Transport and optical properties of warm dense aluminum in the
two-temperature regime: Ab initio calculation and semiempirical
approximation

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This work is devoted to the investigation of transport and optical properties of liquid aluminum in the
two-temperature case. At first, all physical properties, static electrical and thermal conductivities were obtained
in the \textit{ab initio} calculation. The \textit{ab initio} calculation is based on the quantum molecular dynamics, density
functional theory and the Kubo-Greenwood formula. The semiempirical approximation was constructed based
on the results of the \textit{ab initio} calculation. The approximation yields the dependences \(\sigma_{\text{lec}} \propto 1/T_i^{0.25}\) and
\(\kappa \propto T_i/T_i^{0.25}\) for the static electrical conductivity and thermal conductivity, respectively. The approximation
is valid for liquid aluminum at \(\rho = 2.70\ \text{g/cm}^3\), \(3\ \text{kK} \leq T_i \leq 20\ \text{kK}\). Our results are well described
by the Drude model with the effective relaxation time \(\tau \propto T_i^{-0.25}\). We have compared our results with a
number of other models. They are all reduced in the low-temperature limit to the Drude model with different
expressions for the relaxation time \(\tau\). Our results are not consistent with the models in which \(\tau \propto T_i^{-1}\) and
support the models which use the expressions with the slower decrease of the relaxation time.

I. INTRODUCTION

The experiments on the interaction of femtosecond
lasers with matter are widespread nowadays\textsuperscript{1–4}. During
the ultrafast heating the matter passes through the two-
temperature state with hot electrons and relatively cold
ions. Different approaches may be used to simulate these
experiments. Two-temperature hydrodynamic\textsuperscript{5,6} and
combined continuum-atomistic modeling\textsuperscript{7} are widely
used.

The information on the properties of matter is neces-
sary for the practical implementation of the computa-
tional schemes. The necessary properties may differ
depending on the type of simulation.

For thin targets at initial stage only the information on
optical properties, electron and ion heat capacities, and
electron-ion coupling is necessary\textsuperscript{8}. The study of the optical
properties is possible both using modern picosecond
diagnostics\textsuperscript{9–12} and computational methods\textsuperscript{6,7}.

Thermal conductivity is necessary, in addition, for the
simulation of thick targets\textsuperscript{13,14}. During the initial stage
of experiment the density of the target remains almost
constant, so the study of the matter properties along the
normal isochor is of the paramount importance.

If the whole process of the target heating and post-
evolution is to be studied, the full hydrodynamic simu-
lation is necessary\textsuperscript{15}. Two-temperature equation of state,
valid in the broad region of densities and temperatures,
should be available.

The properties of matter in the two-temperature
regime differ significantly from those in the equilib-
rrium case. This has been investigated previously
for structural properties\textsuperscript{16–18}, optical properties\textsuperscript{19}, melt-
ing temperatures\textsuperscript{20–22}, density of states\textsuperscript{23–25}, phonon
spectra\textsuperscript{26}, electron-ion coupling factor\textsuperscript{27} and equations
of state\textsuperscript{28,29}.

In this work we focus on the investigation of the op-
tical properties, static electrical and thermal conductiv-
ities of liquid aluminum at normal density in the two-
temperature case.

The usual approach to obtain transport and optical
properties in the wide range of parameters is to interpo-
late between high- and low-temperature asymptotics\textsuperscript{5,18,19}.

At high temperatures the electrons are non-degenerate
and the ions are not correlated. The Spitzer theory\textsuperscript{30} is
valid for the non-degenerate fully ionized plasma with
a small non-ideality. At lower temperatures coupling,
degeneracy corrections\textsuperscript{31} and partial ionization\textsuperscript{32} should
be taken into account.

At low temperatures the electrons become degenerate
and should be treated within the quantum mechanical
approach. The optical properties may be obtained using
the average atom models\textsuperscript{33,34}. However, at low tempera-
tures ion-ion correlations become important, and the
cohert scattering of electrons by the ions should be taken
into account. The average atom models do not allow for
ion-ion scattering and do not give correct static electrical
and thermal conductivities\textsuperscript{24}.

The correct treatment of ion-ion correlations and co-
herent electron scattering is crucial for the calculations
at relatively low temperatures. There are several ap-
proaches to deal with the problem.

The simplest approach is to use the Drude model with
the effective collision frequency of the crystalline-like
form \(\nu_{\text{eff}} = A T_i + B T_i^{2/3}\).
In the more complicated approximations the temperature growth of the effective collision frequency in the liquid phase is limited by some maximum value. This approach is often used in the simulations of femtosecond laser heating.

The ionic structure factor may be calculated by solving the integral equations for distribution functions. The transport and optical properties are then obtained via the Ziman theory. However, the treatment of the band excitation in the metals with complex electronic structure is difficult within this formalism.

The method based on the quantum molecular dynamics (QMD), density functional theory (DFT) and the Kubo-Greenwood formula is widely used to treat the structure of materials. Since that time the method was applied to the wide variety of materials. The QMD simulation is performed. At each ionic step the electronic structure is calculated in the frame-works. The electronic structure is calculated according to the Kubo-Greenwood formula. The static Onsager coefficients \( L_{mn} \), \( m, n = 1, 2 \) connect the applied electric field \( E \) and the electron temperature gradient \( \nabla T_e \) with the emerging electric \( j \) and heat \( j_q \) current densities:

\[
  j = \frac{1}{e} \left( e L_{11} E - \frac{L_{12} \nabla T_e}{T_e} \right),
\]

\[
  j_q = \frac{1}{e^2} \left( e L_{21} E - \frac{L_{22} \nabla T_e}{T_e} \right).
\]

Here \( e \) is the electron charge. For the sake of convenience we also introduce the Onsager coefficients \( \sigma_{mn} \), \( m, n = 1, 2 \) which are connected with \( L_{mn} \) via the following relations:

\[
  L_{11} = \sigma_{11}, \quad L_{12} = \frac{L_{12}}{e T_e}, \quad L_{21} = \frac{L_{21}}{e}, \quad L_{22} = \frac{L_{22}}{e^2 T_e}.
\]

The dynamic Onsager coefficients \( \sigma_{mn}(\omega) \), \( m, n = 1, 2 \) are calculated according to the Kubo-Greenwood formula:

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

Here \( \Psi_{i,k} \) and \( \epsilon_{i,k} \) are the electronic wave function and energy eigenvalue respectively, corresponding to the particular band \( i \) and point in the Brillouin zone \( k \). This information is obtained during the precise resolution of the band structure. \( f(\epsilon_{i,k}) \) is the Fermi-weight of the particular band, \( W(k) \)—the weight of the particular \( k \)-point. \( \mu \) is the chemical potential, \( \omega \)—the frequency of the applied electric field, \( \Omega \)—the volume of the supercell. \( h \) is the reduced Planck constant, \( m_e \) is the electron mass.

The delta-function in the Kubo-Greenwood formula is broadened by the Gaussian function. The intuitively clear derivation of the Kubo-Greenwood formula for \( \sigma_1(\omega) = \sigma_{11}(\omega) \) may be found in the paper. The derivation of the Kubo-Greenwood formula in the form was performed in the paper. It is worth noting, that the energy eigenvalues half-sum \( \frac{\epsilon_{i,k} + \epsilon_{j,k}}{2} \) is used during
the calculation. This was first established in the paper\textsuperscript{39}, some additional discussion is also present in our previous paper\textsuperscript{39}.

The real part of the dynamic electrical conductivity is readily obtained as \( \sigma_1(\omega) = L_{11}(\omega) \). The imaginary part is reconstructed via the Kramers-Kronig relation. If the dynamic electrical conductivity is known, we may calculate other optical properties\textsuperscript{39,39}, complex dielectric function, complex refraction index, reflectivity, and absorption coefficient.

If we calculate the transport properties, the static Onsager coefficients \( L_{mn} \) and \( L_{nm} \) are obtained by the simple linear extrapolation to the zero frequency\textsuperscript{39}. Except for the \( L_{11}(\omega) = \sigma_1(\omega) \), no physical meaning is assigned to the dynamic Onsager coefficients. They are necessary only to calculate the static ones. Then the transport properties are expressed as follows:

\[
\sigma_{\text{DC}} = L_{11},
\]

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

Here \( \sigma_{\text{DC}} \) stands for the static electrical conductivity, whereas \( K \)—for electron thermal conductivity. The thermal conductivity \( K \) contains not only the \( L_{22} \) Onsager coefficient. Additional positive contribution, called thermoelectric term, is also subtracted. At low temperatures the relative contribution of the thermoelectric term is small\textsuperscript{42}.

The experimentally discovered Wiedemann-Franz law exists\textsuperscript{15}:

\[
\frac{K(T)}{\sigma_{\text{DC}}(T) \cdot T} = \text{const} = L = \frac{\pi^2 k^2}{3 e^2}.
\]

The static electrical conductivity \( \sigma_{\text{DC}}(T) \) and thermal conductivity \( K(T) \) depend on the temperature, whereas the ratio \( L \), called the Lorenz number, does not depend on the temperature. The value \( L = \frac{\pi^2 k^2}{3 e^2} = 2.44 \cdot 10^{-8} \text{ W}\cdot\Omega\cdot\text{K}^{-2} \) is called the ideal value. The Wiedemann-Franz law was discovered at low temperatures in the equilibrium case \( T_e = T_i \). In this work we obtain the static electrical and thermal conductivities and check the validity of the Wiedemann-Franz law at high temperatures in the non-equilibrium case.

The QMD simulation and the band structure calculation are performed using Vienna \textit{Ab initio} Simulation Package (VASP)\textsuperscript{40,45}. The special parallel program module was created to compute the dynamic Onsager coefficients, extrapolate them to zero frequency and calculate transport properties. This module uses information from the VASP package.

### III. CALCULATION PARAMETERS

The optimal choice of technical parameters was described in detail in our previous paper\textsuperscript{39}. Here we will only specify the values of technical parameters.

The QMD simulation is performed for the supercell, containing 256 atoms. Initially the atoms are placed to the nodes of the fcc lattice. The Newton’s motion equations are integrated using the Verlet algorithm. The integration step is 2 fs. 1500 steps of the QMD simulation are performed. The ultrasoft pseudopotential (USPP) of Vanderbilt\textsuperscript{46} together with the local density approximation (LDA) for the exchange correlation functional are used during the QMD simulation. According to the paper\textsuperscript{39} the influence of the inner electrons on the thermodynamic properties becomes significant only at \( T_e \lesssim 80 \text{ kK} \). In this work \( T_e \leq 50 \text{ kK} \), so only three outer electrons were taken into account. The electronic structure is calculated for 1 k-point in the Brillouin zone (Γ-point) and energy cut-off \( E_{\text{cut}} = 100 \text{ eV} \). The number of bands is different for different temperatures. The number of bands is selected as described in\textsuperscript{39}. Every 100 steps the configuration (except for the initial configuration) is selected for the further calculation of the transport and optical properties.

During the precise resolution of the band structure the electronic structure is calculated with the same pair USPP, LDA, as during the QMD simulation. The energy cut-off is increased to \( E_{\text{cut}} = 200 \text{ eV} \). The higher number of bands, chosen as shown in\textsuperscript{39}, is used. As well as during the QMD simulation, Γ-point only is used.

The dynamic Onsager coefficients are calculated for the frequencies from 0.005 eV up to 10 eV with the step 0.005 eV. The optimal broadening of the δ-function in the Kubo-Greenwood formula \( \Delta E = 0.1 \text{ eV} \) was found\textsuperscript{39}. The static Onsager coefficients were calculated by the linear extrapolation of the dynamic coefficients to the zero frequency (see\textsuperscript{39} for details).

All the \((\rho,T_i,T_e)\) points in this work were calculated with the parameters specified above. The only exception are the points with \( T_e = 50 \text{ kK} \). They were calculated with 108 atoms while all other parameters were kept the same.

The error of the static electrical conductivity calculation was estimated as 20% for liquid aluminum at \( \rho = 2.249 \text{ g/cm}^3, T = 1273 \text{ K} \) in our previous paper\textsuperscript{39} by variation of the technical parameters of the method.

Our previous works\textsuperscript{39,47} contain the comparison of our calculation with the similar computations of other authors, experimental and reference data. The agreement of our data with other results was permanently good.

### IV. RESULTS AND DISCUSSION

#### A. The results of ab initio calculation

The calculations were performed for aluminum at normal density. The temperatures of electrons and ions were in the range from 3 kK up to 50 kK. Three basic types of the calculations were performed: 1) the equilibrium case with \( T_e = T_i \) varied from 3 kK up to 20 kK; 2) at fixed
ion temperature $T_i = 3$ kK with $T_e$ varied from 3 kK up to 20 kK; 3) at fixed electron temperature $T_e = 20$ kK with $T_i$ varied from 3 kK up to 20 kK. The variation of only one temperature with another one kept fixed makes possible to examine the influence of each temperature on transport and optical properties.

The frequency dependences of the real part of dynamic electrical conductivity for different temperatures are shown in Fig. 3a. All the curves have the Drude-like shapes.

In the equilibrium case (Fig. 1a) the curves change significantly as the temperature is varied. At a fixed low frequency (ω ≲ 1 eV) the conductivity decreases with temperature rise, at a high frequency (ω ≳ 2 eV)—increases.

If $T_i$ is kept fixed at 3 kK, the curves for different $T_e$ almost coincide (Fig. 1b).

The temperature dependences of the static electrical conductivity are shown in Fig. 2.

In Fig. 2a the electron temperature $T_e$ is varied. If it is changed together with the ion temperature, $T_i = T_e$, the conductivity decreases. But if $T_i$ is kept fixed at 3 kK, the conductivity changes not so drastically. For the temperatures from 3 kK up to 20 kK the conductivity remains almost constant.

In Fig. 2b, the ion temperature $T_i$ is varied. The equilibrium dependence $T_i = T_e$ is obviously the same as in Fig. 2a. If $T_e$ is kept fixed at 20 kK, and only $T_i$ is varied, the results almost coincide with the equilibrium data (Fig. 2b).

The temperature dependences of the thermal conductivity are shown in Fig. 4.

The dependences of the thermal conductivity on the electron temperature $T_e$ are shown in Fig. 3a. In the equilibrium case, $T_i = T_e$, the thermal conductivity increases as the temperature grows. In the non-equilibrium case $T_i$ is kept fixed at 3 kK, and thermal conductivity increases even more rapidly.

The dependences of the thermal conductivity on the ion temperature $T_i$ are shown in Fig. 3b. In the equilibrium case $T_e = T_i$ we have the same dependence as in Fig. 3a. If $T_e$ is kept fixed at 20 kK and $T_i$ is varied from 3 kK up to 20 kK, thermal conductivity decreases.

The dependences of the thermoelectric term on the electron temperature $T_e$ are shown in Fig. 5. In the equilibrium case, the contribution of the thermoelectric term grows as the temperature increases. If $T_i$ is kept fixed the thermoelectric contribution also increases as $T_e$ grows.

The dependences of the thermoelectric term on the ion temperature $T_i$ are shown in Fig. 3b. The equilibrium results in Fig. 3b are obviously the same as in Fig. 3a: the thermoelectric term increases with the temperature growth. If $T_e$ is kept fixed the thermoelectric term is almost independent on the ion temperature $T_i$.

If thermal conductivity and static electrical conductivity are known, the Wiedemann-Franz law may be checked. The Wiedemann-Franz law was discovered at rather low temperatures. At those conditions $T_e = T_i$ and $K ≈ L_{22}$: the law is presented in form (7). In our case $T_e$ and $T_i$ may differ; at rather high temperatures $K$ and $L_{22}$ differ also (Fig. 3b). Therefore, the question arises, what expression for the Lorenz number should be used. In this work we tested the expressions $K_{1DC}/T_e$ and $L_{22}/T_e$. The results for the Lorenz number are shown in Fig. 4.

The dependences of the Lorenz number on the electron temperature $T_e$ are shown in Fig. 4a. The Lorenz numbers for temperatures $T_e$ lower than 20 kK are close to the ideal value, both in equilibrium and non-equilibrium cases, both calculated using $L_{22}$ and $K$. The relative difference of all the points from the ideal value is within 9%. This is smaller than the estimated error calculation of about 20% (see section III and paper(24)). Thus we can conclude that the Wiedemann-Franz law is approximately valid for the points considered. The Lorenz numbers calculated using the $L_{22}$ coefficient seem to be closer to the ideal value (discrepancy not larger than 3%), than those calculated with $K$ (discrepancy not larger than 9%).

The dependences of the Lorenz number on the ion temperature $T_i$ are shown in Fig. 4b. All the points presented are close to the ideal value (the discrepancy less than the estimated error of calculation). The points calculated using $L_{22}$ values are closer to the ideal value (discrepancy not larger than 3%), than those calculated with $K$ (discrepancy not larger than 9%).

The results obtained lead us to the following conclusions for liquid aluminum at normal density for the temperatures 3 kK ≤ $T_i ≤ T_e ≤ 20$ kK.

The optical properties do not depend on $T_e$, but only on $T_i$. Particularly, in the equilibrium case the static electrical conductivity decreases as the temperature grows. And this decrease is entirely due to the $T_i$ growth. In the non-equilibrium case the static conductivity is fully determined by $T_i$.

The behavior of the thermal conductivity is determined by the behavior of the $L_{22}$ Onsager coefficient. The $L_{22}$ Onsager coefficient depends both on $T_e$ and $T_i$. The growth of $T_e$ leads to the increase of $L_{22}$, growth of $T_i$ leads to the decrease of $L_{22}$. Consequently, in the equilibrium case, we have the struggle of two opposite mechanisms. The influence of $T_e$ turns out to be more powerful and $L_{22}$ still increases as the temperature grows. In the non-equilibrium case with $T_e > T_i$, typical for the femtosecond laser heating, the thermal conductivity is larger than in the equilibrium case with the same $T_i$. The contribution of the thermoelectric term is rather small (the maximum relative contribution is 10% at $T_i = T_e = 20$ kK). The thermoelectric term does not depend on $T_i$ and increases with the growth of $T_e$.

The values of the Lorenz numbers calculated according to the formulas $K_{1DC}/T_e$ and $L_{22}/T_e$ are close to the ideal value (discrepancy lower than the calculation error). The values calculated using the $L_{22}$ value seem to be even closer to the ideal value than those calculated.
using thermal conductivity $K$.

Two points at normal density—$T_i = T_e = 50$ kK and $T_i = 3$ kK, $T_e = 50$ kK—were calculated for the temperatures larger than 20 kK. At these temperatures some of the conclusions drawn above become incorrect. The optical properties and static electrical conductivity start to depend on $T_e$ (Fig. 1b) and Fig. 2a). The thermoelectric term turns out to give significant contribution to the thermal conductivity (Fig. 3b). The Lorenz number becomes significantly different from the ideal value (Fig. 4b).

B. The construction of approximation

We have also built the approximation based on the results of our $ab$ *initio* calculation. The points with the temperatures $3$ kK $\leq T_i \leq 20$ kK were used for the construction of the approximation. The procedure was as follows.

First of all, the results on static electrical conductivity and the $L_{22}$ Onsager coefficient (Figs. 2-3) were plotted in the double logarithmic scale. In this scale all the dependences were successively fitted by the straight lines, both slope and intercept were adjusted. Hereafter all linear fits were performed by the "Fit Linear" option of the...

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Figure 1. (Color online) The frequency dependences of the real part of dynamic electrical conductivity for different temperatures. a) Equilibrium case $T_e = T_i$. b) Non-equilibrium case, $T_i$ is fixed at 3 kK.

Figure 2. (Color online) Temperature dependences of static electrical conductivity. a) Dependences on the electron temperature $T_e$. Squares—equilibrium case $T_i = T_e$; triangles—non-equilibrium case, $T_i = 3$ kK, $T_e$ is varied. Solid line—approximation (15) in equilibrium case, dashed line—approximation (15) at fixed $T_i = 3$ kK. b) Dependences on the ion temperature $T_i$. Squares—equilibrium case $T_i = T_e$; triangles—non-equilibrium case, $T_e = 20$ kK, $T_i$ is varied. Solid line—approximation (15) both for equilibrium and non-equilibrium cases.
Origin software. The slope of the line equals therefore the power $\alpha$ in the approximation $\propto T_{ei}^\alpha$. The following approximations were obtained:

$$\sigma_{1DC}(T)|_{T_{ei}=T_i} \propto T_i^{0.279},$$  \hspace{1cm} (8)

$$L_{22}(T)|_{T_{ei}=T_i} \propto T_i^{0.7420/2},$$  \hspace{1cm} (9)

$$L_{22}(T_{ei})|_{T_{ei}=3 \text{ kK}} \propto T_i^{0.986},$$  \hspace{1cm} (10)

$$L_{22}(T_i)|_{T_{ei}=20 \text{ kK}} \propto \frac{1}{T_i^{2.2418}}.$$  \hspace{1cm} (11)
The powers obtained are close to the values 0.25, 0.75, 1. This, together with the conclusions of the \textit{ab initio} calculations drawn in the previous subsection, brings to the mind the idea to test the following form of approximation:

\begin{align}
\sigma_{1DC}(T_i, T_e) &= \frac{A}{T_i^{0.25}}, \\
L_{22}(T_i, T_e) &= B \frac{T_e}{T_i^{0.25}}, \\
L &= \frac{L_{22}}{\sigma_{1DC} \cdot T_e} = \frac{B}{A}.
\end{align}

Here \(A\) and \(B\) are adjustable constants to be determined. It is worth noting, this form of approximation yields the correct Wiedemann-Franz law \((14)\).

The coefficients \(A\) and \(B\) were determined as follows. The \textit{ab initio} \(\sigma_{1DC}(T)|_{T_e=T_i}\) dependence was plotted in the double logarithmic scale and fitted by the straight line. Now the slope was set exactly to -0.25 and the intercept only was adjusted. The intercept yielded the \(A\) value. Then \(L_{22}(T_e)|_{T_i=3 \text{ kK}} \text{ \textit{ab initio}}\) dependence was plotted in double logarithmic scale and fitted by the straight line. The slope was set exactly to 1 and intercept was adjusted. The intercept yielded the \(B\) value, taking into account the ionic temperature of 3000 K.

Thus we come to the following approximation of the transport properties:

\begin{align}
\sigma_{1DC}(T_i, T_e) &= 2.844 \cdot 10^7 \frac{\Omega^{-1} \text{m}^{-1}}{(T_i[\text{K}])^{0.25}}, \\
L_{22}(T_i, T_e) &= 0.720 \cdot \frac{T_e}{(T_i[\text{K}])^{0.25}}, \\
L &= 2.533 \cdot 10^{-8} \left[\text{W m}^{-1} \text{K}^{-1}\right].
\end{align}

The comparison of the approximations with the \textit{ab initio} data is presented in Figs. (2) - (4). The comparison is to be performed only for the temperatures 3 kK \(\leq T_i \leq T_e \leq 20\) kK. The error of the static electrical conductivity approximation is not larger than 7\% (Fig. 2). The error of the thermal conductivity approximation is not larger than 5\% (Fig. 3). The discrepancy between the Lorenz numbers calculated using the \(L_{22}\) coefficient and the approximate value \((17)\) is not larger than 8\% (Fig. 4).

Thus the approximation rather well reproducing the transport properties was constructed. Only thermoelectric coefficients \(L_{12}\) and \(L_{21}\) and thermoelectrical contribution to the thermal conductivity were not described for the following reasons. The constructed approximation works well for the temperatures less than 20 kK. At those temperatures the thermoelectrical term is small, the precision of its calculation is low, and it can hardly be investigated properly (it is also not necessary due to its negligible contribution). At the temperatures higher than 20 kK the thermoelectrical term is evidently important (Fig. 5). But at those temperatures the current approximation is not valid and should be further reworked.

We have also extended the approximation to describe the optical properties.

The dynamic electrical conductivity was approximated by the Drude formula:

\[\sigma_1(\omega) = \frac{\sigma_{1DC}}{1 + \omega^2 \tau^2}.\]

The Drude formula was linearized:

\[\frac{1}{\sigma_1(\omega)} = \frac{1}{\sigma_{1DC}} + \frac{\tau^2}{\sigma_{1DC} \omega^2}.\]

The frequency dependences of the dynamic electrical conductivity for each temperature point 3 kK \(\leq T_i = T_e \leq 20\) kK were plotted in \(\frac{1}{\sigma_1(\omega)}\) vs. \(\omega^2\) plot. The \textit{ab initio} data were fitted by the straight line. The intercept was kept fixed at the values \(\frac{1}{\sigma_{1DC}}\), obtained previously by the linear extrapolation to zero frequency (see Section 11). The slope was adjusted to fit the \textit{ab initio} data. The effective relaxation time \(\tau\) was expressed via the slope of the fitting straight line. Thus we get a number of \(\tau(T)\) points.

The set of \(\tau(T)\) values along with the corresponding \(\sigma_{1DC}(T)\) values already provides an approximation. It enables the calculation of the dynamic electrical conductivity for the given temperature according to the formula \((13)\). The error of such an approximation is not larger than 9\% for all frequencies \(\omega \leq 10\) eV. However it is more convenient to approximate \(\tau(T)\) dependence by the smooth curve as it has been done previously for \(\sigma_{1DC}(T)\).

Having plotted \(\tau(T)\) in the double logarithmic scale and fitted it by straight line, we have received the approximation:

\[\tau(T)|_{T_i=T_e} \propto \frac{1}{T^{0.288}}.\]

This leads us to the idea to approximate \(\tau(T)\) dependence by the expression:

\[\tau(T)|_{T_i=T_e} = \frac{C}{T^{0.25}}.\]

This particular choice of the power of 0.25 possesses the following advantage. This power is the same as one in the approximation of the static electrical conductivity \((15)\). So \(\tau(T)\) and \(\sigma_{1DC}(T)\) become proportional to each other. This is natural for the Drude approach\(22\), where the ratio of \(\sigma_{1DC}(T)\) and \(\tau(T)\) is a constant (for a given density) connected with the plasma frequency:

\[\frac{\sigma_{1DC}(T)}{\tau(T)} = \omega_p^2 \varepsilon_0.\]

The latter formula is presented in SI units and \(\varepsilon_0\) is the dielectric permittivity of vacuum.

One more time the dependence \(\tau(T)\) was plotted in the double logarithmic scale. The points were fitted by the straight line. This time the slope was kept fixed at -0.25 and only the intercept was adjusted. This yielded
us the $C$ value. Thus we receive the approximation for the relaxation time $\tau$:

$$\tau [{\text{eV}}^{-1}] = \frac{7.876}{(T_i[\text{K}])^{0.25}},$$

and the final approximation for the dynamic electrical conductivity:

$$\sigma_1(T_i, T_e, \omega) [\Omega^{-1} \text{m}^{-1}] = \frac{2.844 \times 10^9}{(T_i[\text{K}])^{0.25}} \frac{7.876}{(T_i[\text{K}])^{0.25}} \left(\frac{\omega [\text{eV}]}{\omega [\text{eV}]}\right)^2.$$  

(24)

The approximation also gives the value of plasma frequency:

$$\omega_{pl} = 16.83 \text{ eV}.$$  

(25)

The discrepancy between the approximation and the results of the $ab$ initio calculation is not larger than 13% for all points at the normal density; 3 kK $\leq T_i \leq T_e \leq 20$ kK, $\omega \leq 10$ eV. The latter restrictions determine the region where the approximations (15)–(17), (23)–(25) are valid.

The example of the comparison of the $ab$ initio data with the approximation (24) is presented in Fig. 5. When the temperature is changed from 3 kK to 20 kK, at low frequencies the dynamic electrical conductivity increases almost by a factor of 2, at high ones—decreases by a factor of 2. The difference of the approximation from the $ab$ initio curves is not higher than 13% for all the temperatures and frequencies considered. So the error of approximation is significantly lower than the characteristic changes of the curves under temperature variation. This is an argument for the applicability of the approximation developed. The error of approximation is lower than the estimated error of our $ab$ initio calculation (see Section 1111 and paper 22), this also supports the approximation constructed.

C. Comparison with other models

1. The Drude model

The simplest model, frequently used for the description of two-temperature electrical and thermal conductivity is based on the Drude approach. The thermal conductivity is expressed via the volume-specific heat capacity $C_e$ and the electron relaxation time $\tau_e$.

$$K = \frac{1}{3} v_F^2 C_e \tau_e,$$  

(26)

where $v_F$ is the Fermi velocity. The static electrical conductivity is expressed via the electron relaxation time $\tau_e$ and electron concentration $n_e$:

$$\sigma_{1DC} = \frac{n_e e^2 \tau_e}{m_e},$$  

(27)

where $m_e$ and $e$ are the electron mass and charge, respectively.

The temperature dependence of the heat capacity is considered to be linear, $C_e = \gamma T_e$, that corresponds to the ideal Fermi-gas at $T_e \ll T_F$, $T_F$ is the Fermi temperature. Simplest assumptions are made for the electron relaxation time $\tau_e$: $1/\tau_e = 1/\tau_{e-ph} + 1/\tau_e$ ph, where $\tau_{e-ph}$ and $\tau_e$ ph are the electron-electron and electron-phonon relaxation times, respectively; their temperature dependencies are $1/\tau_{e-ph} = AT_i$ and $1/\tau_{e} = BT_e^2$ expressions are used to describe the temperature dependences of the relaxation times. The expression for $K$ is obtained:

$$K = \frac{1}{3} v_F^2 \frac{\gamma T_e}{AT_i + BT_e^2}. $$  

(28)

Here $A$ and $B$ are dimensional coefficients. The assumption $1/\tau_{e-ph} = AT_i$ is based on the linear dependence of the number of phonons on the ion temperature. The very concept of phonons is based on the idea of a solid phase and small displacements of atoms from their equilibrium positions. Expression (28) is used in the paper only for the crystalline phase and the temperatures slightly above melting. Also, paper claims that the term $1/\tau_{e-ph} = BT_e^2$ may be neglected for the temperatures significantly below the Fermi temperature.

We may obtain the similar expression for the static electrical conductivity:

$$\sigma_{1DC} = \frac{n_e e^2}{m_e} \frac{1}{AT_i + CT_e^2}. $$  

(29)

The electron-electron collisions in the latter expression are described by the term $CT_e^2$. The coefficient $C$ is smaller or equal than the coefficient $B$ in expression
This difference is introduced to take into account the probably different influences of the electron-electron collisions on thermal conductivity and electrical conductivity.

Expressions (28) and (29), with electron-electron collision term neglected, ensure the validity of the Wiedemann-Franz law in the form:

$$\frac{K}{\sigma_{1DC} \cdot T_e} = \text{const.}$$  \hspace{1cm} (30)

In this work we have performed ab initio calculations of static electrical conductivity and thermal conductivity and constructed the approximations based on the calculations. Therefore we may verify expressions (28). We work at $T_i$ significantly above melting, and $T_e$ significantly below the Fermi temperature $T_F$ (for aluminum at normal density it is about 135 kK, taking 3 electrons into account).

The statement on the negligibility of the $CT^2$ in (29) is proved by our data: the static electrical conductivity does not depend on $T_e$. In that case according to (29) $\sigma_{1DC}$ should be $\propto T_e^{-1}$. This is not proved by our data: $\sigma_{1DC}$ decreases slower, as $\propto T_e^{-0.25}$. We do not assign any physical meaning to our approximation (29), the coefficients and the powers of the approximation may be slightly different, but the lower rate of the $\sigma_{1DC}$ decrease is obvious. We have also tried to approximate our ab initio data by the expression $\sigma_{1DC} \propto \frac{1}{A \cdot T_e + \text{const}}$ with no result. Thus the expression (29) is not supported by our data.

The same conclusions may be drawn for the thermal conductivity, if the ratio $K/T_e$ is investigated and expression (28) is taken as a model for $K$.

Thus we have checked, that our ab initio data can not be described by the Drude model with these particular expressions for the relaxation times (28)–(29). However our data do not contradict to the Drude model (28)–(27) with expression (23) for the relaxation time. The electron concentration $n_e$ in (27) is connected with the atom concentration $n_a$:

$$n_e = Z n_a = Z^2 \frac{\rho}{\mu} N_A.$$  \hspace{1cm} (31)

Here $\rho$ is the density of material (normal density of aluminum is 2.70 g/cm$^3$), $\mu$ is its molar mass (26.98 g/mol for aluminum), $N_A$ is the Avogadro constant. The ion charge $Z$ is taken to be 3. The volume-specific heat capacity at constant volume $C_v$ in (28) is calculated via the low-temperature asymptotic formula for the degenerate ideal Fermi-gas:

$$C_v = \left(\frac{\pi}{3} \right)^{2/3} \frac{m_e}{h^2} k_B n_e^{1/3} T_e.$$  \hspace{1cm} (32)

Here $k_B$ is the Boltzmann constant, $h$ is the reduced Planck constant. The square of the Fermi velocity $v_F^2$ in (20) is calculated for the ideal Fermi gas at zero temperature:

$$v_F^2 = \frac{E_F}{2m_e} = \frac{k^2}{4m_e^2} \left(3\pi^2\right)^{2/3} n_e^{2/3}.$$  \hspace{1cm} (33)

The results of the comparison of the ab initio data with the results of the Drude model, $Z = 3$. Squares—ab initio data, equilibrium case, $T_i = T_e$; triangles—ab initio data, non-equilibrium case, $T_i = 3$ kK. Solid line—the Drude model, equilibrium case, $T_i = T_e$; dashed line—non-equilibrium case, $T_i = 3$ kK. a) Static electrical conductivity. b) The $L_{22}$ Onsager coefficient.

Figure 6. (Color online) The comparison of the ab initio data with the results of the Drude model, $Z = 3$. Squares—ab initio data, equilibrium case, $T_i = T_e$; triangles—ab initio data, non-equilibrium case, $T_i = 3$ kK. Solid line—the Drude model, equilibrium case, $T_i = T_e$; dashed line—non-equilibrium case, $T_i = 3$ kK. a) Static electrical conductivity. b) The $L_{22}$ Onsager coefficient.
The effective charge $Z_{\text{eff}}$ may be calculated by the formula:

$$Z_{\text{eff}} = \frac{\omega_{\text{pl}}^2}{m_e c^2} \sqrt{\frac{e}{m_e^*}}.$$  \hfill (34)

The calculation yields $Z_{\text{eff}} = 3.23$. If the Drude model is calculated with this effective charge, we immediately receive the approximation \(^{(15)}\) for static electrical conductivity and better agreement with the ab initio data (compare Fig. 2 and Fig. 9). It is also worth noting, that $Z_{\text{eff}} = 3.23$ value is not that far from 3.

The results on the $L_{22}$ Onsager coefficient are shown in Fig. 6b. The derivation of the Drude expression \(^{(20)}\) presented in \(^{(22)}\) neglects the thermoelectric terms. Consequently it is more correct to use $L_{22}$ ab initio values rather than $K$ for the comparison with the Drude model.

Thus the results of the ab initio calculation may be satisfactorily described by the Drude model, but the frequency of the electron-ion collisions should not grow $\propto T_i$. The rate of its growth should be smaller, in this work it was approximated as $\propto T_i^{0.25}$.

2. The Anisimov model

Another analytical model, describing the two-temperature thermal conductivity was proposed in paper \(^{(49)}\):

$$K = C \frac{(t_e^2 + 0.16)^{3/4}(t_e^2 + 0.44)}{(t_e^2 + 0.092)^{1/2}} \frac{t_e}{\beta t_i + t_e^2},$$  \hfill (35)

where $t_e = T_e/T_F$ and $t_i = T_i/T_F$ are the dimensionless temperatures of electrons and ions, respectively. $C$ and $\beta$ coefficients may be derived from experimental data. The density dependence is accounted by the $T_F(\rho)$. Hereafter the model \(^{(35)}\) will be called the Anisimov model. This model gives the correct high-temperature Spitzer asymptotics $K \propto T_e^{5/2}$ for $T_e \gg T_F$. In this work, however, we will consider the Anisimov model only at low temperatures $T_i \leq T_e \ll T_F$.

The coefficients $C = 770$ W m$^{-1}$K$^{-1}$ and $\beta = 1.2$ are presented in paper \(^{(50)}\). The coefficient $C$ was chosen to obtain the correct experimental value of thermal conductivity at $T_i = T_e = 1$ kK. In our previous work \(^{(22)}\) we achieved good agreement with the experiment at $\rho = 2.35$ g/cm$^3$, $T_i = T_e = 1$ kK. So in these conditions the results of the Anisimov model are close to ours.

In Fig. 7 we present the comparison of our results with the Anisimov model in equilibrium (Fig. 7a) and non-equilibrium (Fig. 7b) cases. It should be mentioned that at $T_e < 20$ kK the first factor in \(^{(35)}\) is almost constant, and all the changes in the thermal conductivity may be described by the reduced expression:

$$K = C \frac{0.16^{3/4} \cdot 0.44}{0.092^{1/2}} \frac{t_e}{\beta t_i + t_e^2}. $$  \hfill (36)

Figure 7. (Color online) Comparison of the ab initio data on the thermal conductivity with the Anisimov model. Squares—ab initio data. Solid line—the Anisimov model \(^{(35)}\), dashed line—the reduced Anisimov model \(^{(36)}\). a) Equilibrium case $T_i = T_e$. b) Non-equilibrium case $T_i = 3$ kK.

This reduced expression is simply the Drude model in the form \(^{(25)}\). As before the term $\beta t_i$ in the denominator is due to the electron-phonon collisions, the term $t_e^2$—due to the electron-electron ones. The results of the calculation both according to the full \(^{(35)}\) and reduced \(^{(36)}\) expressions are shown in Fig. 7.

In the equilibrium case (Fig. 7a) the reduced expression yields the values almost equal to that at $T_i = T_e = 1$ kK. The electron-phonon collisions significantly dominate electron-electron collisions in \(^{(36)}\) (their contributions become equal only at $T_i = T_e = 162$ kK). Thus we have $\propto T_e/T_i$ dependence that in the equilibrium case yields the constant thermal conductivity. The constant temperature behavior of the thermal conductivity is a characteristic of the crystalline phase \(^{(25)}\). The Anisimov model shows this behavior even at very high tempera-
tures. Our calculations give the different, increasing dependence. Particularly, at $T_i = T_e = 3$ kK our values significantly exceed the results of the Anisimov model.

In the non-equilibrium case our dependences also differ significantly. Already at $T_i = T_e = 3$ kK our results are significantly higher due to the reasons mentioned above. At constant $T_i = 3$ kK at first the Anisimov model gives the curve that increases $\propto T_e$. Our dependence also has $\propto T_e$ shape, though the slope is different. But already at 22 kK the contributions of the electron-phonon and electron-electron collisions in (35) become equal. The term $t^2_e$ in the denominator prevents the Anisimov curve from further increase.

Thus the differences between our results and the Anisimov model are due to the following two reasons. Firstly, the Anisimov model at low temperatures has the dependence $\propto T_e$, whereas we predict different behavior, $\propto T_i/T_e^{0.25}$. Secondly, in the non-equilibrium case in the Anisimov model the electron-electron collisions become significant already at rather moderate $T_e$ (of about 20 kK).

3. The Inogamov-Petrov model

We have also compared our results with the Inogamov-Petrov model. This approach yields the wide-range expression $K^{WR}_{sum}$ for the thermal conductivity, valid for $T_i, T_e \lesssim 330$ kK. It is an interpolation between the condensed matter expression $K^{pl}_{sum}$ and the plasma one $K^{pl}_{sum}$.

The plasma expression is obtained from the Spitzer theory. The contribution of $K^{pl}_{sum}$ to $K^{WR}_{sum}$ is negligible for the temperature region $T_i \leq T_e \leq 50$ kK considered in our work. Thus, we assume $K^{WR}_{sum} \approx K^{pl}_{sum}$.

The condensed matter expression $K^{c}_{sum}$ is composed of the electron-electron contribution $K^{ee}_{c}$ and the electron-ion one $K^{ei}_{c}$ according to the formula:

$$\frac{1}{K^{c}_{sum}} = \frac{1}{K^{ee}_{c}} + \frac{1}{K^{ei}_{c}}$$

(37)

The electron-electron contribution $K^{ee}_{c}$ in the Inogamov-Petrov paper is calculated by solving of the linearized Boltzmann equation, with the $\tau$-approximation for the collision term. To compute the energy dependent electron-electron relaxation time $\tau_{ee}(\epsilon)$ the scattering of all free electrons on each other is considered. The electrons are supposed to interact via the screened Coulomb potential, with the Thomas-Fermi length as the screening radius. In the most of similar works the strongly degenerate case only is considered, and only the collisions of the electrons close to the Fermi sphere are taken into account. In the Inogamov-Petrov work the electrons, far from the Fermi sphere are also taken into account. After $K^{ee}_{c}$ is obtained, the integral electron-electron relaxation time $\tau_{ee}^{c}$ may be calculated according to the Drude expression (20) with the ideal gas expressions (22) and (33) for $C_e$ and $v^2_F$, respectively.

In the Inogamov-Petrov work the electron-electron relaxation time $\tau_{ee}^{c}(T_e)$ depends on $T_e$ only. At low temperatures $\tau_{ee}^{c}(T_e)$ has the common $\sim T_e^{-2}$ asymptotics. At high enough temperatures $T_e \gtrsim 10$ kK it decreases slower than $\sim T_e^{-2}$ with the temperature growth. The calculation of the $K^{ee}_{c}$ term is the main contribution of the Inogamov-Petrov work.

To describe the electron-ion term $K^{ei}_{c}$ Inogamov and Petrov involve the results of the ab initio calculation. Ab initio data are approximated by the Drude expression (23) with ideal gas expressions (22) and (33) for $C_e$ and $v^2_F$, respectively. The semiempirical formula

$$\tau_{ei}^{c}(T_i) = \frac{A + BT_i - \frac{C}{T}}{DT_i}$$

(38)

is used to approximate the electron-ion relaxation time $\tau_{ei}^{c}(T_i)$ which depends only on $T_i$. Here $A$, $B$, $C$ and $D$ are dimensional coefficients. The expression different from the common expression $\sim T_i^{-1}$ is used: the $BT_i$ term in the numerator of (35) prevents $\tau_{ei}^{c}(T_i)$ from the too fast $\sim T_i^{-1}$ decrease. Ab initio calculations provide results for aluminum at $\rho = 2.35$ g/cm$^3$ and 1 kK $\leq T_i \leq 10$ kK.

The comparison of our results with the Inogamov-Petrov model is presented in Fig. 8. Since Inogamov and Petrov do not take the thermoelectric term into account, our results on the $L_{22}$ Onsager coefficient are presented. The comparison will be performed for 3 kK $\leq T_i \leq T_e \leq 20$ kK.

Fig. 8h shows the results in the equilibrium case $T_i = T_e$.

Since the $K^{ei}_{c}$ data in the Inogamov-Petrov model is based on the ab initio calculation, it should, in principle, coincide with our results. However the discrepancy is present. Both our and $K^{ei}_{c}$ data are well approximated by the $\sim T^{0.75} \kappa$ dependence; the difference is by a constant factor of approximately 1.4. The sources of this discrepancy are easily found. Our results for the density 2.35 g/cm$^3$ are larger than the corresponding values of Rechouds by a factor of approximately 1.15. This discrepancy is most probably due to the used technical parameters (discussed in our previous work). The approach of Inogamov and Petrov also neglects the difference connected with the change of density from 2.35 g/cm$^3$ to 2.70 g/cm$^3$. This change of the density increases thermal conductivity approximately by a factor 1.21. The product of 1.15 and 1.2 yields the resulting factor 1.4 of the discrepancy between our results and $K^{ei}_{c}$ data of Inogamov and Petrov. However, this is not crucial, because the $K^{ei}_{c}$ data may be adjusted to reproduce our results.

The contribution of electron-electron collisions may be estimated if we compare $K^{ei}_{c}$ data with $K^{c}_{sum}$ (Fig. 8c). At $T_i = T_e = 10$ kK $K^{ei}_{c}$ is 10% lower than $K^{c}_{sum}$; at $T_i = T_e = 20$ kK--24% lower.

The results in the non-equilibrium case $T_i = 3$ kK are similar (Fig. 8h).
Both our results and $K_{ei}^c$ data are well approximated by the $\sim T_e$ dependence; the difference by a constant factor of approximately 1.35 is present (Fig. 8(b)). The reasons of this difference are the same as mentioned above for the equilibrium case.

At $T_e = 10$ kK $K_{sum}^c$ is 15% lower than $K_{ei}^c$; at $T_e = 20$ kK—35% lower (Fig. 8(b)). If the ion temperature is kept fixed, the influence of the electron-electron collisions is even larger than in the equilibrium case. This may be easily explained. The total relaxation time is determined according to the inverse summation law $1/\tau = 1/\tau_{ei} + 1/\tau_{ee}$. According to this law the total relaxation time is mainly determined by the smallest of the relaxation times. If $T_i$ is kept fixed and $T_e$ is increased, $\tau_{ei}$ remains constant, but $\tau_{ee}$ decreases and soon starts to dominate in the total thermal conductivity. In the equilibrium case both $\tau_{ei}$ and $\tau_{ee}$ decrease simultaneously, and the role of $\tau_{ee}$ in the total thermal conductivity is less.

The comparison with the Inogamov-Petrov model brings us to following conclusions. Similar to our work, the Inogamov-Petrov model has the expression for $\tau_{ei}$, that decreases with the temperature growth slower than $\sim T_i^{-1}$. Though the expression of $K_{ei}^{Coulomb}$ differs from ours, it gives the correct temperature dependences of the thermal conductivity (neglecting the electromagnetic term). Some quantitative discrepancies of $K_{ei}^c$ with our work may be removed by the adjustment of the Inogamov-Petrov model. The contribution of the electron-electron collisions, calculated in [18], turns out to be significant, especially in the non-equilibrium case.

4. The Lee-More model

We have also compared our results with the well-known model of Lee and More [18]. It is based on the kinetic Boltzmann equation for the free electrons. The interaction of electrons with ions is described by the collision term in the approximation of the relaxation time $\tau$, which is defined differently for plasma and liquid. The electron-electron collisions are neglected.

Two different approaches for plasma exist.

In the first plasma approach the Thomas-Fermi potential of ions is calculated. Then the phase shifts and $\tau_c(\epsilon)$ are obtained from the numerical solution of the Schrödinger equation with this potential. The results obtained by this method are depicted by separate points in Fig. 9, and marked with the label ”phase shift”. The usage of the Thomas-Fermi theory restricts the field of this method by rather high temperatures only.

In the second plasma approach the ion potential is considered to be the Coulomb one with upper and lower cutoffs which depend on the temperatures of electrons and ions and their concentrations. The degeneracy and strong coupling effects are taken into account by choosing appropriate cutoffs. In the second plasma approach the electrical and thermal conductivities are expressed by the integrals over analytic functions. The results obtained by this method are depicted by the solid line in Fig. 9, and marked with the label ”Coulomb with cutoffs”.

In the liquid case the electron gas is degenerate, the model is reduced to the simple Drude expressions [20]-[22] with [23] expressions for the heat capacity and the square of the Fermi velocity. Also unlike the plasma case in the liquid case the ionic structure factor $S(q)$ is different from unity, therefore the coherent scattering of electrons on ions should be taken into account. Lee and More do not go deep into the investigation of this...
matter and adopt the Bloch-Grüneisen expression $\tau_c \propto T_i^{-1}$. Moreover, some approximate theories, based on the Lindemann melting criterion, are involved to calculate the coefficient in the Bloch-Grüneisen expression.

The liquid and plasma approaches are conjugated in the intermediate region.

The comparison of our \textit{ab initio} results with the Lee-More model is presented in Fig. 9. Though the Lee-More model allows different temperatures of electrons and ions, only equilibrium curves $T_e = T_i$ are available in the paper\textsuperscript{21}. The Lee-More results are available for the density $2.5$ g/cm$^3$. We did not perform calculation for that particular density, but our data for the surrounding densities $2.35$ g/cm$^3$ and $2.70$ g/cm$^3$ are available.

The results on the static electrical conductivity are shown in Fig. 9a. At high temperatures the Lee-More model yields the results consistent with the Spitzer theory. At temperature lowering the Spitzer results decrease rapidly. The Lee-More model demonstrates the slower decrease of the electrical conductivity. Though the treatment of the non-ideal plasma within the Lee-More model is approximate, this behavior, different from the Spitzer results is the important feature of this model. The Lee-More transport coefficients from the phase shift calculation are consistent with the results obtained using the Coulomb potential with cutoffs (Fig. 9). At low temperatures the Lee-More model reduces to the Drude model with the electron-ion relaxation time $\propto T_i^{-1}$. So when the temperature increases, $\sigma_{\text{loc}}$ decreases faster than our results, approximately described by expression (18). The inconsistency of our values with those of Lee-More may also be explained by the inaccurate coefficient used by Lee and More in the Bloch-Grüneisen expression. The two branches of the Lee-More model, low-temperature and high-temperature, yield the minimum of the static electrical conductivity. In this region some approximation is used for the electron-ion relaxation time, and, therefore the position of the minimum is inaccurate. However, the very existence of this minimum and the construction of the wide range model are the significant advantages of the Lee-More work.

The results on the thermal conductivity are shown in Fig. 9b. Again at high temperatures the Lee-More model is consistent with the Spitzer model. At lower temperatures the two methods of Lee-More yield consistent results slightly different from the Spitzer model. At low temperatures the thermal conductivity increases as the temperature grows. The rate of this increase is smaller than that of our \textit{ab initio} data. Again this is explained by the electron-ion relaxation time $\propto T_i^{-1}$. In fact this behavior of the Lee-More model is similar to the constant behavior demonstrated by the Anisimov model (see Fig. 7).

5. The Apfelbaum model

We have also compared our results with the Apfelbaum model\textsuperscript{21,52}.

As well as the Lee-More model the Apfelbaum calculation of transport properties is based on the kinetic Boltzmann equation with the collision term in the approximation of relaxation time.

Unlike the Lee-More model, where electron-electron collisions are neglected, in the Apfelbaum model they are taken into account by the introduction of the so-called generalized Spitzer factor\textsuperscript{21}.

The Lee-More model considers some average ionization
The wide-range approximations of the transport and optical properties are commonly built to combine the results of different models in the form applicable for practical use. The Povarnitsyn et al. model is the example of such an approximation.

At temperatures, significantly lower than the Fermi one, the thermal conductivity in the Povarnitsyn model is calculated according to the Drude expression. At temperatures above melting, the relaxation time $\tau_e$ is calculated according to the common expression $1/\tau_e = AT_i + BT_i^2$. This relaxation time decreases if $T_i$ and $T_e$ grow. However, some minimal relaxation time $\tau_{min}$, is introduced. Here $v_F$ is the Fermi velocity, $r_0$ is the average interatomic distance, $C$ is the dimensionless constant. If $1/(AT_i + BT_i^2) < \tau_{min}$ the relaxation time is set to $\tau_{min}$ which is almost independent of the temperatures at $T_i, T_e < 50$ kK.

At the temperatures comparable with the Fermi one the Drude dependence is damped exponentially and the Spitzer expression is smoothly switched on.

The Povarnitsyn model contains parameters which may be adjusted to fit the results of different calculations. The results of the Povarnitsyn model, together with discussed already Inogamov-Petrov, Apfelbaum models and ab initio data of this work are presented in Fig. 10.

At rather low temperatures in the equilibrium case $AT \gg BT^2$ and the Povarnitsyn model yields the constant behavior, characteristic of the crystalline phase (Fig. 10). This is not supported by our results and was discussed previously in connection with the Anisimov model. However, already starting from the temperature $T = 5$ kK the relaxation time is kept fixed at $\tau_{min}$ and, therefore, the thermal conductivity exhibits $T$ behavior. Our approximation in the equilibrium case yields $T^{0.75}$ behavior. Nevertheless, the linear growth of the Povarnitsyn model is better than the constant behavior. At higher temperatures we see the smooth transition from the metallic Drude behavior to the Spitzer $T^{5/2}$ behavior. The high temperature branch of the Povarnitsyn approximation reproduces well the Apfelbaum results.

In the double logarithmic scale the Povarnitsyn wide-range model well reproduces the results of all works depicted in Fig. 10

6. The wide-range Povarnitsyn expression

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V. CONCLUSIONS

1. We have performed ab initio calculations of optical properties, static electrical and thermal conductivities of liquid aluminum in the two-temperature regime.

2. Based on the results of ab initio calculations we have built the semiempirical approximation of static electrical and thermal conductivities, and optical properties. The approximation is valid for liquid aluminum at normal density $\rho = 2.70$ g/cm$^3$, 3 kK $\leq T_i \leq T_e \leq 20$ kK.

3. We have found out that our results are well described by the Drude model if $\tau \propto T_i^{-0.25}$ expres-
4. The models we have considered are all reduced at low temperatures to the Drake model with different expressions for the relaxation time. Ivanov, Anisimov and Lee-More models use a crystallinelike $\tau \propto T^{-1}$ expressions which are not consistent with our results. Inogamov-Petrov and Povarnitsyn models use the expressions that decline slower than $\propto T^{-1}$ with the temperature rise in agreement with our ab initio data.

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