation for macroscopic fields,
E, *D*, *B*, *H*

Constitution relation

$$D = D[E] = \varepsilon(\omega)E$$

Quantum Mechanics:

Perturbation theory to calculate linear susceptibilities,
$\varepsilon(\omega)$

As the light intensity increases, nonlinear effects appear

Quantum mechanics is useful to calculate nonlinear susceptibilities as well.

$$D = D[E] = \varepsilon(\omega)E + 4\pi\chi^{(2)}E^2 + 4\pi\chi^{(3)}E^3 + \cdots$$

Extreme intensity of laser pulse

⇩

We need to solve couple Maxwell + Schroedinger dynamics.

We need to solve couple Maxwell + Schroedinger dynamics.

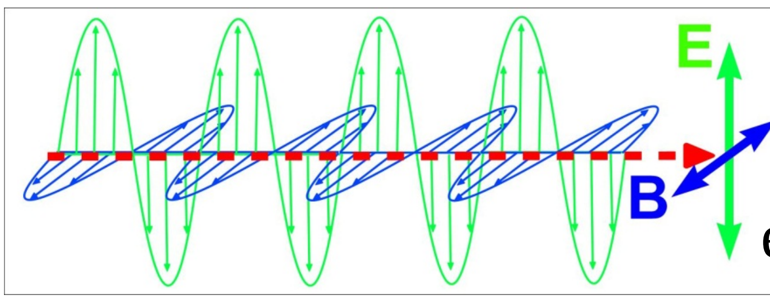
Two spatial scales

Maxwell equation
describing electromagnetic field

$$E(\vec{r},t),\quad B(\vec{r},t)$$

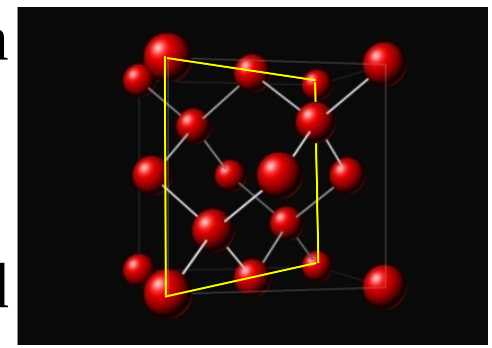
Time-dependent density-functional theory
describing electron dynamics

$$\psi_i(\vec{r},t)$$



polarization

external field



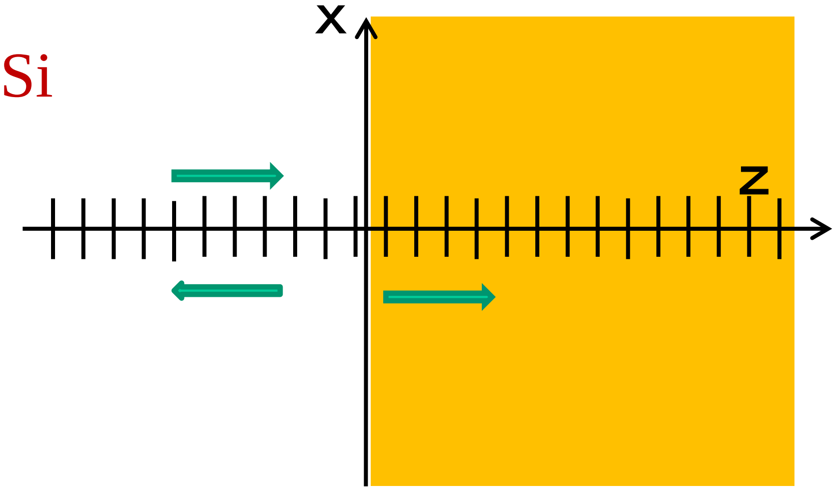
[μm]

Different spatial scales

[nm]

We introduce two spatial grids and achieve “multiscale simulation”

We consider a problem:
Laser pulse irradiation normal on bulk Si



Macroscopic grid

Maxwell eq.

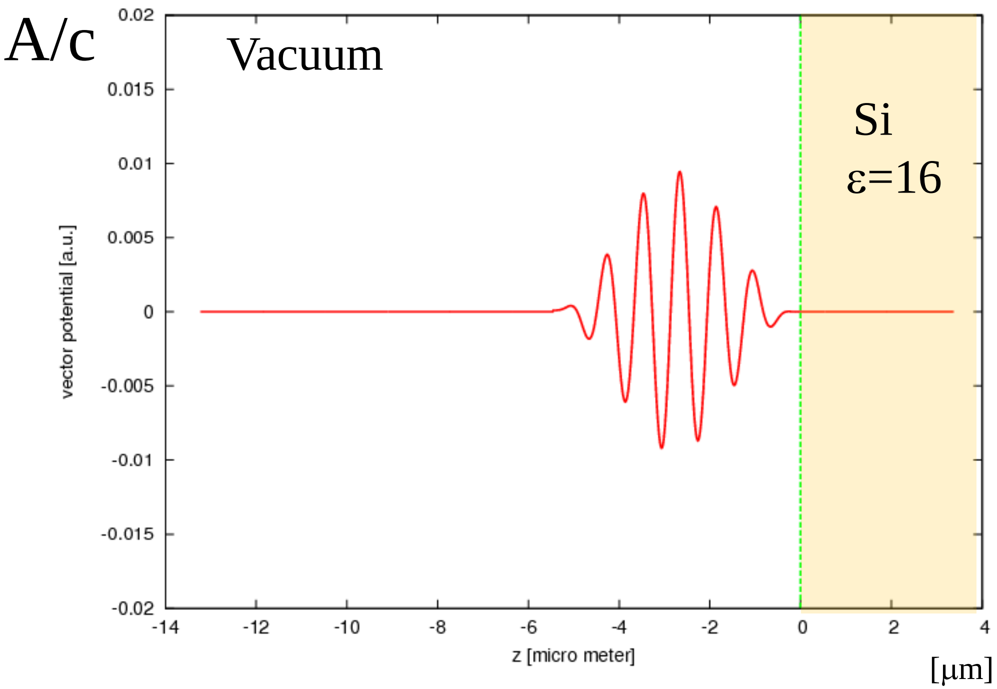
$$\frac{\varepsilon(z)}{c^2}\frac{\partial^2}{\partial t^2}A(z,t)-\frac{\partial^2}{\partial z^2}A(z,t)=0$$

Propagation z-direction, polarization x-direction

$$\vec{A}(\vec{r},t)=A(z,t)\hat{x}$$

Laser frequency below direct bandgap

$$\lambda=800\text{nm},\quad \hbar\omega=1.55\text{eV}$$



Index of refraction

$$n=\sqrt{\varepsilon}$$

Reflectance

$$R=\left(\frac{1-n}{1+n}\right)^2$$

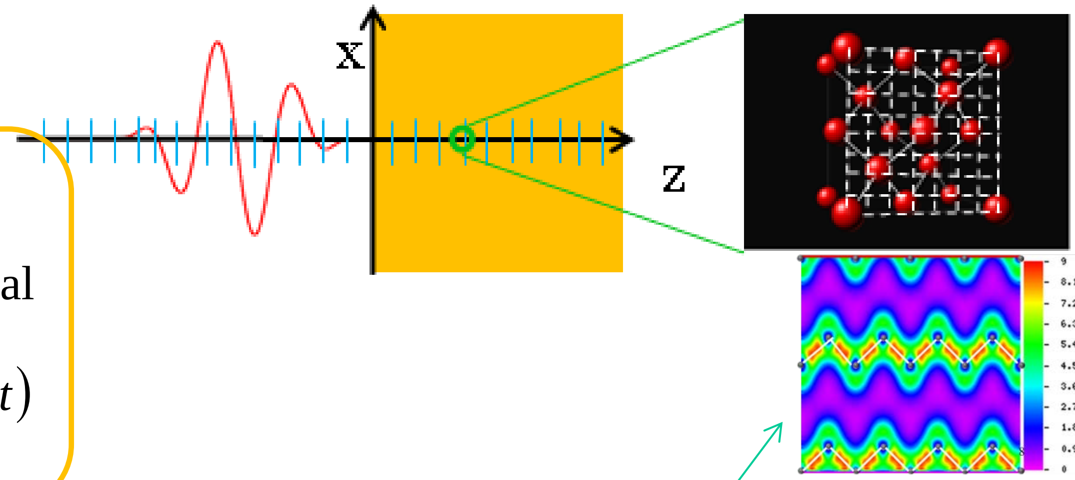
Velocity of wave

$$v=\frac{c}{n}$$

Multiscale simulation: Formalism

At each macroscopic grid point,
We consider a unit cell and prepare microscopic grid.

K. Yabana, T. Sugiyama, Y. Shinohara, T. Otobe, G.F. Bertsch, Phys. Rev. B85, 045134 (2012).



Macroscopic grid points (μm) to describe macroscopic vector potential

$$\frac{1}{c^2}\frac{\partial^2}{\partial t^2}A(Z,t)-\frac{\partial^2}{\partial Z^2}A(Z,t)=\frac{4\pi}{c}J(Z,t)$$

$J(Z,t)$

Exchange of information by macroscopic current and macroscopic vector potential.

$A(Z,t)$

$$J(Z,t)=\int_\Omega d\vec{r}\,\vec{j}_{e,Z}$$

$$\vec{j}_{e,Z}=\frac{\hbar}{2mi}\sum_i\left(\psi_{i,Z}^*\vec{\nabla}\psi_{i,Z}-\psi_{i,Z}\vec{\nabla}\psi_{i,Z}^*\right)-\frac{e}{4\pi c}n_{e,Z}\vec{A}$$

At each macroscopic points, Kohn-Sham orbitals $\psi_{i,Z}$ are prepared, and described in microscopic grids.

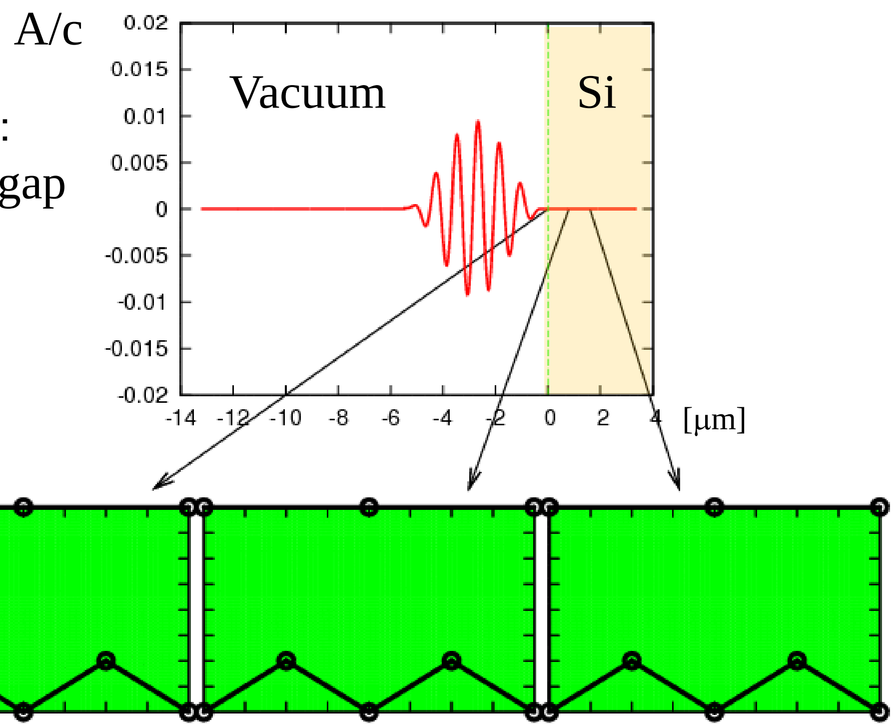
$$i\hbar\frac{\partial}{\partial t}\psi_{i,Z}=\frac{1}{2m}\left(-i\hbar\vec{\nabla}+\frac{e}{c}\vec{A}\right)^2\psi_{i,Z}-e\phi_Z\psi_{i,Z}+\frac{\delta E_{xc}}{\delta n}\psi_{i,Z}$$

$$\vec{\nabla}^2\phi_Z=-4\pi\left\{en_{ion}-en_{e,Z}\right\}$$

Propagation of weak pulse
(Linear response regime, separate dynamics of electrons and E-M wave)

$I = 10^{10} W/cm^2$

Laser frequency : 1.55eV :
lower than direct bandgap
2.4eV(LDA）



Z=0 [μm]　Z=0.8 [μm]　Z=1.6 [μm]

Propagation of weak pulse

(Linear response regime, separate dynamics of electrons and E-M wave)

$I=10^{10}W/cm^2$

Laser frequency : 1.55eV :
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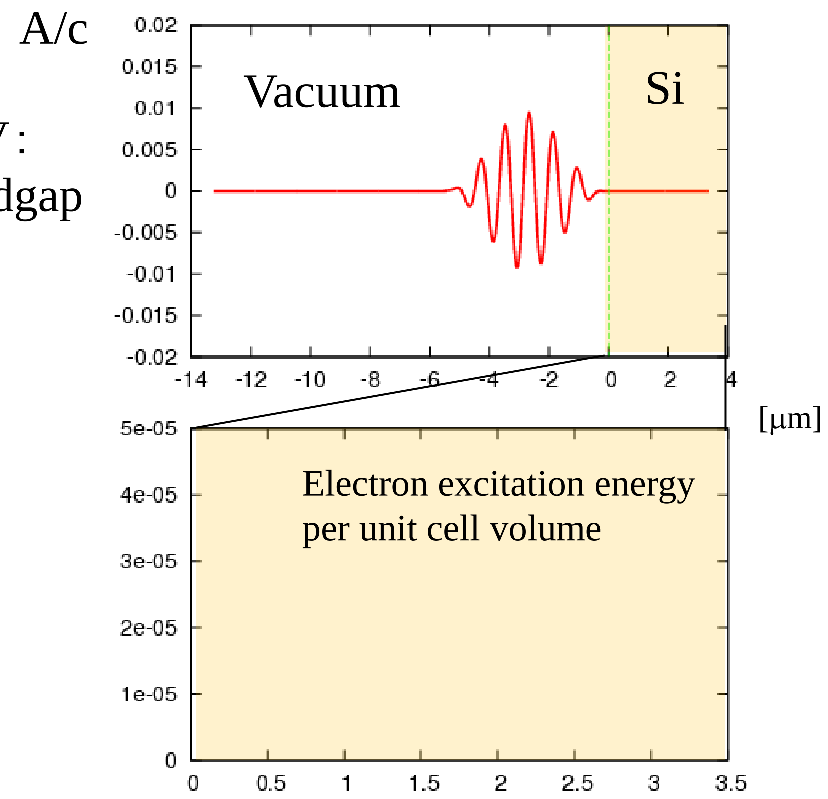
2.4eV(LDA)

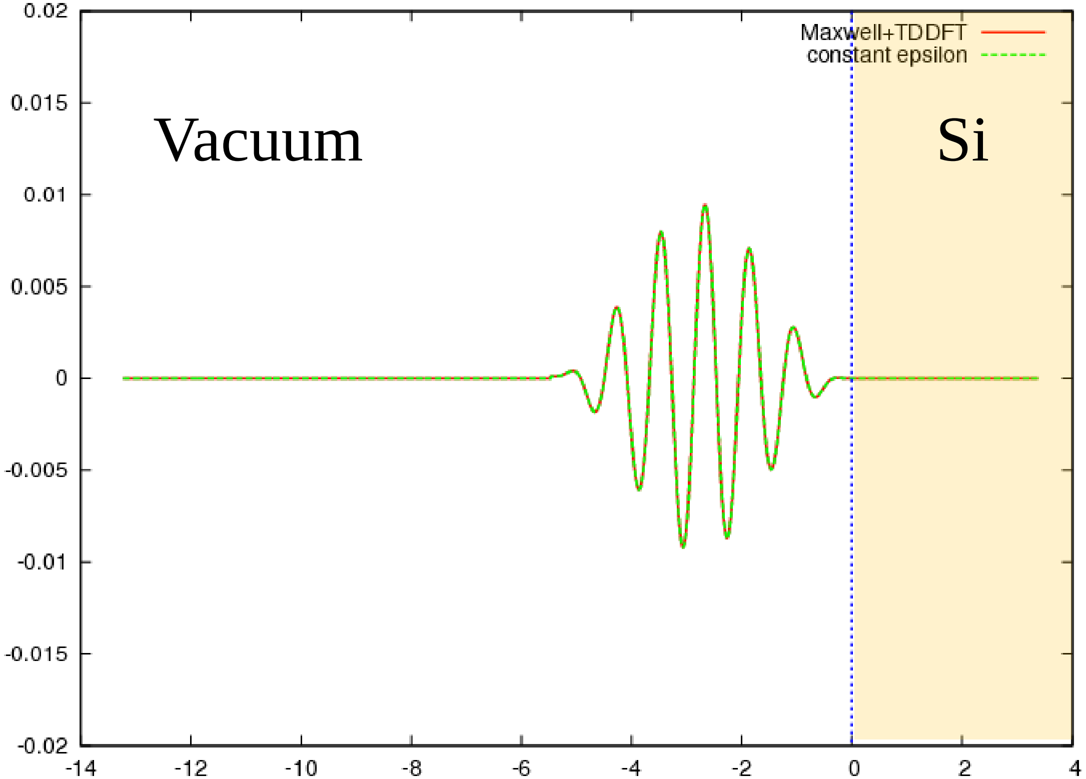


Maxwell+TDDFT vs Maxwell only (constant ε)

Red = Maxwell + TDDFT

Green = Maxwell $\frac{\varepsilon}{c^2}\frac{\partial^2}{\partial t^2}A(z,t)-\frac{\partial^2}{\partial z^2}A(z,t)=0 \qquad \varepsilon=16$

A/c



[μm]

In linear regime,
dispersion of dielectric function
Induces

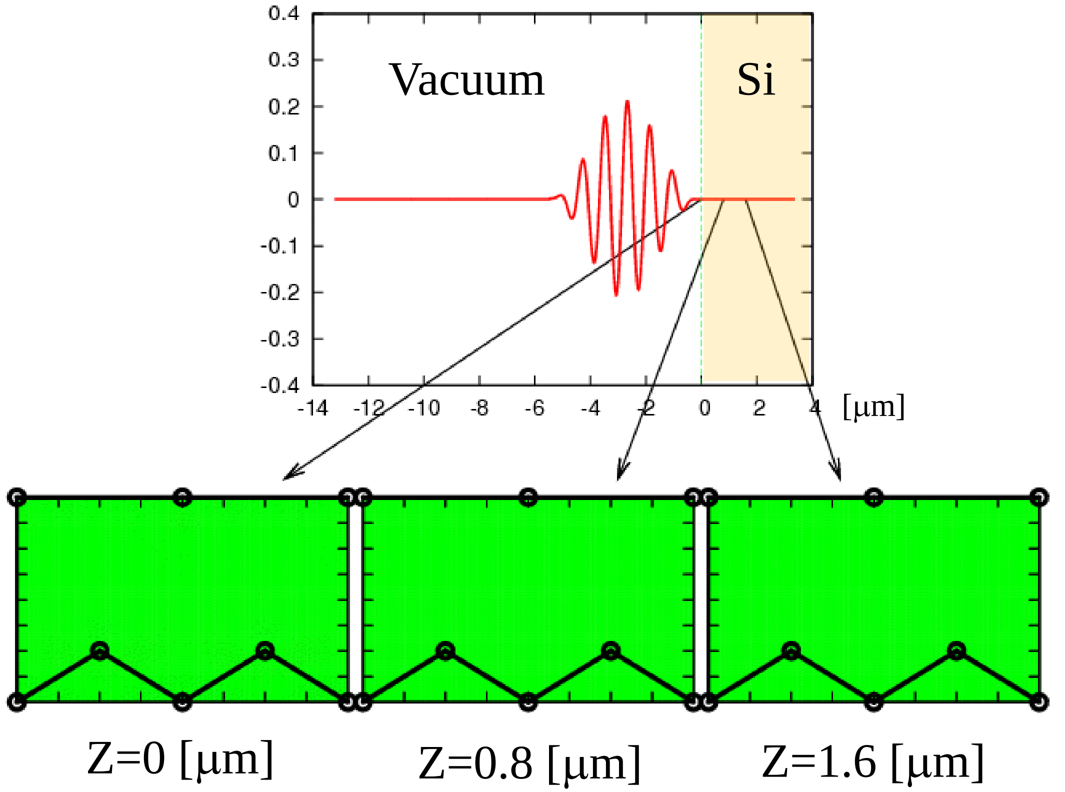
Phase velocity vs group velocity

$$v=\frac{c}{\sqrt{\varepsilon}} \qquad v_g=\frac{c}{\sqrt{\varepsilon}\left(1+\frac{\omega}{2\varepsilon}\frac{d\varepsilon}{d\omega}\right)}$$

Chirp effect is also seen

More intense laser pulse
Maxwell and TDKS equations no more separate.

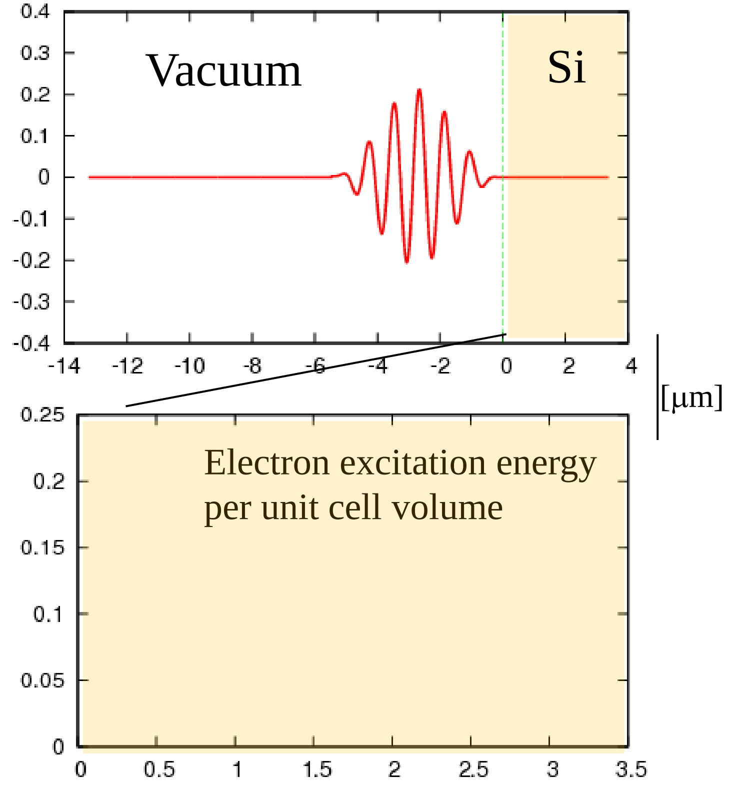
$I = 5 \times 10^{12} W/cm^2$



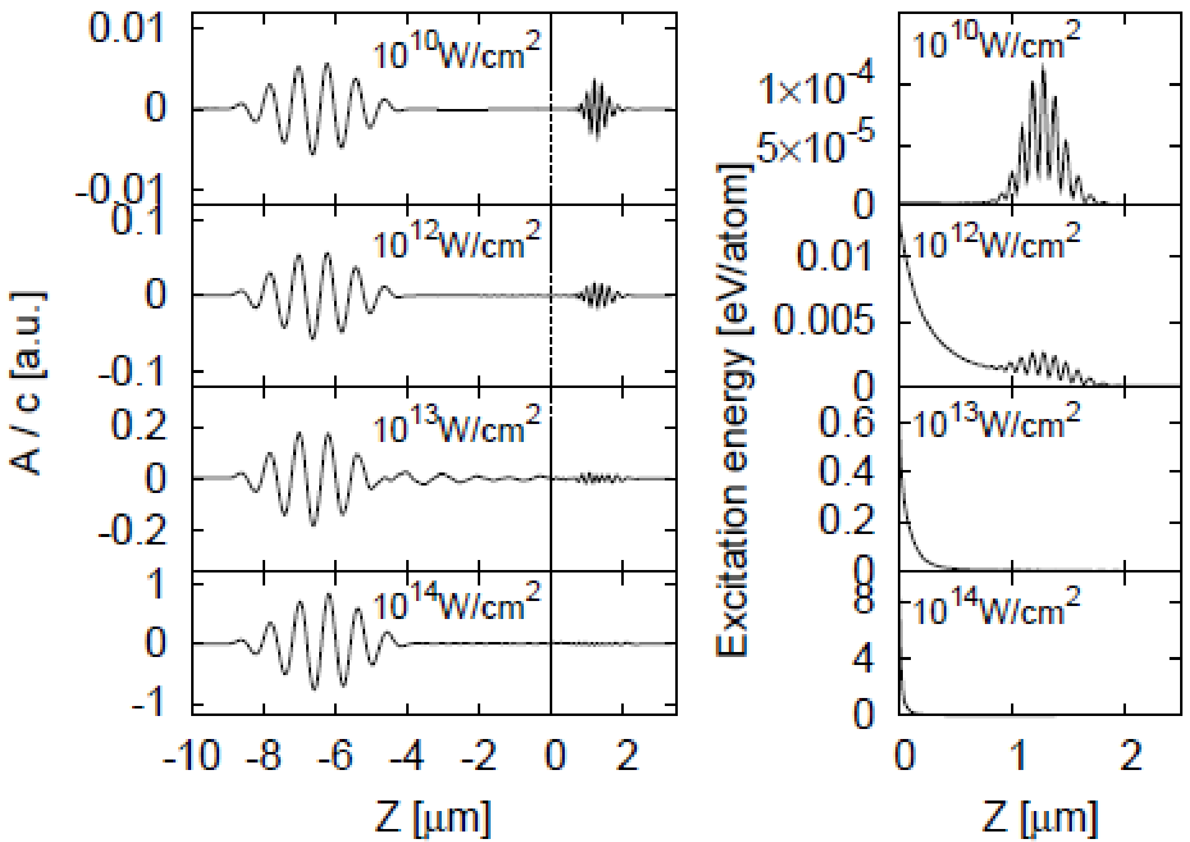
More intense pulse
(2-photon absorption dominates)

$I = 5 \times 10^{12} W/cm^2$

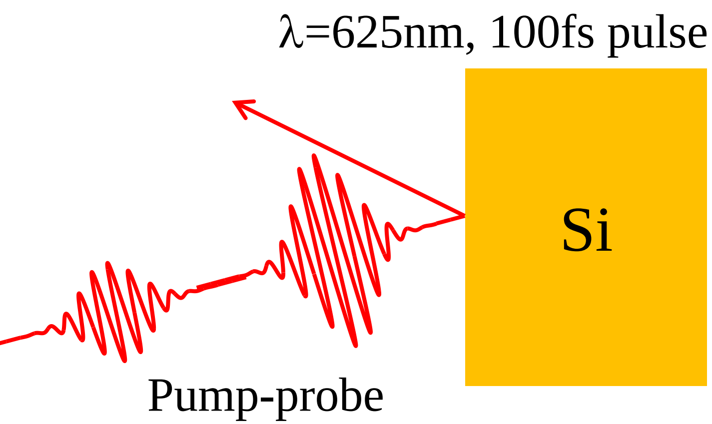
Laser frequency : 1.55eV :
lower than direct bandgap
2.4eV(LDA)



Vector potential and electronic excitation energy after the laser pulse splits into reflected and transmitted waves

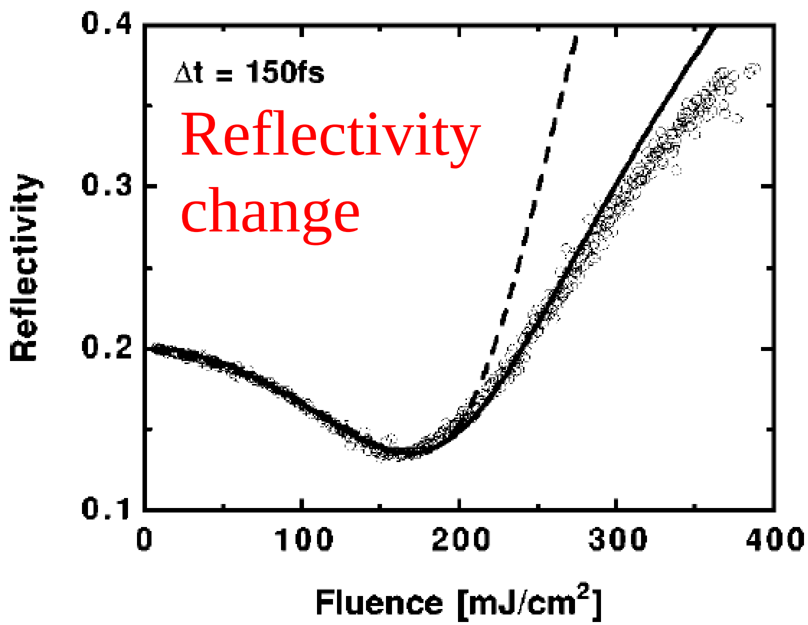


Dense electron-hole plasma generation at the surface modifies dielectric properties at the surface.



Strong pump-pulse excites electrons at the surface, forming dense electron-hole plasma

K. Sokoowski-Tinten, D. von der Linde, Phys. Rev. B61, 2643 (2000)



Pump-pulse intensity

Probe-pulse measures change of Dielectric properties.

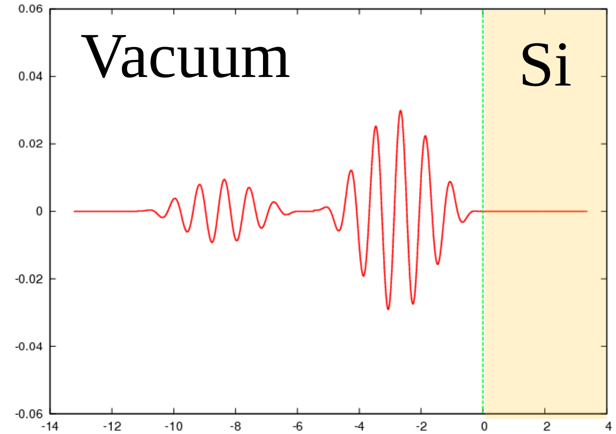
Drude model fit

$$\varepsilon(n_{ph}) = \varepsilon_{gs} - \frac{4\pi e^2 n_{ph}}{m^*} \frac{1}{\omega\left(\omega + \frac{i}{\tau}\right)}$$

$m^*=0.18$, $\tau=1$fs

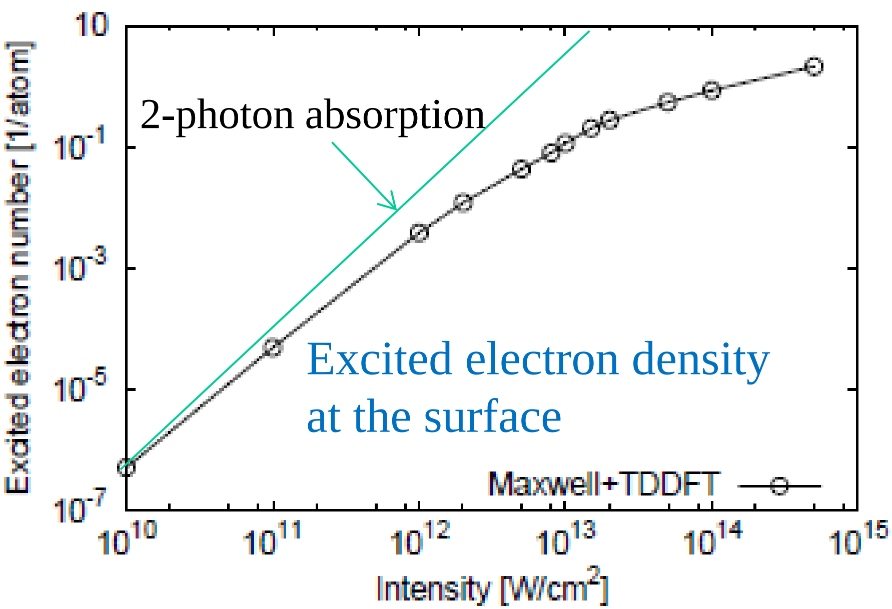
"Numerical Pump-Probe Experiment"

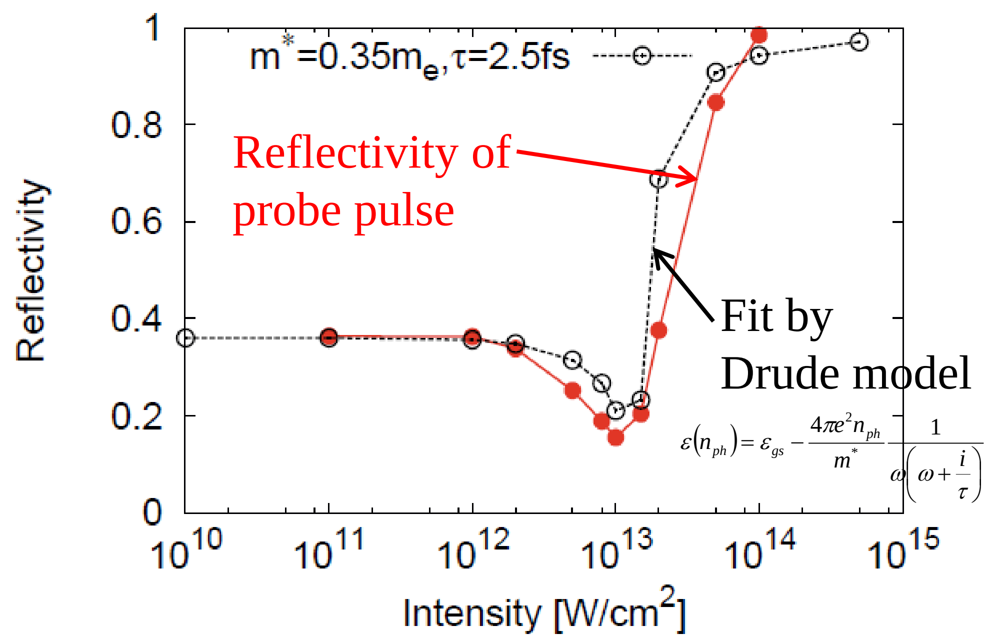
I=1x10^{11}W/cm^2,
$h\nu$=1.55eV



We can calculate

excited electron density at the surface by pump-pulse / reflectivity of probe pulse

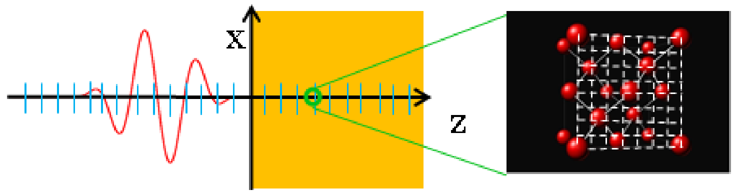




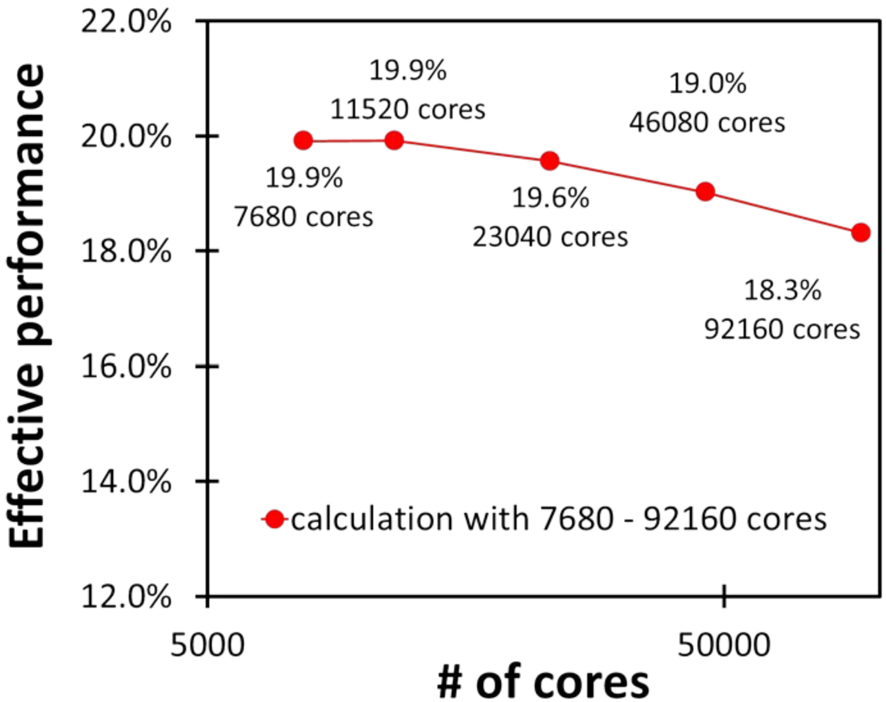
Computational Aspects

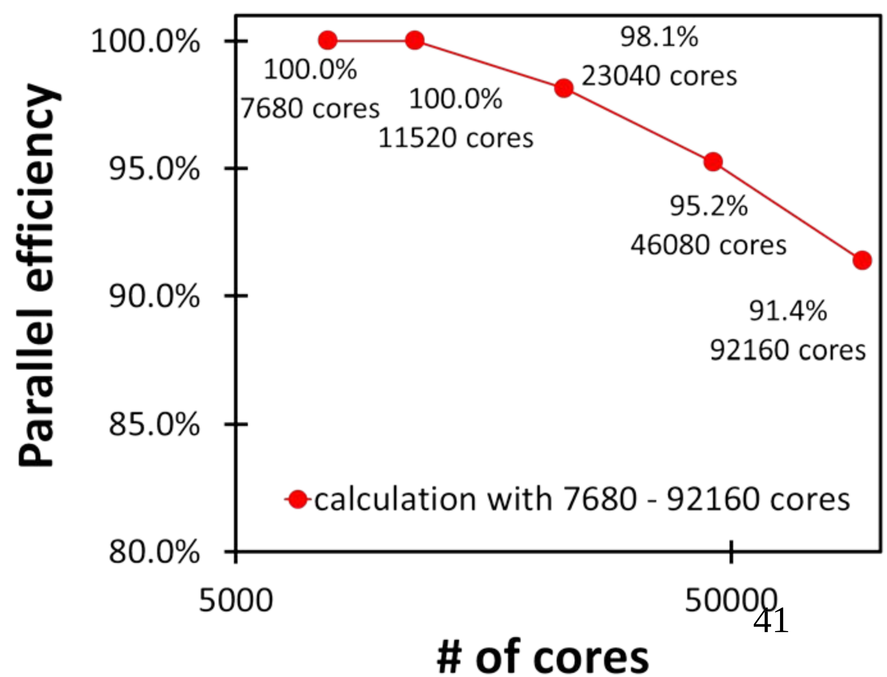
Large computational resources required for multi-scale calculation

1,000 cores, 10 hours (SGI Altix, U. Tokyo)
20,000 cores, 20 min (K-computer, Kobe)
macroscopic grid: 256
microscopic grid: 16^3
k-points 8^3 -> 80 (too small)
time step: 16,000

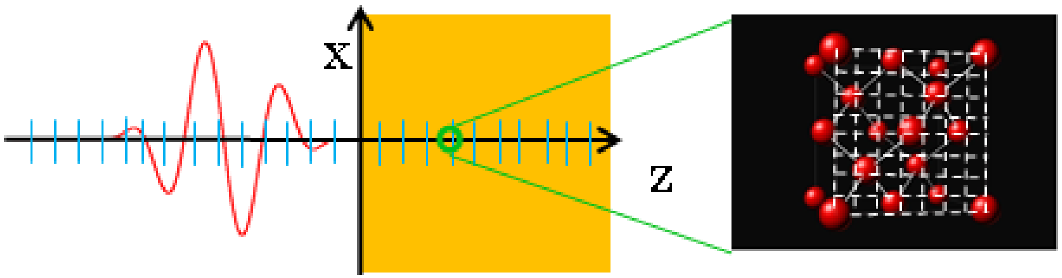


Performance at K-Computer in Kobe (in early access)





Future Prospects: Multi-dimensional wave propagation



At present, 1-dim propagation (macroscopic grid)

Si, diamond:

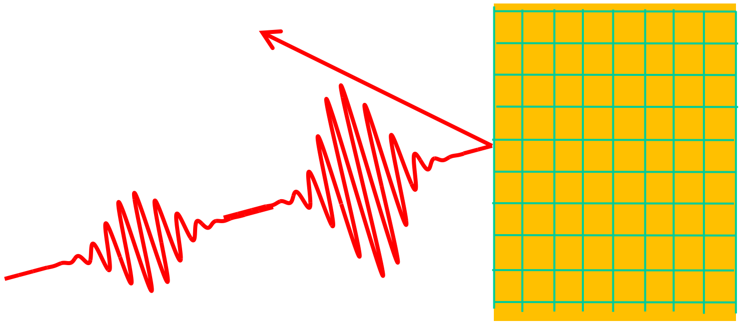
1,000 cores, 10 hours

20,000 cores, 20 min (K-computer, Kobe)

SiO_2 (α-quartz)

30,000 cores, 2 hours

Oblique incidence, 2-dim



$\times 50$

3-dim

- Self focusing
- Circular polarization

A million of macro-grid points

$\times 1{,}000$

need to wait next generation supercomputers

Summary

Electron dynamics in bulk periodic solid by real-time TDDFT

- First-principles description of electron dynamics in femto- and atto-second time scale
- Applications to
    - dielectric function (linear response)
    - coherent phonon generation
    - optical breakdown

Coupled Maxwell + TDDFT multi-scale simulation

- Promising tool to investigate laser-matter interaction
- Requires large computational resources, a computational challenge

Further developments necessary

- Surface dynamics, electron emission
- Collision effects (electron-electron, electron-phonon)