Coulomb logarithm in femtosecond-laser–matter interaction

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In femtosecond-laser–matter interaction, collisional absorption plays an important role during the early stages of the interaction, when the laser intensity and the plasma temperature still have moderate values. We propose a cutoff impact parameter $b_{\max}$ for the Coulomb logarithm $\lambda = \ln \Lambda$ in the electron-ion collision rate which takes into account, for an overdense plasma, the crystalline structure of the ion background. Calculations are presented for a bcc lattice and generalized to sc and fcc lattices. The results are applicable for laser intensities $I_l \leqslant 10^{17}\,\mathrm{W\,cm^{-2}}$ and when the Debye theory is valid, that is to say, when the Landau length is distinctly less than the minimum ion distance, and when the Debye screening is unaffected by the electron quiver motion in the laser field. We present the space angle dependence of the cutoff $b_{\max}$ as also its spatial average, and we discuss the ensuing corrections to the Coulomb logarithm due to the improved values of $b_{\max}$. Finally, we present the pertinent $\langle\lambda\rangle$ values, averaged over a Maxwellian distribution function, which are needed for applications of the ballistic model for collisions. [S1063-651X(99)05108-9]

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When an intense femtosecond laser pulse impinges solid matter, collisional absorption in the generated overdense plasma ($\omega_{pe} > \omega$, where ω is the laser frequency and ω_{pe} the plasma frequency) plays an important role during the early stages of the interaction, i.e., as long as the local laser intensity I_l and the electron temperature $k_B T_e$ still have moderate values. For a laser wavelength $\lambda_l = 0.815\,\mu$m, intensity $I_l \leqslant 10^{17}\,\mathrm{W\,cm^{-2}}$, electron temperature $k_B T_e \leqslant 300$ eV, and density $n_e \approx 5\times 10^{23}\,\mathrm{cm^{-3}}$, the electron-ion collision frequency is of the order of $10^{13}\,\mathrm{s^{-1}}$.

The most complete theory describing electron-ion interaction in solid matter is the dielectric model (see, for instance, [1–3]). For practical purposes, it has, however, appeared more convenient to use simpler models based on the ballistic collision theory. This approach has been recently revisited by Mulser *et al.* [4], who provide for laser-matter interaction a time-dependent collision frequency, which in fact represents the collisional energy absorption rate.

In the following, we denote by $b_\perp(v) = Z e^2/4\pi\varepsilon_0 m_e v^2$ the impact parameter corresponding to a 90° deflection, where v is the colliding electron velocity, Z the ion charge number, ε_0 the vacuum permittivity, e the elementary electric charge, and m_e the electron mass. The cutoff $b_{\max}$ is the maximum interaction distance corresponding to the minimum meaningful deviation angle $\chi_{\min}$, and $b_{\min}(v)$ the minimum interaction distance corresponding to the maximum deviation angle $\chi_{\max}$. According to quantum-mechanical considerations, $b_{\min}(v)$ is equal to the de Broglie wavelength $\lambda_B = \hbar/m_e v$.

For a bare Coulomb potential, the calculation of the collision frequency generates a Coulomb logarithm $\lambda = \ln\Lambda$:

$$\lambda_1(v) = \int_{\chi_{\min}}^{\chi_{\max}} \cot(\chi/2)\; d(\chi/2) = \frac{1}{2}\ln\left(\frac{1+b_{\max}^2/b_\perp^2}{1+b_{\min}^2/b_\perp^2}\right), \tag{1}$$

where χ is the deviation angle, related to the impact parameter b by $\tan(\chi/2) = b_\perp/b$. The physical ''cutoff'' is related to $b_{\max}$ only; the term $b_\perp$ enters into Eq. (1) in order to simplify notation. The bare Coulomb potential approximation is valid here since we investigate impact parameters shorter than or close to the Debye length. Some more precise formulas are given in [5] to take into account the Debye screening, but for one ion only—not for an ion lattice.

The rough formula, Eq. (1), could be replaced by a more detailed one,

$$\lambda_2(v) = \frac{1}{2}\ln\left(\frac{1+b_{\max}^2/b_\perp^2}{1+b_{\min}^2/b_\perp^2}\right) + \frac{1}{2}\left(\frac{1}{1+b_{\max}^2/b_\perp^2} - \frac{1}{1+b_{\min}^2/b_\perp^2}\right), \tag{2}$$

which takes into account the energy conservation of the electron colliding elastically with a much heavier fixed ion [6].

One can also find in the literature (see, e.g., [7,8]) another approximate formula for $\lambda = \ln\Lambda = \ln(b_{\max}/b_0)$, where $b_0 = \max(\lambda_B, b_\perp)$. This can be derived from Eq. (1) in the limit $b_{\max} \gg b_\perp$: if $\lambda_B > b_\perp$, we get $\lambda_1(v) \approx \ln(b_{\max}/\lambda_B)$; if $\lambda_B < b_\perp$, we get $\lambda_1(v) \approx \ln(b_{\max}/b_\perp)$.

When $b_{\max}$ is less than $b_{\min}$, there is no interaction and the collision frequency vanishes. For $b_{\max} < b_\perp$, meaning that trajectories are strongly curved, the absorption cannot be described anymore by the ballistic model. The absorption is then heavy since electrons are turning backwards. As shown in Fig. 1, where we have chosen $b_{\max}$ according to this paper—see Eq. (9)—this occurs for densities below $2.2\times 10^{24}\,\mathrm{cm^{-3}}$, and for a narrow electron velocity range below $2.2\times 10^6\,\mathrm{m\,s^{-1}}$. For instance, for $n_i = 5\times 10^{22}\,\mathrm{cm^{-3}}$, it occurs for velocities between about $6\times 10^5\,\mathrm{m\,s^{-1}}$ and $10^6\,\mathrm{m\,s^{-1}}$. The fact that some electrons are experiencing such deviations can be neglected to a first approximation for solid density plasmas.

Generally, for slow electron velocities ($v < 0.1\,c$), one can neglect the term $b_{\min}^2/b_\perp^2$ in Eqs. (1) and (2). Usually the cutoff parameter $b_{\max}$ is approximated either by the Debye

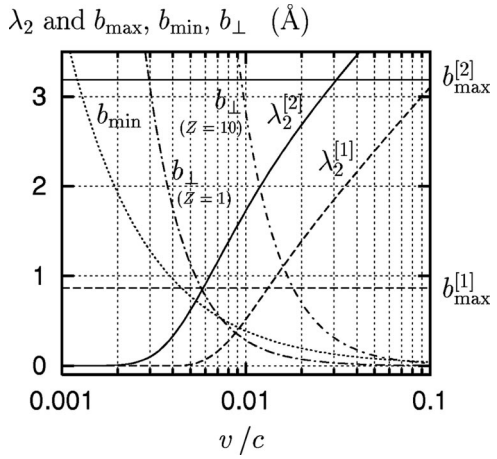

FIG. 1. The impact parameters $b_{\min}=\lambda_B$, $b_\perp$, and $b_{\max}$ (in Å) and the Coulomb logarithm λ_2 vs v/c for $n_i^{[1]}=5\times10^{23}\ \mathrm{cm}^{-3}$ and $n_i^{[2]}=10^{22}\ \mathrm{cm}^{-3}$, and $Z=1$.

length $\lambda_D=v_{\mathrm{th}\,e}/\omega_{p\,e}$ or in the dielectric theory [1] by $\lambda_o=v/\omega_{p\,e}$, where $v_{\mathrm{th}\,e}$ is the electron thermal velocity (ions are treated here as immobile).

Another limitation of the ballistic model arises for high density plasma where predominant electron-ion collisions are no longer binary: the lattice has to be taken into account, since a test electron can interact with several ions simultaneously. Consequently, the $b_{\max}$ term appearing in Eq. (2) has to be reduced to take into account the surrounding ions [9,10]. In this paper we propose an improved cutoff $b_{\max}$ for the formula (1). The idea is to compute the potential seen by the colliding electron with an ion placed at the origin, *including the ion lattice*, too.

The relevant parameter describing the plasma degeneracy is $\Gamma=l_L/a$, where the Landau length $l_L=Z^2e^2/4\pi\varepsilon_0 k_B T_e$ is the minimum approach distance between ions and $a=(\frac{4}{3}\pi n_i)^{-1/3}$ the radius of a sphere containing one ion; $n_i=\overline{n_0}/Z$ is the ion density, $\overline{n_0}$ the background electron density to be defined later, T_e the electron isothermal fluid temperature, and k_B the Boltzmann constant. In terms of the Debye length $\lambda_D=\sqrt{\varepsilon_0 k_B T_e/\overline{n_0}\,e^2}$, the coupling parameter Γ can be written as $\Gamma=\frac{1}{3}Z\,(a/\lambda_D)^2$, which reveals the importance of the ratio a/λ_D.

In the case of nondegenerate plasmas ($\Gamma<1$, i.e., $a/\lambda_D<1$), the Debye-Hückel theory applies and the potential created by each ion is the Debye one. For *one ion*, the Debye potential is obtained by solving the Poisson equation and the equation of motion for the electrons:

$$\varepsilon_0\nabla^2\Phi(\mathbf{r},t)=-Ze\,\delta(\mathbf{r})+en_e, \tag{3}$$

$$m_e\left[\frac{\partial\mathbf{v}}{\partial t}+(\mathbf{v}\cdot\nabla)\,\mathbf{v}\right]=-e(\mathbf{E}+\mathbf{v}\times\mathbf{B})-k_B T_e\,\frac{\nabla n_e}{n_e}. \tag{4}$$

We use in Eqs. (3) and (4) the following notation: $\Phi(\mathbf{r},t)$ and n_e are, respectively, the scalar potential and the electron density at the position $\mathbf{r}$ and time t; $\delta(\mathbf{r})$ is the Dirac distribution function, implying that the ion is localized at the origin; $\mathbf{v}$ is the electron velocity.

Setting $\mathbf{E}=-\partial\mathbf{A}/\partial t-\nabla\Phi$, where $\mathbf{A}$ is the vector potential used with the Coulomb gauge ($\nabla\cdot\mathbf{A}=0$), we get

$$\mathbf{E}+\mathbf{v}\times\mathbf{B}=-\frac{d\,\mathbf{A}}{d\,t}-\nabla\Phi=-\frac{\partial\,\mathbf{A}}{\partial\,t}-(\mathbf{v}\cdot\nabla)\,\mathbf{A}-\nabla\Phi. \tag{5}$$

For moderate laser intensities ($I_l\leqslant 10^{17}\,\mathrm{W\,cm}^{-2}$), we use the dipole approximation [11], that is to say, the convective terms $(\mathbf{v}\cdot\nabla)\,\mathbf{A}$ and $(\mathbf{v}\cdot\nabla)\,\mathbf{v}$ are neglected in Eqs. (4) and (5), or in other words, magnetic field effects are ignored. We assume a linearly polarized field with a wave vector $\mathbf{k}$, oscillation frequency ω, and the corresponding vector potential $\mathbf{A}=\mathbf{A}_0\exp(-i\,\omega\,t+i\,\mathbf{k}\cdot\mathbf{r})$. The electron motion is dominated by the quiver motion in the laser field: $\mathbf{v}=\mathbf{v}_0\exp(-i\,\omega\,t+i\,\mathbf{k}\cdot\mathbf{r})$. Making these insertions, we obtain from Eq. (4)

$$e\,\nabla\Phi=k_B T_e\,\nabla(\ln n_e)+i\,\omega\,(e\,\mathbf{A}-m_e\,\mathbf{v}). \tag{6}$$

The plasma potential is $\Phi=\Phi_0+\delta\Phi$, with $\delta\Phi=\delta\Phi_i+\delta\Phi_l$, where Φ_0 is the constant spatial background potential, $\delta\Phi_i$ the perturbation caused by the ion at the origin, and $\delta\Phi_l$ the perturbation caused by the laser. Actually, the second term in the right-hand side of Eq. (6) equals $e\,\nabla\delta\Phi_l=i\,\omega\,(e\,\mathbf{A}-m_e\,\mathbf{v})$ and is of the order of $m_e\,\nu_{ei}\,\mathbf{v}$, where ν_{ei} is the electron-ion collision frequency [4], which is negligible compared to $e\,\nabla\delta\Phi_i=k_B T_e\,\nabla(\ln n_e)$, the first term in the right hand side of Eq. (6). For instance, for $k_B T_e=100\,\mathrm{eV}$ and $n_e=5\times10^{22}\,\mathrm{cm}^{-3}$ the typical scale length is the Debye length $\lambda_D\approx3\times10^{-10}\,\mathrm{m}$. Thus the force $|k_B T_e\,\nabla(\ln n_e)|$ is approximately $5\times10^{-6}\,\mathrm{N}$; and $|m_e\,\nu_{ei}\,\mathbf{v}|\ll5\times10^{-6}\,\mathrm{N}$, since $\nu_{ei}\leqslant10^{16}\,\mathrm{s}^{-1}$ for $v<c/100$. So, assuming that the temperature is high enough, i.e., $e\,\delta\Phi\ll k_B T_e$, we can write the Boltzmann distribution function as $n_e=n_0\exp(e\,\Phi/k_B T_e)=\overline{n_0}+\delta n_e$ where $\delta n_e=(\overline{n_0}\,e/k_B T_e)\,\delta\Phi$, is the density perturbation with the equilibrium electron density $\overline{n_0}=n_0\exp(e\,\Phi_0/k_B T_e)$. Thus Eq. (3) reduces to $\nabla^2\delta\Phi-\delta\Phi/\lambda_D^2=-(Z\,e/\varepsilon_0)\,\delta(r)$.

That the screening length is not influenced by the collective electron oscillation can be explained by the fact that the oscillation of the electrons only slightly changes the local electron density, which is perturbed mainly by the ion at the origin and by the screening caused by the collisional Maxwellian electrons. In fact, the linearly polarized laser field causes only transverse perturbations since magnetic field effects are neglected; ions, in contrast, introduce three-dimensional perturbations.

The computations of the cutoff parameter $b_{\max}$ have been performed for a body-centered-cubic (bcc) lattice. The ions are considered fixed during the time when collisions are of importance in femtosecond-laser–matter interaction. Actually, ions are initially at a temperature of a few hundredths of eV and during the short time electron-ion collisions are of importance, they do not reach a sufficient temperature for appreciable hydrodynamic motion. As long as the lattice is not totally disordered, ions quiver around their average position, as in a solid lattice.

The lattice parameter is $\mathcal{A}=(4/\sqrt{3})\,a$, since the minimum distance between two ions in the bcc lattice is one-half of the cube diagonal. We choose the spherical coordinate system (r,θ,ϕ) shown in Fig. 2. Due to the symmetry of the bcc lattice, it suffices to consider the range $r\geqslant0$, $0\leqslant(\theta,\phi)\leqslant\pi/2$.

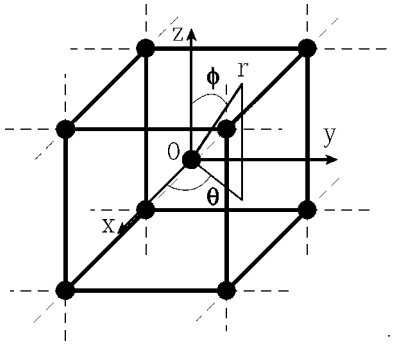

FIG. 2. Definition of the coordinate system for a bcc lattice.

Normalizing all the lengths to the Debye length, the force exerted by an ion j at position $\mathbf{r}_j$ on the colliding electron at position $\mathbf{r}_e$ can be written as $\mathbf{f_j}=-e\,\boldsymbol{\nabla}\,\delta\Phi(\Delta r_j)$ where $\delta\Phi(\Delta r_j)=(Z\,e/4\,\pi\,\varepsilon_0)\,[\exp(-\Delta r_j/\lambda_D)/\Delta r_j]$ and $\Delta r_j=\|\mathbf{r}_j-\mathbf{r}_e\|$. We compute the total force $\mathbf{F}=(F_r,F_\theta,F_\phi)$ on the colliding electron by including all the ions at a distance less than an arbitrarily chosen value of five Debye lengths, i.e., $\mathbf{F}=\Sigma_{\Delta r_j\leqslant 5\lambda_D}\mathbf{f_j}$.

The physical boundary of the possible interaction area defining $b_{\max}$ between the colliding electron and the ion at origin occurs when the radial force F_r on the electron vanishes, i.e., when the electron effectively leaves the ion interaction ''cell.'' Thus the condition ''$F_r=0$'' is chosen as the criterion to compute the cutoff $b_{\max}$. For numerical work it turns out to be more convenient to solve the problem with the following equivalent condition: ''$\partial|F_r|/\partial r$ changes its sign.''

We present in Fig. 3(a) the smoothed (small numerical irregularities have been suppressed) surface of the normalized cutoff $b_{\max}/\lambda_D$ for $a/\lambda_D=0.5$ versus the direction angles θ and ϕ. The minimum cutoff is obviously obtained for $\theta=\phi=\pi/4$. The lattice geometry creates other variations on the surface: the local minima at ($\phi=0$) and ($\phi=\pi/2$, $\theta=0$ or $\pi/2$) are due to the three closest body-centered ions in the surrounding cells. Crests for ($\phi\approx\pi/4$, $\theta=0$ or $\pi/2$) and ($\phi=\pi/2$, $\theta\approx\pi/4$) are due to the three body-centered ions on the diagonal. The three saddle regions between them are due to more distant ions of the neighboring cells. We also want to point out the fact that the bcc ion lattice and the associated Debye potential causes the force acting on the test electron to vanish before the half-distance between two ions, contrary to intuitive expectations, for particular directions of the lattice: ($\theta=0$, $\phi=\pi/4$), ($\theta=\pi/2$, $\phi=\pi/4$), ($\theta=\pi/4$, $\phi=0$) as demonstrated in Fig. 3(b). A similar phenomenon occurs for fcc and sc lattices, in other special directions.

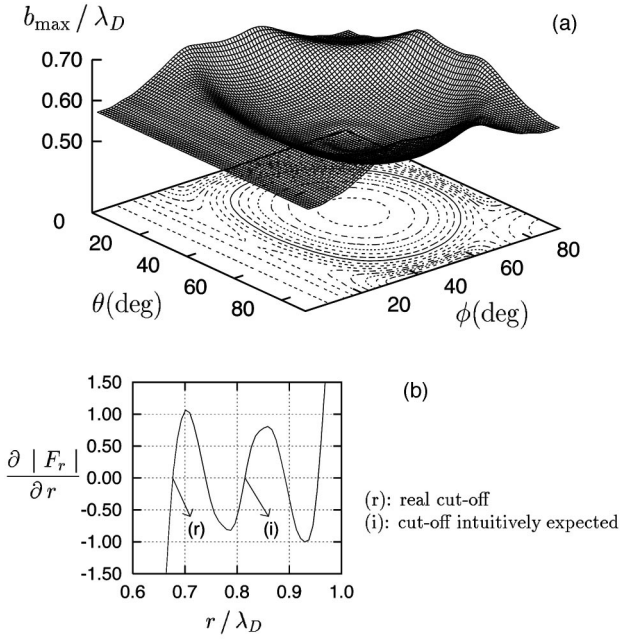

FIG. 3. (a) Cutoff $b_{\max}/\lambda_D$ vs angles θ and ϕ for a bcc lattice and for $a/\lambda_D=0.5$; (b) $\partial|F_r|/\partial r$ vs r/λ_D showing an ''anomaly'' in the particular direction $\theta=0$ and $\phi=45°$.

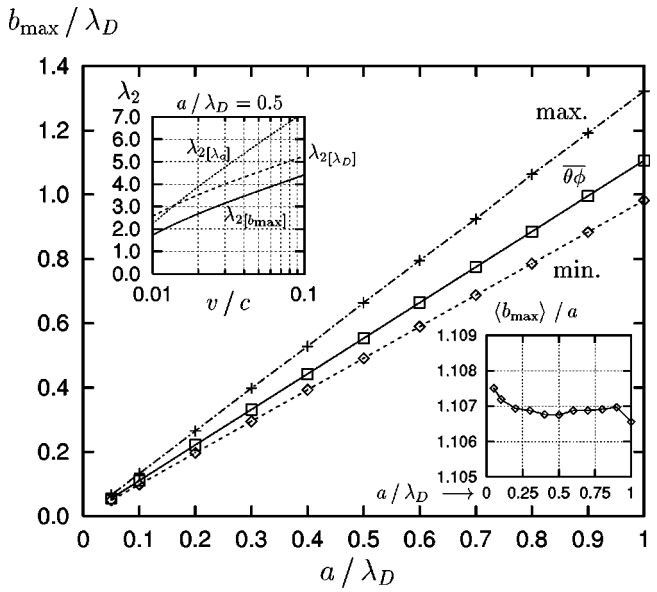

FIG. 4. Maximum, minimum, and average values of the cutoff $b_{\max}/\lambda_D$ vs a/λ_D for a bcc lattice. The top left inset shows the Coulomb logarithm λ_2 vs v/c for the corresponding cutoffs: $\lambda_{2\,[b_{\max}]}$, $\lambda_{2\,[\lambda_D]}$, and $\lambda_{2\,[\lambda_o]}$ ($n_i=10^{22}$ cm^{-3}, $Z=1$, $k_BT_e=100$ eV, and $a/\lambda_D=0.5$). The bottom right inset presents the ratio between the cutoff and the ion-sphere radius $\langle b_{\max}\rangle/a$.

The relatively moderate variations ($\approx 30\%$) in the cutoff value suggest averaging over the angles θ and ϕ. In Fig. 4 we show as a function of a/λ_D the minimum, the maximum, and the average value $(b_{\max}/\lambda_D)_{\min}$, $(b_{\max}/\lambda_D)_{\max}$, and $\langle b_{\max}/\lambda_D\rangle_{\overline{\theta\phi}}$, respectively. For a/λ_D much less than unity, the cutoff is largely reduced from both the dynamical screening length λ_o and the static Debye length λ_D.

The Coulomb logarithm λ_2, Eq. (2), is presented in the top left inset of Fig. 4, as a function of v/c using in Eq. (2) the three different cutoff parameters $b_{\max}$, λ_D, and λ_o. For the plasma parameters we have chosen the values $n_0=10^{22}$ cm^{-3}, $k_BT_e=100$ eV, $Z=1$. We notice that for velocities less than $0.03\,c$, that is to say for laser intensities less than 3×10^{16} W cm^{-2}, the variation of λ_2 can exceed 25% from the commonly used value based on the screening length.

In Fig. 5, we present some typical values of $\langle\lambda_2\rangle_{\text{Maxwell}}$,

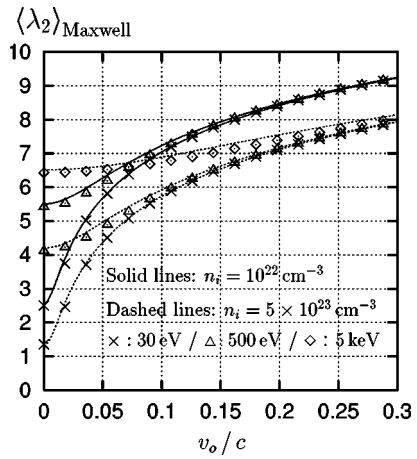

FIG. 5. Coulomb logarithm $\langle \lambda_2 \rangle_{\text{Maxwell}}$ averaged over a Maxwellian distribution function for $n_i = 10^{22}\,\text{cm}^{-3}$ (solid lines) and $n_i = 5 \times 10^{23}\,\text{cm}^{-3}$ (dashed lines) for three electron temperatures 30 eV, 500 eV, and 5 keV. The points represent the exact computations, Eq. (7), and the lines the fit formula, Eq. (8).

the average over a Maxwellian distribution function of λ_2, for different densities and isotropic electron temperatures:

$$\langle \lambda_2 \rangle_{\text{Maxwell}} = \left(\frac{m_e}{2\,\pi\,k_B T_e} \right)^{3/2} \int_0^{+\infty} \int_{-\infty}^{+\infty} \exp\left(\frac{-m_e\,v_\perp^2}{2\,k_B T_e} \right) \times \exp\left(\frac{-m_e\,v_\parallel^2}{2\,k_B T_e} \right) \lambda_2 [\sqrt{v_\perp^2 + (v_\parallel + v_o)^2}] \times 2\,\pi\,v_\perp\;\; d\,v_\parallel\;\; d\,v_\perp\,, \tag{7}$$

where v_o is the electron quiver velocity; $v_\perp$ and $v_\parallel$ are, respectively, the perpendicular and the parallel individual electron velocities with respect to the oscillatory electron motion in the laser field. A good fit to $\langle \lambda_2 \rangle_{\text{Maxwell}}$ is given by

$$\langle \lambda_2 \rangle_{\text{Maxwell}} \approx \lambda_2(v_f), \;\; v_f = \sqrt{v_o^2 + 3/2\;\; v_{\text{th}\,e}^2}\,, \tag{8}$$

where we use Eq. (2) for λ_2.

In conclusion, we have devised a method which takes into account in femtosecond-laser–matter interaction in a simple way the effect of surrounding ions in electron-ion collision frequency. For the cutoff $b_{\max}$ appearing in the Coulomb logarithm, Eqs. (1) and (2), instead of the Debye length, one should use

$$\langle b_{\max} \rangle \approx 1.107\,a, \;\; a < \lambda_D \tag{9}$$

for a bcc lattice ($\mathcal{A} = 4\,a/\sqrt{3}$) according to the bottom right inset in Fig. 4. The modification is obviously particularly important for small a/λ_D values.

The computation above has been performed for a bcc lattice but can be easily generalized for any type of lattice. The numerical value in the previous equation changes somewhat without affecting the essential dependence $\langle b_{\max} \rangle = \alpha\,a$. For a sc lattice ($\mathcal{A} = 2\,a$), we propose $\langle b_{\max} \rangle \approx 1.211\,a$ with $a < \lambda_D$, and for a fcc lattice ($\mathcal{A} = 4\,a/\sqrt{2}$), $\langle b_{\max} \rangle \approx 1.107\,a$ with $a < \lambda_D$.

The rather moderate influence of the lattice type on the α coefficient shows that even when the lattice deformation starts, due to individual motion of heated ions, the relevant parameter is still the ion-sphere radius a.

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