Dielectric response of laser-excited silicon at finite electron temperature

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Abstract

We calculate the dielectric response of excited crystalline silicon in electron thermal equilibrium by adiabatic time-dependent density functional theory (TDDFT) to model the response to irradiation by high-intensity laser pulses. The real part of the dielectric function is characterized by the strong negative behavior at low frequencies due to excited electron-hole pairs. The response agrees rather well with the numerical pump-probe calculations which simulate electronic excitations in nonequilibrium phase immediately after the laser pulse irradiation. The thermal response is also compared with the Drude model which includes electron effective mass and collision time as fitting parameters. We find that the extracted effective masses are in the range of 0.22-0.36 and lifetimes are in the range of 1-14 fs depending on the temperature. The short Drude lifetimes show that strong damping is possible in the adiabatic TDDFT, despite the absence of explicit electron-electron collisions.
I. INTRODUCTION

Properties of dielectrics irradiated by high-intensity and ultra-short laser pulses have been attracting substantial interests from both fundamental and technological points of view [1–5]. We are investigating the theory of the dielectric response of materials to high fields at times shorter than the full local equilibration time. Time-domain electron dynamics simulation based on the time-dependent density functional theory (TDDFT) is quite promising for describing the earliest time. This is the subject of a companion paper, Ref. [6], where we reported numerical simulations of pump-probe experiments. This theory should describe the formation of electron-hole excitations in insulating materials and the energy deposited in them. At the next time scale, the electron-hole excitations will come to an equilibrium, allowing one to treat the system as a thermalized electron-hole plasma with fixed numbers of electrons and holes. The dielectric properties of this state are the subject of the present paper. We will discuss them in crystalline silicon as in Ref. [6]. At even later times, the atomic degrees of freedom will be thermalized as well. That complete plasma equilibrium is beyond the scope of the present work. The two-temperature model assuming much smaller time-scale of electronic equilibrium than that of phonons is well established, see Ref. [7]. We will consider the response of thermalized electrons ignoring atomic motions, keeping them at equilibrium positions in the ground state. This treatment should be reasonable at times before substantial part of the electronic excitation energies is transferred to lattice motions.

We employ a static density functional theory (DFT) at finite temperature to describe the thermalized electronic state. An extension of the DFT to nonzero electronic temperature was first considered in [8], employing the grand canonical ensemble and introducing a chemical potential for the electrons. Recent developments of finite temperature DFT include discussions on basic aspects of the theory such as the conditions for the validity of the adiabatic connection formula [9] and applications to electrochemical reactions [10]. The finite temperature DFT has been applied to the properties of matter excited by intense and ultra-short laser pulses. For example, in Ref. [11], lattice properties of laser-excited solids were investigated using density functional perturbation theory with the Fermi-Dirac distribution for electrons. In Ref. [12], finite temperature DFT results were utilized to analyze solid aluminum excited by XUV pulses.

Our implementation of finite temperature DFT will use the grand canonical ensemble
for the occupation in the static solution. We then calculate the dielectric response in the linear response using a real-time method [14, 15]. To interpret the results, we compare the thermal response with the response of numerical pump-probe experiments [6]. We will show that many features of response in the elaborated numerical pump-probe experiments may be reproduced even at a quantitative level with the finite temperature calculation. We also compare with a simple Drude response embedding the free electrons in a dielectric medium [17–19].

The construction of the paper is as follows. In Sec. II, we describe the theoretical framework of finite temperature model and present calculated results. In Sec. III, we compare the results with the Drude model. In Sec. IV, we compare results of the finite temperature model with results of numerical pump-probe experiments. Our findings are summarized in Sec. V.

II. ELECTRONIC THERMAL MODEL

A. Ground state

We model the electronic state of crystalline silicon after irradiation of a high-intensity laser pulse by static DFT for a thermal ensemble of electrons. Atomic positions are kept at their equilibrium positions in the ground state, assuming that electron thermalization time is so short that atomic motions may be ignored. The Kohn-Sham equation for orbitals is given by

\[
\left\{-\frac{\hbar^2}{2m_e} \nabla^2 + V_{\text{ion}} + \int d\vec{r}' \frac{e^2}{|\vec{r} - \vec{r}'|} \rho^T(\vec{r}') + \mu_{xc}\right\} \phi_i(\vec{r}) = \epsilon_i \phi_i(\vec{r}).
\]

(1)

The electron density at temperature \(T\), \(\rho^T(\vec{r})\), is given by

\[
\rho^T(\vec{r}) = \sum_i n_i^T |\phi_i(\vec{r})|^2,
\]

(2)

where \(n_i^T\) is the temperature-dependent occupation number of Fermi-Dirac distribution,

\[
n_i^T = \frac{1}{1 + e^{(\epsilon_i - \mu)/k_B T}}.
\]

(3)

Here \(\epsilon_i\) is the energy of electron orbitals, \(\mu\) is the chemical potential, and \(k_B T\) is the temperature in energy units. We note that all the quantities related to the orbitals, \(\phi_i\), \(\epsilon_i\), and \(\mu\) depend on the temperature \(T\) due to the self-consistency requirement.
For the present purpose, it is essential to use a functional which reproduces both indirect and direct band gaps. The reproduction of the indirect band gap is important to produce correct density of electron-hole pairs for a given electronic temperature. The reproduction of the direct band gap is important for reasonable descriptions of the optical properties. We choose the meta-GGA (generalized-gradient approximation) potential of Tran and Blaha \[20\] for the exchange-correlation potential, \( \mu_{xc} \). The meta-GGA potential depends on the density \( \rho^T(\vec{r}) \), the gradient of the density \( |\nabla \rho^T(\vec{r})| \), and the kinetic energy density \( \tau^T(\vec{r}) = \sum_i n_i^T|\nabla \phi_i(\vec{r})|^2 \). The Tran-Blaha meta-GGA potential is known to resolve to some extent the band gap problem inherent to the local density approximation. It includes a parameter \( c \) to which the band gap is sensitive \[21\]. We treat it empirically, determining \( c = 1.04 \) which reproduces the measured indirect band gap of silicon at 1.17 MeV. The optical band gap is also found to be described reasonably.

Practical calculations are achieved as follows. We consider only valence electron orbitals treating electron-ion interaction by a norm-conserving pseudopotential \[22, 23\]. We use a three-dimensional grid representation to represent orbital wave functions. The cubic unit cell of a side length \( a = 10.26 \) a.u. containing eight silicon atoms is discretized into \( 20^3 \) grid points. The \( k \)-space is also discretized into \( 32^3 \) grid points.

In Fig. 1, we show the calculated number density of electron-hole pairs as a function of electron temperatures for crystalline silicon. As seen from the figure, the number density of excited electrons monotonically increases as the electron temperature increases. At electron temperature of 1.00 eV, which corresponds to 11,600K, the number density of electron-hole pairs is 0.2 per atom, indicating excitations of 5% of valence electrons. Figure 2 shows occupation distributions at various temperatures, as well as the density of states shown by black solid line. At temperatures around 1 eV, we find a substantial excitations of electrons from orbitals within 3 eV below the highest occupied orbital to orbitals within 5 eV above the lowest unoccupied orbitals.

**B. Linear response**

We calculate dielectric properties of the medium in the adiabatic TDDFT, using the same Tran-Blaha meta-GGA potential for the response calculation. Numerically, we solve the following time-dependent Kohn-Sham equation in real time to calculate the dielectric
FIG. 1: The number density of electron-hole pairs is shown as a function of electronic temperature in the thermal DFT calculation of crystalline silicon.

FIG. 2: Occupation number distribution of silicon at various temperatures. The density of states is also shown by black-solid line.

\[
\begin{align*}
\psi_i(\vec{r}, t) &= \left\{ \frac{1}{2m_e} \left( \vec{p} + \frac{e}{c} \vec{A}(t) \right)^2 + V_{\text{ion}} + \int d\vec{r}' \frac{e^2}{|\vec{r}' - \vec{r}|} \rho(\vec{r}', t) + \mu_{xc} \right\} \psi_i(\vec{r}, t). \\
\end{align*}
\]

The density \( \rho(\vec{r}, t) \) is constructed from time-dependent orbitals as \( \rho(\vec{r}, t) = \sum_i n_i^T |\psi_i(\vec{r}, t)|^2 \), using the occupation numbers in the ground states. To explore the dielectric property, we apply a distorting vector potential of step function in time \[15, 16\].

\[
\vec{A}(t) = \vec{\epsilon}_\beta A_0 \theta(t),
\]

\[
\]
where \( \vec{e}_\beta \) is a unit vector in the \( \beta \) direction. We calculate the current flowing within the unit cell from the solution by

\[
\vec{J}(t) = -\frac{e}{\Omega} \sum_i n_i^T \int _\Omega d\vec{r}d\vec{r}' \psi_i^*(\vec{r},t) \vec{v}(\vec{r},\vec{r}') \psi_i(\vec{r}',t), \tag{6}
\]

where \( \Omega \) is a volume of the unit cell and the velocity operator \( \vec{v}(\vec{r},\vec{r}') \) is defined by

\[
\vec{v}(\vec{r},\vec{r}') = -\frac{i\hbar}{m_e} \vec{V} \delta(\vec{r},\vec{r}') + \frac{1}{i\hbar} \left[ \vec{r}V^{NL}_{ps}(\vec{r},\vec{r}') - V^{NL}_{ps}(\vec{r},\vec{r}')\vec{r}' \right], \tag{7}
\]

where \( V^{NL}_{ps} \) is the nonlocal part of the pseudopotential. The conductivity is calculated from the induced current by

\[
\sigma_{\alpha\beta}(\omega) = -\frac{c}{A_0} \int_0^T dt e^{i\omega t} W(t/T) J_\alpha(t), \tag{8}
\]

where \( J_\alpha(t) \) is the \( \alpha \) component of \( \vec{J}(t) \), and \( T \) is the duration of time evolution. We use the mask function \( W(x) \) given by \( W(x) = 1 - 3x^2 + 2x^3 \) \[13\]. The dielectric function is obtained from the conductivity by

\[
e_{\alpha\beta}(\omega) = \delta_{\alpha\beta} + \frac{4\pi i\sigma_{\alpha\beta}(\omega)}{\omega}. \tag{9}
\]

In silicon, only diagonal element appears in the thermal model, \( e_{\alpha\beta}(\omega) = \delta_{\alpha\beta} e(\omega) \).

In time evolution calculations, we use the same grid points in the real space and the \( k \)-space as those in the static calculation. The time propagation is computed using a fourth-order Taylor expansion method \[14\], with a time step of \( \Delta t = 0.04 \) a.u. The total duration of the time evolution is \( T = 1,280 \) a.u. with the number of time steps \( N_T = 32,000 \).

In Fig. 3 we show dielectric functions of silicon at several electron temperatures. In the real part of the dielectric function, all responses at finite temperatures show a strong negative behavior at low frequencies. This Drude-like behavior comes from excited electron-hole pairs. The low energy component of the imaginary part shows absorptive contributions at low frequencies, increasing monotonically as the temperature increases. In our previous study employing numerical pump-probe experiments \[6\] which catch nonequilibrium distributions of electron-hole pairs, we have observed a similar behavior of Drude-like divergence in the real part. However, the absorptive contribution in the imaginary part was not observed.

A convenient way to exhibit the plasmon contribution to the response is to plot the imaginary part of the inverse dielectric function, \( \text{Im} e^{-1} \). This is shown in Fig. 4 for several temperatures up to \( k_BT = 1.4 \) eV. At the lowest temperature, one sees a very sharp plasmon
FIG. 3: The dielectric function of silicon in the finite temperature model at several temperatures. Top panel shows the real part of the dielectric function, and the bottom panel shows the imaginary part.

peak, located at an energy of \( \sim 0.4 \) eV. The plasmon excitation energy increases with temperature, due to the increased density of electron-hole pairs. We note that the width of the plasmon also increases with temperature, up to about \( k_B T \approx 0.6 \) eV. Beyond that, the width does not change very much, up to the maximum temperature considered.

III. COMPARISON WITH FREE-CARRIER MODELS

The dielectric response of solids excited by intense and ultrashort laser pulses is often modeled by a simplified dielectric function, adding a Drude-like component to the dielectric function in the ground state \[ \text{[18, 19]} \]. In this section, we will show that a model of this kind can reproduce quite well our calculated finite-temperature response.

We consider a model proposed by Sokolowski-Tinten and von der Lind \[ \text{[17]} \], which we
shall call the SL model. They consider three physical effects for the dielectric response of laser-excited semiconductor: (i) state and band filling, (ii) renormalization of the band structure, and (iii) the free-carrier response. The SL dielectric function is parameterized as

$$
\epsilon_{SL}(\omega) = 1 + \left[ \epsilon_0(\omega + \Delta E_{gap}) - 1 \right] \frac{n_0 - n_{eh}}{n_0} - 4\pi \frac{e^2 n_{eh}}{m^* \omega (\omega + i/\tau)}.
$$

Here $\epsilon_0(\omega)$ is the dielectric function in the ground state for which we employ the one calculated at zero temperature. $\Delta E_{gap}$ is the change of the band gap by the laser irradiation for which the calculated shift of the gap energy is used. $n_{eh}$ is the electron-hole pair density for which we use the calculated values. Three other parameters are: the effective mass $m^*$; the Drude damping time $\tau$; and the active number of valence electrons $n_0$. These are treated as fitting parameters.

The fit is carried out by minimizing the mean square error as given by

$$
I_{error} = \int_{\omega_i}^{\omega_f} d\omega \left| \epsilon_{T}^{-1}(\omega) - \epsilon_{SL}^{-1}(\omega) \right|^2,
$$

where $\epsilon_{T}(\omega)$ is the dielectric function in the thermal model. We take the interval $\hbar \omega_i = 0.3$ eV and $\hbar \omega_f = 6.0$ eV. The quality of the fit is shown in Fig. 5 for temperatures of $k_B T = 1.4$ and 0.4 eV in the thermal model. The fit is very good except for the Im$\epsilon$ at the lowest frequencies. In particular, the plasmon peak in the inverse dielectric function is very well reproduced.
FIG. 5: Comparison of the thermal model and a fit with the SL model. The electronic temperature in the thermal model is $k_B T = 0.4$ eV (left) and 1.4 eV (right).

In Fig. 6 we show the fitted effective mass $m^*$ and the collision time $\tau$ as functions of the temperature in the thermal model. The top panel shows that the effective mass $m^*$ increases as the temperature increases. We have found a similar behavior in the numerical pump-probe experiments in Ref. [6]. The change of effective mass may be understood by the change of the distribution of the electron-hole pairs in $k$-space.

The bottom panel of Fig. 6 shows that the damping time $\tau$ becomes very small as the electron temperature increases. The value of $\tau$ monotonically decreases and reaches a value of 1.0 fs at $k_B T \approx 1.4$ eV. At first sight this is puzzling, because there are no explicit collision effects in either the TDKS equation or in the thermal model in the adiabatic meta-GGA which we adopted. In spite of this, our plasmon peak has a large damping, corresponding to collision times as short as 1.0 fs in the thermal model. We consider that the damping arises from the elastic scattering of electrons from ionic core potentials. We note that TDDFT treatment of linear response describes the dielectric function of metals fairly well, including the width of plasmon seen in the inverse dielectric function [15].

IV. COMPARISON WITH NUMERICAL PUMP-PROBE EXPERIMENTS

In the preceding paper [6], we have carried out numerical pump-probe experiments to extract dielectric properties of laser-excited silicon immediately after irradiation by the laser pulse. This method catches fully the nonequilibrium nature of the excited electrons. The difference between the numerical pump-probe calculations and the present thermal model comes entirely from the different electron-hole distributions in the excited system to be
In this subsection, we compare their predicted dielectric functions.

In the numerical pump-probe calculation, we solve the TDKS equation in real time where the electric fields of both pump and probe pulses are included. The pump electric field $E_P(t)$ excites electrons and probe electric field $E_p(t)$ is used to extract dielectric properties of excited silicon. The dielectric properties are examined from the currents induced by the electric fields. In practice, we performed two calculations. In one calculation, we include both pump and probe electric fields, $E_P(t) + E_p(t)$, in the TDKS equation. We denote the current in this pump-probe calculation as $J_{Pp}(t)$. The other calculation includes only the pump field $E_P(t)$ and we denote the current as $J_P(t)$. The difference of the currents, $J_p(t) = J_{Pp}(t) - J_P(t)$ brings information of excited silicon. The electric conductivity $\sigma(\omega)$ of excited silicon is given by

$$\sigma(\omega) = \frac{\int dt J_p(t)e^{i\omega t}}{\int dt E_p(t)e^{i\omega t}}, \quad (12)$$

and the dielectric function by $\epsilon(\omega) = 1 + 4\pi i\sigma(\omega)/\omega$. In the numerical pump-probe experiment, we note that the responses are not isotropic but depend on the angle between electric fields of pump and probe fields. We consider two cases: the pump and probe electric fields
FIG. 7: The number density of electron-hole pairs of the crystalline silicon in the final state following the pulsed excitation as a function of the maximum pump intensity determined as \( I = cE_0^2 / 8\pi \). The critical density is indicated by the horizontal line. The squared intensity line normalized at \( 10^{10} \text{ W/cm}^2 \) is also shown by blue-dotted line. Taken from [6].

are parallel and perpendicular to each other.

To compare results of the thermal model with those of the numerical pump-probe experiments, we first need to assume a correspondence between the excited systems that we wish to compare. Since the plasmon characteristics are closely tied to the number of electron-hole pairs, we shall use that measure to make the comparison.

In Ref. [6], we reported calculations solving the TDKS equation with the electric field of the applied laser pulse whose vector potential is given by

\[
A(t) = \begin{cases} 
-\frac{E_0}{\omega} \cos(\omega t) \sin^2(\pi t/\tau_L) & (0 < t < \tau_L) \\
0 & (\text{otherwise}) 
\end{cases}
\]

(13)

where \( \omega \) and \( \tau_L \) is the average frequency and the time length of the laser pulse, respectively. \( E_0 \) is the maximum electric field strength in the medium. We denote the maximum intensity of the pulse given by \( I = cE_0^2 / 8\pi \). Using the laser pulse of the frequency \( \hbar\omega = 1.55 \text{ eV} \) and the duration of the pulse \( \tau_L = 18 \text{ fs} \), the number density of excited electrons is calculated for laser pulses of several intensities. We show the result in Fig. 7 which is taken from [6]. Combining Fig. 7 and Fig. 11 we can relate the laser intensity \( I \) and the electronic temperature \( k_B T \) through the number density of electron-hole pairs \( n_{eh} \). For example, in the TDKS calculation using the laser pulse of \( I = 1.0 \times 10^{12}\text{W/cm}^2 \) excites electron
FIG. 8: Comparisons of the dielectric function of the numerical pump-probe calculation and the thermal model. Left-hand panels: $n_{eh} = 0.016$ /Atom; right-hand panels: $n_{eh} = 0.31$ /Atom.

hole pairs of $n_{eh} = 0.016$ /Atom. From Fig. 7, the corresponding temperature is given by $k_B T = 0.4$ eV. For the laser pulse of $I = 5.0 \times 10^{12}$ W/cm$^2$, the density of electron-hole pair is $n_{eh} = 0.31$ /Atom. Corresponding temperature is $k_B T = 1.4$ eV. In the following, we use $n_{eh}$ to specify calculations of the finite temperature model and the numerical pump-probe experiments.

We show a comparison of dielectric function by two methods for two cases, $n_{eh} = 0.016$ /Atom and $n_{eh} = 0.31$ /Atom, in Fig. 8. The black lines show dielectric function of thermal model. The red-dashed line and the blue-dotted line show the results of the numerical pump-probe calculations for probe polarization parallel and perpendicular to the pump, respectively.

As seen from the figure, the real part of the dielectric function of silicon excited by the pump pulse is close to the thermal model for two cases. At lower excitation of $n_{eh} = 0.016$ /Atom, the thermal model is close to the pulsed excitation in the parallel probing. At higher excitation of $n_{eh} = 0.31$ /Atom, the thermal model is again close to the pulsed excitation in the parallel probing at higher frequencies ($\hbar \omega > 1$ eV) and is between the parallel and perpendicular probings at low frequencies ($\hbar \omega < 1$ eV). The imaginary part of the dielectric function looks rather different. While the thermal model predicts positive imaginary part below the band gap, the pulse-excited silicon shows much smaller value, even negative in certain frequencies.
We thus conclude that the thermal model describes the real part of the dielectric function quite well, provided the density of electron-hole pairs is the same. The difference between two calculations comes from the nonthermal distribution of electron-hole pairs in pump-probe simulation. It seems that the difference is more evident for the imaginary part. A nonequilibrium phase of electronic excitations manifests more sensitively in the imaginary part of the dielectric function.

V. SUMMARY

We investigated the change of dielectric response induced by intense and ultrashort laser pulses by a thermal model, assuming electronic equilibrium. This description is expected to apply to excited matter after a few tens of femtosecond following the laser irradiation. We first solved the static Kohn-Sham equation with finite temperature Fermi-Dirac function occupation factors. Its dielectric response was then computed by applying the linear response theory using the real-time method.

The calculated thermal dielectric function is characterized by the strong negative behavior in the real part at low frequencies caused by excited electron-hole pairs. The imaginary part shows absorptive contributions at low frequencies, increasing monotonically as the temperature increases. Plotting it in the inverse dielectric function, a sharp plasmon feature manifests clearly. The frequency of the plasmon increases monotonically with temperature due to the increased density of electron-hole pairs. The width also increases at low temperature region, then becomes almost constant.

The thermal dielectric function is compared with a simple Drude model of free-electron dynamics, embedded in the dielectric medium corresponding to the ground state. There are three basic parameters determining the electron-hole plasma properties, namely the density of electron-hole pairs, their effective mass $m^*$, and the collision time $\tau$. The density of electron-hole pairs is known from the thermal ground state calculation, but the other quantities are fit. We find the collision time of as short as 1.0 fs gives reasonable fit. This short value for the collision time is unexpected, since there are no explicit collision terms in the time-dependent Kohn-Sham equation that we solve. We consider the short collision time comes from the elastic scattering of electrons from atoms.

We also compared the thermal dielectric function with that derived from numerical pump-
probe calculation in which electronic response is derived from time evolution of Kohn-Sham orbitals under electric fields of both pump and probe pulses. The difference comes from the distributions of electrons and holes in \(k\)-space. The numerical pump-probe simulation describes the response of excited matter in the nonequilibrium state reached just after the pulse has been applied. We find the real part of the dielectric function shows reasonable correspondence if we compare them at the same number density of electron-hole pairs. However, the imaginary part shows marked difference. The thermal dielectric function shows positive imaginary part, while the numerical pump-probe calculation gives small contribution in the imaginary part, even negative contribution.

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