Transport and optical properties of CH$_2$ plastics: Ab initio calculation and density-of-states-based analysis

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Abstract. This work covers an ab initio calculation of transport and optical properties of plastics of the effective composition CH$_2$ at density 0.954 g/cm$^3$ in the temperature range from 5 kK up to 100 kK. The calculation is based on the quantum molecular dynamics, density functional theory and the Kubo–Greenwood formula. The temperature dependence of the static electrical conductivity $\sigma_1^{DC}(T)$ has an unusual shape: $\sigma_1^{DC}(T)$ grows rapidly for 5 kK $\leq T \leq 10$ kK and is almost constant for 20 kK $\leq T \leq 60$ kK. The additional analysis based on the investigation of the electron density of states (DOS) was performed. The rapid growth of $\sigma_1^{DC}(T)$ at 5 kK $\leq T \leq 10$ kK is connected with the increase of DOS at the electron energy equal to the chemical potential $\epsilon = \mu$. The frequency dependence of the dynamic electrical conductivity $\sigma_1(\omega)$ at 5 kK has the distinct non-Drude shape with the peak at $\omega \approx 10$ eV. This behavior of $\sigma_1(\omega)$ was explained by the dip at the electron DOS.

1. Introduction

The carbon-hydrogen plastics are widely used in the experiments in high energy density physics. The contrast improvement of intense laser pulses is one of the many fruitful applications of plastics [1]. In those experiments [1] the plastic film is used to reduce the action of the prepulse on the target.

The numerical simulation is necessary to choose the correct thickness of the film. The two-temperature hydrodynamic simulation may be applied to describe the action of the prepulse [1,2]. The two-temperature hydrodynamic model [3–5] requires the knowledge of the matter properties: two-temperature equation of state, optical properties (complex dielectric function), thermal conductivity, electron-ion coupling.

It is rather convenient to describe matter properties during the simulation by the wide-range semi-empirical analytical model [6]. The measurements or calculations of matter properties in various regions of phase diagram are required to construct such a model [7, 8]. The separate experimental and computational results are then joined to the wide-range model. This work covers the calculation of transport and optical properties in one region of the phase diagram.
At first under the action of the prepulse the matter is heated almost isochorically, so the investigation of the matter properties along the normal isochor is especially important. The quantum molecular dynamics (QMD) simulation in conjunction with the Kubo–Greenwood formula is well suited to calculate matter properties during the near-isochoric heating. In this work, we are focused on the investigation of transport and optical properties along the normal isochor via the QMD simulation and the Kubo–Greenwood formula.

The QMD simulation together with the Kubo–Greenwood formula has been widely used to calculate transport and optical properties [9–14]. In our previous works [15–17] we have employed this technique to calculate transport and optical properties of aluminum.

The carbon-hydrogen plastics have been also recently explored by the QMD technique [18–24]. However, the research was mainly focused on the calculation of the principal Hugoniots and the properties of plastics in the compressed state. The attention was also scattered among the plastics of various chemical compositions. The transport and optical properties were reported only in some works.

There is certain lack of the results on the plastic properties at the normal density. This motivated us to perform the current work. This work covers the investigation of the properties of plastics of the effective composition CH$_2$ at the normal isochor 0.954 g/cm$^3$. This composition and normal density correspond to the high-density polyethylene used for the contrast improvement of intense laser pulses [1].

2. Computation method

Here we will present only the brief description of the computation technique. The computation method was described in detail in our previous paper [16] and earlier works [9–11, 25].

Three main stages are included to the calculation: QMD simulation; precise resolution of the band structure in the framework of density functional theory (DFT); calculation of the transport and optical properties according to the Kubo–Greenwood formula.

At the first stage the atoms of carbon and hydrogen in the necessary proportion are placed to the supercell with periodic boundary conditions, the QMD simulation is used to calculate ionic trajectories in the further moments. The QMD simulation is performed using the Vienna ab initio simulation package (VASP) [26].

At the second stage the precise resolution of the band structure is performed. We select several independent ionic configurations from the equilibrium section of the MD run. For these selected configurations we calculate the electronic structure; the larger cut-off energy, number of bands, number of k-points in the Brillouin zone than during the QMD simulation may be used. Energy eigenvalues, corresponding wave functions and occupation numbers are obtained during the precise resolution of the band structure. This information is used at the third stage to calculate the dynamic Onsager coefficients according to the Kubo–Greenwood formula [27]:

\[
L_{mn}(\omega) = (-1)^{m+n} \frac{1}{e^{m^{-1}(eT)n^{-1}} \frac{2\pi e^2 \hbar^2}{3m^2 \omega \Omega}} \times \sum_{i,j,\alpha,k} W(k) \left( \frac{\epsilon_{i,k} + \epsilon_{j,k}}{2} - \mu \right)^{m+n-2} |\langle \Psi_{i,k} | \nabla_\alpha | \Psi_{j,k} \rangle|^2 \times (f(\epsilon_{i,k}) - f(\epsilon_{j,k})) \delta(\epsilon_{j,k} - \epsilon_{i,k} - \hbar \omega). 
\]

We use the VASP module optics.f90 to calculate matrix elements $\langle \Psi_{i,k} | \nabla_\alpha | \Psi_{j,k} \rangle$. We have also created special parallel program module that uses matrix elements obtained from VASP to calculate the dynamic Onsager coefficients according to the Kubo–Greenwood formula (1).

The dynamic Onsager coefficients calculated for different ionic configurations are averaged. The real part of the dynamic electrical conductivity $\sigma_1(\omega)$ is simply the $L_{11}(\omega)$ Onsager
coefficient. Other dynamic Onsager coefficients are necessary only to obtain the static Onsager coefficients via the extrapolation to the zero frequency. The static electrical conductivity \( \sigma_{\text{1 DC}} \equiv L_{11} \); the thermal conductivity \( K \) is expressed via the static Onsager coefficients as follows:

\[
K = L_{22} - \frac{L_{12}L_{21}}{L_{11}}.
\]

It should be mentioned, that \( K \) contains the additional second term in equation (2), called the thermoelectric term. In this work we check the relative contribution of the thermoelectric term to the thermal conductivity of plastics at different temperatures.

We have also calculated electron density of states (DOS). During the precise resolution of the band structure the information on the energy eigenvalues was obtained. The whole range of energy eigenvalues \( \epsilon \) (hereafter called the electron energy for simplicity) was divided into the sections of \( \Delta E_{\text{rect}} \) width. The number of bands falling within each section was determined and divided by the width of the section. The obtained value \( g(\epsilon) \) was assigned to the electron energy at the middle of the section. Each band was counted only once, i.e. the spin degeneracy was not taken into account.

3. Calculation parameters

The bulk of our calculations was performed for 120 atoms (40 atoms of carbon, 80 atoms of hydrogen) in the computational supercell. Only several additional runs were made for 249 atoms to check the dependence on the number of atoms.

The QMD step was set to 0.2 fs. We have set the Nosé mass parameter SMASS to 0, thus we let VASP to set SMASS automatically. Thus the SMASS parameter varied from 0.05 at 5 kK to 0.98 at 100 kK. We create an auxiliary simple cubic lattice and put the atoms of carbon and hydrogen to the random positions at the nodes of this auxiliary lattice. Then we perform 15000 steps of simulation. Given the simulation step is 0.2 fs, we track 3 ps of the system evolution.

Following the procedure of configuration generation described above, we need to know only the relative fractions of carbon and hydrogen. Further in this paper we call this unordered state a plastic of the effective composition CH\(_2\).

The setting of the initial ionic configuration of plastics for the QMD simulation is an involved problem; the methods of its construction vary from quite simple to rather complicated. In this work we use the simplest procedure described above to set the initial ionic configuration. We can not assert, that we reach a thermodynamically equilibrium state. But at least we can be sure that we explore a state, that is metastable during the simulation time. The previous works [18, 23] show, that the time of several picoseconds is quite sufficient for chemical bonds to break and form. This ensures that the simple procedure employed in this work is good enough to reasonably reproduce the properties of plastics.

During the QMD simulation we have used the LDA exchange-correlation functional. The exchange part of the functional had a common \( \sim \rho^{1/3} \) dependence, whereas the correlation part had the Ceperley-Alder parametrisation [28]. We have used PAW pseudopotentials [29, 30], 4 electrons per carbon atom and 1 electron per hydrogen one were included in the calculation. During the QMD simulation we have used the energy cut-off \( E_{\text{cut}} = 300 \) eV and 1 k-point (\( \Gamma \)-point) in the Brillouin zone. The number of bands increased as the temperature was increased; the number of bands was selected as described in our previous paper [16]. The bands with the occupation numbers not less than \( 5 \cdot 10^{-6} \) were considered occupied.

We have chosen 15 ionic configurations for the calculation of transport and optical properties: the first one was chosen at step 999 (0.2 ps); the period between neighboring configurations was 1000 time steps. The precise resolution of the band structure was performed for each of the chosen ionic configurations. The exchange-correlation functional, the pseudopotential, the energy cut-off and the number of \( \textbf{k} \)-points during the precise resolution of the band structure
were the same as during the QMD simulation. Only the number of bands was increased to enable the calculation of optical properties for the frequencies up to 40 eV. The number of bands was selected as described in our previous paper [16].

The dynamic Onsager coefficients were calculated for the frequencies from 0.005 eV up to 40 eV with the frequency step of 0.005 eV. The broadening of the $\delta$-function in the Kubo–Greenwood formula was $\Delta E = 0.2$ eV. The simple linear extrapolation was used to obtain the static Onsager coefficients from the dynamic ones (this procedure is described in detail in our previous paper [16]).

The width of the sections $\Delta E_{\text{rect}}$ during the calculation of DOS should be selected the same way as the broadening $\Delta E$ in the Kubo–Greenwood formula (see detailed description in our previous paper [16]).

The comparison of our results with the experimental works, reference data and the calculations of other authors was performed for aluminum in our previous works [15, 16]. Our calculations were permanently in good agreement with other results. This confirms that our results for plastics are reliable, too.

4. Results

Transport and optical properties of plastics of the effective composition CH$_2$ were calculated for the density of 0.954 g/cm$^3$ and the temperatures from 5 kK up to 100 kK.

The results on the dynamic electrical conductivity of plastics are presented in figure 1.

Figure 1a shows frequency dependences of the dynamic electrical conductivity of plastics for 5 temperatures from 5 kK to 10 kK. The curves have the distinct non-Drude shapes. At $T = 5$ kK $\sigma_1(\omega)$ has the prominent peak at the frequency of about 10 eV. The curves change significantly as the temperature grows. At temperature rise the peak becomes smoother and moves to the lower frequencies. The dynamic conductivity grows at low frequencies.

Figure 1b shows frequency dependences of the dynamic electrical conductivity of plastics for 5 temperatures from 20 kK to 100 kK. For the temperature range from 20 kK to 60 kK the curves remain almost invariable if the temperature rises. This is especially noticeable if $\sigma_1(\omega)$ curves for 40 kK and 60 kK are compared. For the temperature range from 60 kK to 100 kK the curves begin to change slightly again. The peak becomes sharper again and moves to even lower frequencies. The dynamic conductivity grows at low frequencies.

The results on the transport properties of plastics are shown in figure 2.
Figure 2. Temperature dependences of the transport properties of CH$_2$ plastics, $\rho = 0.954$ g/cm$^3$. (a) Static electrical conductivity. Squares—120 atoms; triangles—249 atoms. (b) Thermal conductivity. Filled squares—the Onsager coefficient $L_{22}$ (thermoelectric term is neglected), 120 atoms; empty squares—thermal conductivity $K$ (thermoelectric term is taken into account), 120 atoms; empty triangles—thermal conductivity $K$, 249 atoms.

Figure 2a shows the temperature dependence of the static electrical conductivity. The results on the static conductivity show similar behavior as the results on the dynamic one described above. The whole temperature range may be divided into three smaller sections: 1) 5 kK to 10 kK, the conductivity grows rapidly; 2) 20 kK to 60 kK, the conductivity is almost constant as the temperature is varied; 3) 60 kK to 100 kK, slow growth of the static conductivity.

Figure 2b shows temperature dependences of the Onsager coefficient $L_{22}$ and the thermal conductivity $K$. The thermal conductivity grows monotonically in the whole range of temperatures under consideration. At low temperatures $K$ (thermal conductivity with thermoelectric term taken into account) coincides with $L_{22}$ (thermal conductivity with thermoelectric term neglected). The discrepancy between $K$ and $L_{22}$ becomes significant (18%) at the temperature of 40 kK. At $T = 100$ kK $L_{22}$ is 3 times larger than $K$.

5. DOS-based analysis

This section contains the brief discussion of the results on the transport properties.

At first it should be mentioned, that the static electrical conductivity of plastics under the conditions considered has the order of $10^5$ $\Omega^{-1}m^{-1}$. The static electrical conductivity of metals at near-normal densities and temperatures about several tens kK has the order of $10^6$ $\Omega^{-1}m^{-1}$ (see for instance, our previous works [16,17]). The static electrical conductivity of metals at the normal conditions usually has the order of $10^7$ $\Omega^{-1}m^{-1}$.

We think, that the most noticeable result on the transport properties obtained in this work is the rapid growth of the static electrical conductivity in the range of temperatures 5 ÷ 10 kK (see figure 2a). To be sure that this is not the computational error caused by the small number of atoms, we have also performed some additional calculations with larger number of atoms in the supercell. The results are presented in figure 2. Neither the results on the electrical conductivity, nor the results on the thermal conductivity have changed qualitatively at increased number of atoms.

To learn more about the nature of the static electrical conductivity growth at $\rho = 0.954$ g/cm$^3$ (figure 2a) we have chosen two temperatures (5 kK and 10 kK) and compared the electron DOS
related to these temperatures. The results are presented in figure 3.

The density of states \( g(\epsilon - \mu)/\Omega \) calculated as described in Section 2 is plotted by the solid curve. It should be mentioned that the chemical potential \( \mu \) was chosen as the reference point for the electron energies. The DOS was calculated for 249 atoms in the supercell. The occupation numbers \( f(\epsilon - \mu) = \left( \frac{\epsilon - \mu}{\beta} \right)^{-1} \) defined by the Fermi–Dirac distribution. Hatching displays the \( \epsilon - \mu \) values, which give the most significant contribution to the static electrical conductivity. This hatching corresponds to FWHM (full width at half maximum) of the \( \partial f / \partial \epsilon (\epsilon - \mu) \) curve.

The selection of the hatching area is based on the following reasoning. The Kubo–Greenwood formula may be presented in the following continuous fashion (see, for instance, paper [9]):

\[
\sigma_1(\omega) \sim \int |\nabla(\epsilon, \epsilon + \hbar \omega)|^2 \frac{f(\epsilon) - f(\epsilon + \hbar \omega)}{\hbar \omega} g(\epsilon) g(\epsilon + \hbar \omega) d\epsilon. \tag{3}
\]

Here \( |\nabla(\epsilon_1, \epsilon_2)|^2 \) is some continuous form of the matrix elements \( \frac{1}{3} \sum_{\alpha} |\langle \Psi_i \mid \nabla_{\alpha} \mid \Psi_j \rangle|^2 \). The proportionality sign in (3) may contain only fundamental constants and the volume of the supercell \( \Omega \). We call equation (3) the continuous Kubo–Greenwood formula. In the static case \( \omega \to 0 \) equation (3) is reduced to:

\[
\sigma_{1DC} \sim \int |\nabla(\epsilon, \epsilon)|^2 \left( -\frac{\partial f}{\partial \epsilon}(\epsilon) \right) g^2(\epsilon) d\epsilon. \tag{4}
\]

The contribution of too high or too low \( \epsilon \) values is damped by the rapid decay of the \( -\frac{\partial f}{\partial \epsilon}(\epsilon) \) curve. So we may estimate the region, yielding the most significant contribution to \( \sigma_{1DC} \) by the FWHM of the \( -\frac{\partial f}{\partial \epsilon}(\epsilon) \) curve. Also we may notice from (4), that the higher \( g(\epsilon) \) is, the higher is the contribution of the given \( \epsilon \) to \( \sigma_{1DC} \).
The DOS for the temperature 5 kK is shown in figure 3a. The area, giving the most significant contribution to the $\sigma_{\text{DC}}$ corresponds to the dip at the $g(\epsilon - \mu)$ curve. Thus, the low number of bands contributes to the static electrical conductivity and the values of $\sigma_{\text{DC}}$ are relatively low.

Also we may see the peak at the DOS curve at $\epsilon_1 - \mu \approx -5$ eV. The bands located at $\epsilon_1 - \mu \approx -5$ eV are fully occupied. The transition from these bands to the bands located at $-5$ eV $\lesssim \epsilon_2 - \mu \lesssim 0$ eV is damped by the high occupation numbers of the final bands. The transition from $\epsilon_1 - \mu \approx -5$ eV to $0$ eV $\lesssim \epsilon_2 - \mu \lesssim 5$ eV is damped by the low density of states $g(\epsilon_2 - \mu)$. The density of the final states $g(\epsilon_2 - \mu)$ becomes high enough at $\epsilon_2 - \mu \approx 5$ eV. Thus, we consider, that the transition from the bands at $\epsilon_1 - \mu \approx -5$ eV to $\epsilon_2 - \mu \approx 5$ eV gives the prominent $\omega \approx 10$ eV peak at the curves of the dynamic electrical conductivity (figure 1a). This transition is marked by an arrow in figure 3a.

The transition from $\epsilon_1 - \mu \approx -5$ eV to even higher bands $\epsilon_2 - \mu \gtrsim 5$ eV is likely damped by the small values of $|\nabla(\epsilon_1 - \mu, \epsilon_2 - \mu)|^2$ at high $\epsilon_2 - \mu$. This explains the drop of the $\sigma_1(\omega)$ at $\omega \gtrsim 10$ eV (figure 1a). The $\hbar \omega$ factor in the denominator of equation (3) also makes $\sigma_1(\omega)$ drop at high $\omega$.

The DOS for the temperature 10 kK is shown in figure 3b. The area, giving the most significant contribution to the $\sigma_{\text{DC}}$ now corresponds to the small peak at $g(\epsilon - \mu)$. The values of DOS $g(\epsilon - \mu)$ in the hatched area are larger than those in the hatched area at the temperature 5 kK. The larger number of bands contributes to the static electrical conductivity at 10 kK. Consequently, $\sigma_{\text{DC}}$ at 10 kK is larger than at 5 kK (figure 2a).

The smoother DOS curves at 10 kK also yield the smoother curves of the dynamic electrical conductivity (figure 1a).

In this work we have obtained the step-like behavior of $\sigma_{\text{DC}}(T)$ for CH$_2$ plastics along 0.954 g/cm$^3$ isochor. The knee of the $\sigma_{\text{DC}}(T)$ dependence is located at approximately 15 kK. Similar behavior for somewhat different conditions was obtained in the number of previous works.

Static electrical conductivity of CH$_2$ plastics along the principal Hugoniot was investigated in the paper of Theofanis et al. [31] by the wave-packet dynamics method. The step-like behavior of $\sigma_{\text{DC}}(T)$ along the principal Hugoniot was obtained. Though the precision of conductivity calculation in the work [31] is rather low, it may be established that the knee of $\sigma_{\text{DC}}(T)$ dependence is located at approximately 5 kK. The value of conductivity at the plateau in the work [31] is $2 \cdot 4 \cdot 10^3 \, \Omega^{-1} \text{m}^{-1}$, by the order of magnitude it is close to the value at the plateau in our work. The knee of $\sigma_{\text{DC}}(T)$ in the work of Theofanis et al. is located at lower temperature than in our work, this is likely because for the same temperatures the density at the principal Hugoniot is higher than normal. The step-like behavior is called "transition to the metallic state" in the work [31].

The CH plastics along the principal Hugoniot were investigated in the paper [20]. The dependences of the static electrical conductivity $\sigma_{\text{DC}}(u_s)$ and reflectivity $R(u_s)$ on the shock wave velocity $u_s$ demonstrate a step-like behavior. The CH plastics along the principal Hugoniot were also investigated in the paper [24]. The pressure dependence of reflectivity at 532 nm $R(p)$ is reported to have a step-like behavior.

6. Conclusions

(i) In this work we have performed ab initio calculation of transport and optical properties of plastics of the effective composition CH$_2$ at constant density 0.954 g/cm$^3$; the temperature falls within the range 5 kK $\leq T \leq 100$ kK.

(ii) The step-like behavior of $\sigma_{\text{DC}}(T)$ was obtained. Static electrical conductivity grows rapidly for the temperatures 5 kK $\leq T \leq 10$ kK and is almost constant for the temperatures 20 kK $\leq T \leq 60$ kK.
(iii) The behavior of $\sigma_{1\text{DC}}(T)$ was partially explained by the investigation of the electron density of states. The rapid growth of $\sigma_{1\text{DC}}(T)$ at $5 \text{kK} \leq T \leq 10 \text{kK}$ is connected with the growth of the DOS at $\epsilon = \mu$.

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