Supplemental material to the article

"Transport Processes in Metal with Hot Electrons Excited by Laser Pulse"

1. Partial contributions to thermal resistance. As it was pointed out in the main text, energy transport in the d-metals is connected mainly with s-electrons. Dominating contribution to thermal resistance make si, ss, and sd interactions. Collision frequency of an s-electron is equal to $\nu = \nu_{si} + \nu_{se} = \nu_{si} + \nu_{ss} + \nu_{sd}$. This relation follows from the Matthiessen's summation rule for the thermal resistances $S = \kappa^{-1} = \kappa_{si}^{-1} + \kappa_{se}^{-1}$. At the same time, the electron-electron contribution is $S_{se} = \kappa_{ss}^{-1} + \kappa_{sd}^{-1}$, where κ is the electron thermal conductivity. Below we consider first the se-interaction and then the si-interaction. Sum total of these two contributions results in the graphs presented in Fig. 5 of the main text.

2. General expressions for electron-electron collision frequency. The resistance S_{se} is determined by the electron-electron collision frequency. Consider a collision of s-electron having momentum $\mathbf{p}$ with electron having momentum $\mathbf{p}'$: $\mathbf{p}+\mathbf{p}' \to (\mathbf{p}+\mathbf{q})+(\mathbf{p}'-\mathbf{q})$. Here $\mathbf{q}$ is the transmitted momentum. Collision frequency of an s-electron possessing the momentum $\mathbf{p}$ with s- or d-electrons equals

$$\nu(\mathbf{p}) = \frac{2\pi}{\hbar} \int |U_{\mathbf{q}}|^2 \frac{d^3q}{(2\pi\hbar)^3} \int \frac{2d^3p'}{(2\pi\hbar)^3} \, \Phi \, \delta, \tag{1}$$

where $U_{\mathbf{q}} = 4\pi e^2\hbar^2/[q^2\,\epsilon(\mathbf{q})]$ is the matrix element of screened electron-electron interaction and $\epsilon(\mathbf{q})$ is the dielectric constant. In Thomas–Fermi approximation: $\epsilon(\mathbf{q}) = [1 + K^2\,\hbar^2/q^2]^{-1}$, where the screening constant is $K = K(T_e, x)$, and ρ/ρ_0 is the nondimensional density. Correspondingly, the matrix element in (1) takes the form $U_{\mathbf{q}} = 4\pi\, e^2\,\hbar^2/[q^2 + K^2\hbar^2]$.

The factor Φ in (1) is linked to the statistical properties. It depends on the distribution functions of s- and d-electrons. In the ss- and sd-cases we have, respectively:

$$\Phi(\mathbf{p}, \mathbf{p}', \mathbf{q}) = f_s(\mathbf{p}')[1 - f_s(\mathbf{p}+\mathbf{q})][1 - f_s(\mathbf{p}'-\mathbf{q})] +$$

$$+ f_s(\mathbf{p}+\mathbf{q}) f_s(\mathbf{p}'-\mathbf{q})[1 - f_s(\mathbf{p}'-\mathbf{q})],$$

$$\Phi(\mathbf{p},\mathbf{p}',\mathbf{q}) = f_d(\mathbf{p}')[1-f_s(\mathbf{p}+\mathbf{q})][1-f_d(\mathbf{p}'-\mathbf{q})]+$$
$$+ f_s(\mathbf{p}+\mathbf{q})f_d(\mathbf{p}'-\mathbf{q})[1-f_d(\mathbf{p}')],$$

where f_s and f_d are the Fermi distribution functions of s- and d-electrons. In what follows we will consider the sd case only since the ss-collisions were described in [7] of main text.

Delta function

$$\delta = \delta[\varepsilon(\mathbf{p}) + \varepsilon'(\mathbf{p}') - \varepsilon(\mathbf{p}+\mathbf{q}) - \varepsilon'(\mathbf{p}'-\mathbf{q})]$$

in (1) is the energy conservation law.

3. Simplification of the sixfold integral. In our calculations two-parabolic approximation of the electronic spectrum obtained from the DFT simulation (see Ref. [32] in main text) is used. This makes it possible to reduce the order of integration in (1) from six to two. The law of energy conservation for two-parabolic spectrum says:

$$\varepsilon_s + \frac{(\mathbf{p}+\mathbf{q})^2}{2m_s} + \varepsilon_1 + \frac{(\mathbf{p}'-\mathbf{q})^2}{2m_d} = \varepsilon_s + \frac{\mathbf{p}^2}{2m_s} + \varepsilon_1 + \frac{\mathbf{p}'^2}{2m_d},$$

where ε_s, ε_1, ε_2 are the bottom of the s-band, the upper and the lower edges of the d-band, respectively, counted from the Fermi level; see the main text, where the letter E is used in place of ε used here. Let us denote

$$\alpha = \frac{\mathbf{p}^2}{2m_s} - \frac{(\mathbf{p}+\mathbf{q})^2}{2m_s}, \quad \beta = \frac{(\mathbf{p}'-\mathbf{q})^2}{2m_d} - \frac{\mathbf{p}'^2}{2m_d},$$

and $\varepsilon = \mathbf{p}^2/2m_s$, $\varepsilon' = \mathbf{p}'^2/2m_d$. Performing calculations, we obtain the statistical factor for sd-scattering in the following form

$$\Phi(\varepsilon,\varepsilon',\alpha,\beta) = f_d(\varepsilon')[1-f_s(\varepsilon-\alpha)][1-f_d(\varepsilon'+\beta)] +$$
$$+ f_s(\varepsilon-\alpha)f_d(\varepsilon'+\beta))][1-f_d(\varepsilon')],$$

where the Fermi-functions of s- and d-electrons are

$$f_s \equiv f(\varepsilon_s,\varepsilon,\mu,T_e) = [\exp\left(\frac{\varepsilon_s+\varepsilon-\mu}{k_BT_e}\right)+1]^{-1},$$

$f_d = f(\varepsilon_1, \varepsilon', \mu, T_e)$. Substituting the distributions f into Φ, one obtains

$$\Phi(\varepsilon, \varepsilon', \alpha, \beta) = \frac{\exp\left(\frac{\varepsilon_1+\varepsilon'-\mu}{k_B T_e}\right)}{\exp\left(\frac{\varepsilon_s+\varepsilon-\alpha-\mu}{k_B T_e}\right)+1} \times$$

$$\times \frac{\exp\left(\frac{\varepsilon_s+\varepsilon+\beta-\alpha-\mu}{k_B T_e}\right)+1}{\left(\exp\left(\frac{\varepsilon_1+\varepsilon'+\beta-\mu}{k_B T_e}\right)+1\right)\left(\exp\left(\frac{\varepsilon_1+\varepsilon'-\mu}{k_B T_e}\right)+1\right)}.$$

With this result, the delta function of energy conservation in (1) is simplified to $\delta(\alpha-\beta)$. The collision frequency of s-electron having momentum $\mathbf{p}$, with d-electrons can be presented by the integral

$$\nu(p) = \frac{2\pi}{\hbar}\int\left(\frac{4\pi e^2\hbar^2}{q^2+\kappa^2(T_e,x)\hbar^2}\right)^2 \frac{d^3q}{(2\pi\hbar)^3} \times$$

$$\times \int \Phi(\varepsilon, \varepsilon', \alpha, \beta)\delta(\alpha-\beta)\frac{d^3p'}{(2\pi\hbar)^3}. \qquad (2)$$

The six-fold integral appearing in (2) can be reduced to the two-fold one. This permits to construct a computer code for calculation of thermal conductivity using the system Mathematica. The convenience of such code lies in the fact that it permits to vary initial parameters, screenings and temperature T_e and thus to estimate significance of such variations.

4. Reduction of the integration order. Let's introduce the polar angle θ and the azimuthal angle ϕ of the vector of the transmitted momentum $\mathbf{q}$. Let's take that the angle between $\mathbf{p}$ and $\mathbf{q}$ is the angle θ. Then upon integrating with respect to the azimuthal angle ϕ from 0 to 2π we obtain $d^3q = 2\pi\, q^2\, dq\, dt$ $(t = -\cos\theta)$. In accepted variables we have

$$\alpha = (2\,p\,q\,t - q^2)/2m_s, \quad dt = (m_s/p\,q)\,d\alpha. \qquad (3)$$

The integral with respect to α is calculated from $-(2p\,q+q^2)/(2m_s)$ to $(2p\,q-q^2)/(2m_s)$.

Further let us introduce, for given $\mathbf{q}$, the polar angle θ' and the azimuthal angle ϕ' of the vector $\mathbf{p}'$. The angle θ' is the angle between the vectors $\mathbf{p}'$ and $\mathbf{q}$. Hence

$d^3p' = 2\pi\, p'^2\, dp'\, dt'$ $(t' = -\cos\theta')$, and

$$\beta = (2p'\, q\, t' + q^2)/(2m_d), \quad dt' = (m_d/p'\, q)\, d\beta. \tag{4}$$

Using substitutions (3), (4), the part

$$\frac{d^3q}{(2\pi\hbar)^3}\frac{2d^3p'}{(2\pi\hbar)^3}\Phi(\varepsilon,\varepsilon',\alpha,\beta)\delta(\alpha-\beta)$$

of the integrand for $\nu(p)$ in (2) can be transformed to the form

$$\frac{dq}{(2\pi\hbar)^3}\frac{2dp'}{(2\pi\hbar)^3}\times$$

$$\times\,\frac{2\pi m_s}{p}\,2\pi\, m_d\, p'\,\Phi(\varepsilon,\varepsilon',\alpha,\beta)\,\delta(\alpha-\beta)\,d\alpha\,d\beta. \tag{5}$$

After integration of (5) over β we obtain

$$\frac{dq}{(2\pi\hbar)^3}\frac{2dp'}{(2\pi\hbar)^3}\frac{2\pi m_s}{p}\,2\pi\, m_d\, p'\,\Phi(\varepsilon,\varepsilon',\alpha)\,d\alpha, \tag{6}$$

where the statistical factor is

$$\Phi(\varepsilon,\varepsilon',\alpha) = \frac{\exp\left(\frac{\varepsilon_1+\varepsilon'-\mu}{k_BT_e}\right)}{\exp\left(\frac{\varepsilon_1+\varepsilon'-\alpha-\mu}{k_BT_e}\right)+1}\times$$

$$\times\,\frac{\exp\left(\frac{\varepsilon_s+\varepsilon-\mu}{k_BT_e}\right)+1}{\left[\exp\left(\frac{\varepsilon_s+\varepsilon-\alpha-\mu}{k_BT_e}\right)+1\right]\left[\exp\left(\frac{\varepsilon_1+\varepsilon'+\alpha-\mu}{k_BT_e}\right)+1\right]}.$$

It is significant that the indefinite integral (6) with respect to α is integrated analytically

$$\int\Phi(\varepsilon,\varepsilon',\alpha)\,d\alpha = \frac{\exp\left(\frac{\varepsilon_s+\varepsilon-\mu}{k_BT_e}\right)+1}{\exp\left(\frac{\mu-\varepsilon_1-\varepsilon'}{k_BT_e}\right)+1}\times$$

$$\times\,\frac{k_BT_e}{\exp\left(\frac{\varepsilon_s+\varepsilon-\mu}{k_BT_e}\right)\exp\left(\frac{\varepsilon_1+\varepsilon'-\mu}{k_BT_e}\right)-1}\times$$

$$\times \ln \frac{\exp\left(\frac{\alpha}{k_B T_e}\right) + \exp\left(\frac{\mu-\varepsilon_1-\varepsilon'}{k_B T_e}\right)}{\exp\left(\frac{\alpha}{k_B T_e}\right) + \exp\left(\frac{\varepsilon_s+\varepsilon-\mu}{k_B T_e}\right)}\Bigg|_{\alpha_1}^{\alpha_2}.$$

The limits of integration, α_1 and α_2, are determined from the restrictions imposed by sd→sd scattering and by a non-zero result of integration of (5) with respect to β. The integration (5) contains δ-function. The sd→sd scattering is restricted upon the value of the quantity $\varepsilon_1 + (\mathbf{p}' - \mathbf{q})^2/(2m_d)$. This quantity must belong to the interval $[\varepsilon_1, \varepsilon_2]$. This restriction is

$$0 \le \frac{p'^2 + 2p'\,q\,t' + q^2}{2m_d} \le \varepsilon_2 - \varepsilon_1.$$

Here $\varepsilon_2 - \varepsilon_1$ is the width of d-band. Denominating $p_d = \sqrt{2m_d(\varepsilon_2 - \varepsilon_1)}$ – the borderline momentum of d-electron, we obtain the limits $p \le p_d$ and $p'^2 + 2p'\,q\,t' + q^2 \le p_d^2$. These expressions bound the value $t' : t' \le t_0(p', q) = (p_d^2 - p'^2 - q^2)/(2p'\,q)$.

Depending on the position of point t_0 relative to the interval $[-1,\ 1]$ two situations are possible:

In the case 1 we have $t_0 > 1$. In this case the variable t' runs across whole interval $[-1, 1]$.

In the case 2 we have $-1 \le t_0 \le 1$, then t' is bounded between the limits: $-1 \le t' \le t_0$.

Corresponding intervals of integration with respect to β follow from (4). Considering now all options of integration with respect to β in (5) with function $\delta(\alpha - \beta)$, making nonzero contribution (note that α should be situated within the interval of integration with respect to β), we obtain various regions of two-dimensional integration in the plane of variables p', q for the given momentum p. In doing so, the momentum p of an electron is a parameter.

5. Onsager's coefficients. Performing two-dimensional numerical integration with respect to p' and q, over the above described regions, we determine the collision frequency $\nu(p)$ of s-electron having momentum p with d-electrons in the process sd→sd (the process ss→ss was described in [7]). This frequency is used hereafter in the set of kinetic equations for heat flux and electric current density expressed in terms of Onsager coefficients. We require the absence of electric current. Then the

coefficient of heat conduction κ can be expressed as

$$\kappa(T_e, x) = \frac{1}{T_e}\left(I_2 - \frac{I_1^2}{I_0}\right),$$

where

$$I_0 = \frac{1}{3\pi^2\hbar^3 m_s^2}\int \frac{p^4}{\nu(p)}\left(-\frac{\partial f_s}{\partial \varepsilon}\right) dp,$$

$$I_1 = \frac{1}{3\pi^2\hbar^3 m_s^2}\int \frac{p^4}{\nu(p)}\left(-\frac{\partial f_s}{\partial \varepsilon}\right)(\varepsilon - \mu) dp,$$

$$I_2 = \frac{1}{3\pi^2\hbar^3 m_s^2}\int \frac{p^4}{\nu(p)}\left(-\frac{\partial f_s}{\partial \varepsilon}\right)(\varepsilon - \mu)^2 dp.$$

Here $\varepsilon = \varepsilon_s + p^2/2m_s$,

$$-\frac{\partial f_s}{\partial \varepsilon} = \left[4k_B\, T_e\, \cosh^2\left(\frac{\varepsilon_s + p^2/(2m_s) - \mu}{2k_B T_e}\right)\right]^{-1}.$$

6. Effective frequency. We see thus that the thermal conductivity coefficient $\kappa(T_e, x)$ is expressed in terms of above calculated collision frequency $\nu(\mathbf{p})$, depending on electron momentum $\mathbf{p}$. Knowing coefficient κ we find effective collision frequency $\nu(T_e, x)$. The frequency $\nu(T_e, x)$ will be necessary below in section 9 for calculation of electron-electron contribution to electric resistance r. To calculate effective frequency ν we use the Drude formula $\nu(T_e, x) = C_s(T_e, x)[v(T_e, x)]^2/\kappa(T_e, x)$, where C_s is the s-electron heat capacity at constant volume. For Thomas–Fermi screening the electron-electron collision frequencies may be approximated as:

$$\nu_{ss}(T_e, x) = 0.623\, x\, t^2\, \frac{1 + 4.034\, t^{0.7439}}{1 + 1.2178\, t^{2.0939}},$$

$$\nu_{sd}(T_e, x) = 5.32\, x\, \exp\left(-\frac{1.738}{t}\right)\, \frac{1 + 1.64\, t^{-0.761}}{1 + 0.0384\, t^{0.673}}.$$

Here frequencies ν are in units $10^{15}\,\mathrm{s}^{-1} = 1/\,\mathrm{fs}$. These expressions are the approximations of results of the numerical integrations performed according to the above described scheme. Here $t = 6T_e/\varepsilon_F = 6T_e/(\varepsilon_{F0}\, x)$, ε_F is the Fermi energy, ε_{F0} is

the Fermi energy at relative density $x = 1$, $x = \rho/\rho_0$, ρ_0 is density of copper at $T = 0$, $p = 0$. The discussion of the dependence of Fermi energy $\varepsilon_F(x)$ on density is presented in the next section.

In the present calculations the value ε_2 equals to 2.1 eV; the ε_2 is the gap between the upper edge of the d-band and the Fermi level. Note that $e^{-1.738/t} = \exp(-2.7/(T_e\,[\mathrm{eV}]))$ at $\varepsilon_{F0} = 9.2\,\mathrm{eV}$. The value 2.7 eV is larger than the gap $\varepsilon_2 = 2.1\,\mathrm{eV}$. Likely, this is connected with the preexponential factor and with the fact that at the temperatures T_e below $\sim 1\,\mathrm{kK}$ the integration in section 4 using Mathematica system is performed with great difficulty. The above presented approximate formulae provide reasonable accuracy for electron temperatures up to $\sim 5\,\mathrm{eV}$.

7. Final expression for electron-electron contribution to thermal conductivity κ_{se} of copper. Let us make an estimate of dependence of thermal conductivity $\kappa_{se} = 1/S_{se}$ on density. Then we use the expression for S_{se} together with the si contribution to find thermal resistance of copper $S = S_{si} + S_{se}$ in the 2T states.

In the low temperature case we have

$$\kappa_{se}(T_e, x) \sim n\,k_B \frac{k_B T_e}{\varepsilon_F} v_F^2 \frac{\hbar}{\varepsilon_F} \left(\frac{\varepsilon_F}{k_B T_e}\right)^2 \sim$$

$$\sim n\,k_B \frac{\hbar\,v_F}{p_F} \frac{\varepsilon_F}{k_B T_e} \sim \hbar\,k_B \frac{n}{m_s} \frac{\varepsilon_F}{k_B T_e}. \qquad (7)$$

Here k_B is Boltzmann constant, ε_F, v_F, p_F are energy, velocity, and momentum of Fermi, respectively. They depend on density. The letter m_s is effective mass of s-electrons. We performed simulations using the density functional theory (DFT) for gold (see [16] in the main text). It was found [16] that Fermi energy ε_F increases with atomic concentration n as $\varepsilon_F \propto n$. Let's repeat here again that we call ε_F the difference between the chemical potential at $T_e = 0$ and the bottom of the s-band. We increase or decrease atomic concentration by the "cold" compression/refraction. During this process the FCC crystal of gold is homogeneously compressed/expanded at $T_e = T_i = 0$. Similar is the situation with the x-dependence of ε_F in case of copper (Cu).

Therefore in case of Cu near the density $x = 1$ we also have the scaling on density $\varepsilon_F = \varepsilon_{F0}\, x$, where ε_{F0} is Fermi energy at zero external pressure. This scaling is

$$\varepsilon_F = (3\pi^2\, Z_s\, n)^{2/3} \frac{\hbar^2}{2m_s} = (3\pi^2\, Z_{s0}\, n_0)^{2/3} \frac{\hbar^2}{2m_{s0}} \frac{n}{n_0}.$$

In theoretical calculations, we assume that $Z_s = 1$ at low temperatures. The condition $Z_s = 1$ remains during the "cold" ($T_e = T_i = 0$) density variations in our range of compressions/expansions.

In compliance with the previous statement the s-electron effective mass scales as $m_s = m_{s0}\, x^{-1/3}$.

In our theoretical calculations we do not consider deformation of electron spectra caused by increase of electron temperature. But our QMD-KG computations presented in the main text of course include these deformations. The calculations of two-parabolic approximation of electron density-of-states (DoS) for the two-band metals are based on the quantum modeling using DFT for metal at zero temperature.

Using the scaling mentioned above $m_s = m_{s0}\, x^{-1/3}$ and the expression (7), we obtain for the low-temperature limit: $S_{se}(T_e, x) \propto x^{-4/3}(k_B T_e/\varepsilon_F)$. Now we can apply this scaling as function of x for the thermal resistivity S_{se}. We use the points of ss and sd contributions to thermal conductivity which were computed by the method from sections 2–5. As a result, we select an analytical approximation of thermal resistivity

$$S_{se}(T_e, x) = x^{-4/3}\, a_0\, t/(1 + b_0\sqrt{t} + b_1\, t + b_2\, t^2) \tag{8}$$

in the units of [m K/W] with the coefficients $a_0 = 3.803 \cdot 10^{-4}$, $b_0 = -1.9916$, $b_1 = 1.353$, $b_2 = 0.03954$. At fixed density, the electron spectra only slightly depend on a structure factor for given ion configuration. Due to that we use in further calculations of the sums $S_{si} + S_{se}$ the same expression S_{se} (8) for crystal and for liquid.

8. Electron-ion interaction. Thermal conductivity of crystal. Effect of density. We write the expression for the contribution of electron thermal conductivity which is consequence of electron-ion interaction, in the form

$$\kappa_{si} \sim C_s v\, \lambda_{si} \sim n\, k_B\, C(t)\, v_F\, \lambda_{si}, \tag{9}$$

where C_s is thermal capacity of electrons of the copper s-band, v is mean electron velocity, λ_{si} is the mean free path for s-band electrons; $v = (v_F^2 + 3k_B T_e/m_s)^{1/2} = v_F\,(1 + t/4)^{1/2}$, $m_s v_F^2/2 = \varepsilon_F$, $\varepsilon_F = \varepsilon_{F0}\,x$, $m_s = m_{s0}/x^{1/3}$, $v_F = v_{F0}\,x^{2/3}$. A function

$$C(t) = t\,(1 + 11.202\,t^2)/(1 + 3.346\,t^{2.05})$$

is introduced here for copper in analogous manner as it was done for gold in [22] of the main text. The mean free path of s-electrons is equal to $\lambda_{si} = 1/(n\,\Sigma)$, if we consider only scattering caused by electron-phonon collisions. Here Σ is an effective cross-section: $\Sigma \sim u_0^2\,T_i/\theta$, $u_0^2 \sim \hbar^2/(M\,k_B\,\theta)$ is a square of the zero temperature oscillations of atoms with the mass M, and θ is Debye temperature. Thus we have

$$\lambda_{si} \sim \left(n\,\frac{T_i}{\theta}\,\frac{\hbar^2}{M\,k_B\,\theta}\right)^{-1} \sim \frac{M\,k_B}{\hbar^2\,T_i}\,\frac{\theta^2}{n} \sim \frac{\theta^2}{n\,T_i}. \tag{10}$$

Debye temperature θ depends on density. To define this significant dependence, we represent the cold curve of pressure as a function of density in the form of the two power law terms $p_c(x) = (A/V_0)(x^{a+1} - x^{b+1})$, where $x = \rho/\rho_0 = V_0/V$, V is the volume of one atom, and V_0 is initial volume per one atom at $P = 0$ and $T = 0$. Lattice energy of one atom $\varepsilon_c(V) = (A/a)\,[x^a - (a/b)\,x^b]$ has a minimum at $x = 1$. The powers $a = 1.826$ and $b = 1.788$ were found using the cold curve of pressure. The cold curve has been obtained from the wide-range equation of states (EoS) [27–29].

To check an accuracy of the approximation $p_c(x)$ selected above, we have reckoned the sublimation curve

$$p_c(n) + 3\,\Gamma(n)\,n\,k_B\,T = 0, \;\; \Gamma(n) = -d\ln\theta/d\ln V \tag{11}$$

at temperatures $T > \theta$. Here Γ is Grüneisen parameter for ion subsystem. The curve (11) is called also the zero isobar or the coexistence curve between solid state and gas or the sublimation curve. The sublimation curve obtained from our two-terms approximation is in good agreement with the sublimation curve, which corresponds to the EoS [27–29].

Debye energy is $k_B\,\theta = \hbar\,c_s\,k_D$, where $k_D = (6\pi^2\,n)^{1/3}$ is Debye wavenumber, $c_s \propto \sqrt{K/(M\,n)}$ is sound velocity, $K = -V\,dp_c/dV$ is a bulk modulus. After

substitution of the expressions listed above in $\theta^2 \propto c_s^2\, k_D^2$ and differentiation of the expression for cold curve of pressure p_c by V, we obtain

$$\theta^2(x) \propto x^{2/3}\, y, \quad y(x) = \frac{(a+1)\, x^a - (b+1)\, x^b}{a-b}. \tag{12}$$

The function $y \propto (x - x_{\min})$ becomes equal to zero together with the bulk modulus K and sound velocity in the minimum of the pressure cold curve $p_c(x)$ at $x_{\min} = [(b+1)/(a+1)]^{1/(a-b)} = 0.7$, $V_{\min} = 1.43\, V_0$. In this point the copper spinodal [27–29] touches the axis $T = 0$.

The potential well where atoms are oscillating, becomes wider with strain due to decreasing of the modulus K. The decrease of the modulus K is caused by decreasing of density x as it tends to the minimum $x_{\min}$. Accordingly, at fixed temperature (the regime of isothermal strain) the amplitude of thermal oscillations grows because the well becomes wider. This is a factor acting in direction to the increase of the collision frequency. Mean free path $\lambda_{si} \propto \theta^2 \propto (x - x_{\min})$ (10) becomes shorter, and therefore the thermal conductivity κ_{si} (9) decreases.

Now we consider a function

$$\bar{y} = (1+\zeta) x^{2a+1}/(1+\zeta\, x^{a+1}), \quad \zeta = (a-b)/(b+1).$$

The function $\bar{y}(x)$ is close to the function $y(x)$ at the vicinity of the point $x = 1$, but the former is always positive at $x > 0$, in opposition to $y(x)$.

At hydrodynamic modeling of laser ablation of a target in the surrounding vacuum, there is a tail of a rarefaction wave where density strongly decreases. To exclude the troubles with the 2T thermal conductivity during simulations caused by this effects, we replace the function y in (12) by the function $\bar{y}$. In that way, we avoid appearance of small thermal conductivities at the densities near the value $x_{\min}$ which corresponds to rather high densities $x_{\min} = 0.7$.

We substitute the function $\bar{y}$ instead of y in the expression for mean free path (10) and thermal conductivity (9), which both are related to the s-electron scattering on phonons. After substitution, we obtain

$$\lambda_{si} \propto [\bar{y}(x)/x^{1/3}]/T_i, \quad \kappa_{si}^{sol} \propto x^{4/3}\, \bar{y}\, C(t)/T_i. \tag{13}$$

In (13) the prime "sol" is necessary to emphasize that the expression given above is obtained for solid state. The thermal conductivity of molten Cu is considered below separately.

The experimental value of thermal conductivity on the sublimation curve at the room temperature $T_{rt} = 293\,\mathrm{K}$ and density $\rho_{rt} = 8.94\,\mathrm{g/cc}$ is $\kappa_{rt} = 401\,\mathrm{W/(m\ K)}$. Therefore, thermal conductivity of copper in solid phase is given by expression

$$\kappa_{si}^{sol}(T_e, T_i, \rho) = \kappa_{rt} \left(\frac{x}{x_{rt}}\right)^{4/3} \frac{\bar{y}(x)}{\bar{y}(x_{rt})} \frac{T_{rt}}{T_i} \frac{C(t)}{C(t_{rt})},$$

where $x_{rt} = \rho_{rt}/\rho_0$ is relative density at the room temperature T_{rt}, $\rho_0 = 9.02\mathrm{g/cc}$ is the density of copper at $T = 0$ and $P = 0$, $t_{rt} = 6\,k_B\,T_{rt}/(\varepsilon_{F0}\,x_{rt})$.

As a result, we have for thermal conductivity of solid phase the expression:

$$\kappa_{sol}(T_e, T_i, \rho) = [S_{se}(T_e, x) + 1/k_{si}^{sol}]^{-1}, \tag{14}$$

where thermal resistivity S_{se} corresponding to s-electron heat transfer, appears as a result of collisions of s-electron with s- and d-electrons. The resistivity S_{se} is given by the formula (8). The dependencies (14) are used to obtain the curves *1–3* in Fig. 5 of the main text.

9. Electrical conductivity of crystal. We reckon the electrical resistivity r of copper as a function of temperatures T_e and T_i and density. Firstly, we write the expression from Drude theory for contribution of si collisions to electrical resistivity and, at the second step, we derive the general expression, where the contribution of se collisions is also taken into account. The resistivity r_{si} is equal to

$$r_{si} = \frac{m_s\,v}{Z_s\,n\,e^2\,\lambda_{si}} = \frac{(3\pi^2)^{1/3}}{2\pi} \frac{R_0\sqrt{1+t/4}}{Z_s n^{2/3} \lambda_{si}}. \tag{15}$$

In (15) Z_s is the number of s-electrons per atom, v – mean velocity of s-electrons, λ_{si} is the mean free path of s-electrons when the scattering due to electron-phonon interaction is considered, $R_0 = h/e^2 = 25812.8$ Ohm is von Klitzing constant. In (15) we use our estimation of mean velocity which has the form $m_s\,v = p_F\sqrt{1+t/4}$, $p_F = p_{F0}\,x^{1/3}$. The expression for p_F is written in the form which is similar to the expression $\varepsilon_F = \varepsilon_{F0}\,x$. The origin of the factor $\sqrt{1+t/4}$ are discussed in the definition of the formula (9) in section 8.

We substitute the expression for λ_{si} (13) in (15). In addition, we divide the expression (15) by the value of copper resistivity at room temperature $r_{rt} = 16.78\,\text{nanoOhm}\cdot\text{m}$. At room temperatures we can neglect the contribution of the se collisions. As a result, we have

$$r_{si}(T_i, x) = r_{rt}\frac{T_i}{T_{rt}}\left(\frac{x_{rt}}{x}\right)^{1/3}\frac{\bar{y}(x_{rt})}{\bar{y}(x)}\sqrt{1+t/4}. \tag{16}$$

Taking into account also the contribution of electron-electron collisions, we derive the expression for the net electrical resistivity for copper in solid state:

$$r_s(T_e, T_i, x) = r_{si}(T_i, x) + r_{se}(T_e, x) =$$

$$= r_{si}(T_i, x) + r_{at}\,\frac{m_{s0}}{m}\,\frac{\nu_{sd}(T_e, x) + \nu_{ss}(T_e, x)}{Z_s(T_e, x)\,n_0\,a_B^3\,\nu_{at}}. \tag{17}$$

Here $\nu_{at} = me^4/\hbar^3 = 4.1\cdot 10^{16}\text{s}^{-1}$ is atomic unit of frequency, m is mass of a free electron in vacuum, m_{s0} is effective mass of s-electon at $x = 1$, a_B is Bohr radius, $r_{at} = (m\,\nu_{at})/(a_B^{-3}e^2) = \nu_{at}^{-1} = 2.42\cdot 10^{-17}\,\text{sec}$ is atomic unit of electrical resistivity in CGSE units. In units of SI we have $r_{at} = 217.3\,\text{nanoOhm}\cdot\text{m}$. Effective frequencies ν_{ss} and ν_{sd} are reckoned in section 6. The curves 1–3 in the Fig. 3 of the main text are obtained by the formula (17) without the term ν_{ss}.

10. Electrical resistivity of liquid. To describe electron-ion interaction in liquid copper, one have to use (i) experimental data, (ii) the value of resistivity $r_{QMD} = 0.74\,\mu\text{Ohm}\cdot\text{m}$ for the point with equilibrium ($T_e = T_i = T$) temperature $T = 7.5\,\text{kK}$; the point is shown in Fig. 1 of the main text, and (iii) the estimate of electrical resistivity in the critical point of copper: 4–6 $\mu\text{Ohm}\cdot\text{m}$ (see [30] in the main text). We assume that the mean free path of electrons due to electron-ion scattering $\lambda_{si}^{\text{liq}}$ can be factorized as in the case of solid state: $\lambda_{si}^{\text{liq}} = n_0^{-1/3}x^{\beta-1/3}/w(T_i)$. We select a function w using the three sources of data listed above. In order to do that, we write the Drude formula for electrical resistivity which contains a mean free path. We use the same scheme as for the case of (15)

$$r_{si}^{\text{liq}}(T_i, T_e, x) = \frac{p_F\sqrt{1+t/4}}{Z_s(T_e, x)\,n\,e^2\,\lambda_{si}^{\text{liq}}},$$

but the formula for λ is replaced. Thus,

$$r_{si}^{\rm liq}(T_i, T_e, x) = \frac{(3\pi^2)^{1/3}}{2\pi} \frac{R_0}{n_0^{1/3}} \frac{\sqrt{1+t/4}}{Z_s(T_e, x)} \frac{w(T_i)}{x^{\beta+1/3}}. \tag{18}$$

If the conditions (ii) and (iii) are satisfied near the isotherm of the temperature close to the critical point temperature $T_c \approx 8\,\mathrm{kK}$, then we can write an equation which allows us to determine the power β : $r_c/r_{QMD} = (\rho_{QMD}/\rho_c)^{\beta+1/3}$, where $r_c \approx 6\,\mu\mathrm{Ohm}\cdot\mathrm{m}$ is the electrical resistivity in the critical point, $\rho_c \approx 2.5\,\mathrm{g/cc}$ is the density in the critical point of Cu, r_{QMD} is the resistivity in the point QMD-KG presented above (see Fig. 1 of the main text), $\rho_{QMD} = 8\,\mathrm{g/cc}$ is the density in this QMD-KG point.

Solving this equation, we determine that $\beta(T_i = 8\,\mathrm{kK}) + 1/3 = 1.8$. This result is in accordance with the slope of electrical resistivity curve shown in Fig. 1 of Clerouin et al. work (Phys. Rev. B **71**, 064203 (2005)). According to this work, the slope $\beta + 1/3$ weakly decreases in the interval of densities $2 \div 8\,\mathrm{g/cc}$ with increase of equilibrium temperature from 10 to 30 kK. This condition can be satisfied by using of the simple monotonically descending function $\beta = 2.4/(1 + 0.35\,T_i/T_c)$. Thus, for the case of liquid Cu in the region of temperatures $T_i = 2\,\mathrm{kK}$, moderately above the triple point, the slope of a function $r \propto 1/x^{\beta+1/3}$ on the isotherm is equal to $-d\ln r/d\ln x|_{Ti}|_{x=1} \approx 2.2$ in the point $x = 1$.

We emphasize that the dependence of electrical resistivity on density is very strong for the crystal (16): $-d\ln r/d\ln x|_{Ti}|_{x=1} \approx 5$ (!). This slope was obtained from the cold curve for pressure described in section 8. This cold curve has two terms: x^a (compression) and x^b (strain). Our two term approximation is rather good to describe the cold and sublimation curves of copper. Therefore, the sound velocity c_s, the bulk modulus K and the force constant γ in the interval $x_{\min} < x < 1$ are reproduced with sufficient accuracy till the minimum of the pressure cold curve $x_{\min} \approx 0.7$. The force constant defines the behavior of crystal field near the minimum of the potential $u = \gamma\,(\mathbf{r} - \mathbf{r_{eq}})^2/2$, where $\mathbf{r_{eq}}$ is the position of an atom in the lattice site. In Debye theory of crystal the well-known relations are satisfied $\theta^2 \propto (c_s k_D)^2 \propto K/x^{4/3}$, $K = (A/V_0)(a-b)\,y$, $y \approx \bar{y}$. In our case, we obtain $d\ln K/d\ln x|_{Ti}|_{x=1} \approx 4.6$.

In addition, the expression $\gamma = M\omega^2$ allows us to find out the relation between the force constant γ and the frequency of oscillations ω of an atom in the potential well. We can write for a crystal that $\gamma \sim M\omega_D^2$, where ω_D is Debye frequency: $\omega_D = k_B\,\theta/\hbar$, $\theta^2 \propto x^{2/3}\,y$. This means that $d\ln\gamma/d\ln x|_{Ti}|_{x=1} \approx 5.3$. In other words, the potential well becomes more shallow when density is descending and reaches the absolute flatness at $x = x_{\min} = 0.7$ (softening of a crystal as a result of its volume expansion). Thus, due to the formula (10) the strong dependence of the mean free path on x is followed. As we can see, the slope of an electrical resistivity r as a function of x is significantly decreased when copper change its state from solid to liquid.

The function w in (18) is determined using the data for the isochore of density 8 g/cc for the molten copper. We set a requirement that the resistivity (18) should be equal to $r_{si}^{\rm liq} = 0.3\mu{\rm Ohm}\cdot{\rm m}$ at $T_i = T_e = 2\,{\rm kK}$ and $r_{QMD} = 0.74\,\mu{\rm Ohm}\cdot{\rm m}$ in the point $T_e = T_i = 7.5\,{\rm kK}$ of this isochore. The temperatures under consideration are relatively small, thus we can neglect the contribution of the electron-electron collisions to an electrical resistivity at this range of temperatures. In addition, we require the fast saturation of the resistivity growth at the temperatures greater than 10 kK. As a result, we obtain $w(T_i) = 0.0043(1 + 126\,T_i/T_c)/(1 + 0.86\,T_i/T_c)$, which is valid for a liquid phase in the temperature interval below 10 kK. According to the data of the carried out calculations and experiments (see Fig. 2 for Aluminum in the Ref. [39] in the main text and Fig. 1 of the Clerouin et al. work (PRB **71**, 064203 (2005) for copper), the resistivity of copper is almost constant at the temperatures higher than 10 kK and the densities $\rho \sim \rho_0$.

In the 2T states with high electron temperatures, there are necessary to take into account the electron-electron collisions. In our model, this contribution is independent on the particular phases (solid or liquid) of copper. Thus, we can get this contribution from the expression (17) obtained for a crystal. Combining the formulae (17) and (18), we have the result for electrical resistivity of liquid copper in the 2T states which has the form

$$r^{\rm liq}(T_e, T_i, x) = r_{si}^{\rm liq}(T_i, x) + r_{se}(T_e, x).$$

The curves 4–6 in Fig. 3 of the main text are plotted using this expression.

11. Thermal conductivity of liquid. We write the expression for thermal conductivity of liquid copper as a consequence of electron-ion collisions $\kappa_{si}^{\rm liq}(T_e, T_i, x)$. We have for thermal conductivity such a form:

$$\kappa_{si}^{\rm liq}(T_e, T_i, x) \propto C_s(T_e, x)|_V \, v \, \lambda_{si}^{\rm liq} \propto C(t) \, x^{\beta+4/3}/w(T_i).$$

Here we use the function $C(t)$ introduced in section 8. We have taken into account that the thermal capacity C_s of unit of volume, which is included in $C(t)$, satisfies the condition $C_s|_V \propto x$, and that the mean velocity $v \propto v_F \propto x^{2/3}$. Thermal conductivity of liquid copper at the melting point on the binodal is equal to 138 W/m/K. We normalize the expression for thermal conductivity on this value. As a result, the contribution to thermal conductivity of liquid phase, which is related to the si interaction, has the form:

$$\kappa_{si}^{\rm liq}(T_e, T_i, x) = 138 \, \frac{C(t)}{C(t_m)} \, \frac{x^{\beta(T_i)+4/3}}{x_m^{\beta(T_m)+4/3}} \, \frac{w(T_m)}{w(T_i)}.$$

Here $t_m = 6k_B T_m/(x_m \varepsilon_{F0})$, $x_m = 7.91/9.02$ is relative density of liquid copper at the melting point. The net thermal conductivity with consideration of κ_{se} (8) is $\kappa^{\rm liq} = 1/[S_{se}(T_e, x) + 1/\kappa_{si}^{\rm liq}]$. The curves *4–6* in Fig. 5 of the main text are plotted using this formula.