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Lifetimes of low-energy electron excitations in metals

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Abstract

We report theoretical studies of electron and hole lifetimes in a free-electron gas as well as in real metals Al and Nb by means of the *ab initio* many-body method and semi-empirical scattering theory approach. We show that for free-electron-like excitations a simple density-of-state convolution model of the scattering theory approach (STA–DOS) is a good approximation to the *ab initio* lifetimes, the energy dependence of the STA–DOS transition matrix element being rather unimportant. The approximation of energy-independent matrix element appears to also be reasonable for Nb. A good correspondence between the STA–DOS and *ab initio* momentum-averaged results is achieved for Nb with an adjusted matrix element, although the *ab initio* lifetimes disperse greatly with respect to the averaged value.

1. Introduction

The dynamics of low-energy electron excitations in metals is of major importance for the understanding of many chemical and physical phenomena on metal surfaces [1]. A number of experimental tools and theoretical methods has been developed to study the processes of hot-electron de-excitations. One of the most powerful experimental techniques is time-resolved two-photon photoemission spectroscopy, which permits us to measure the excited electron lifetimes on a femtosecond scale [2]. Using this kind of spectroscopy, the hot-electron lifetimes have been measured for non-magnetic metals [3–8] and magnetic transition metals [9,10]. The most potent of the developed theoretical methods are the methods based on the self-energy formalism of many-body theory [11–14]. Such methods were first elaborated for the interacting free-electron gas (FEG) model by Quinn and Ferrell [15,16], who derived basic expressions for the hot-electron lifetimes within the random-phase approximation. The analytical expressions for the lifetime in the limit of small energy—small density parameter were deduced by Quinn and Ferrell [15, 16], and in the limit of small excitation energy by Ritchie and Ashley [17].

In the following research the exchange and correlation effects [18], realistic electron densities within a statistical approximation [19] and band-structure effects [20] were included in the FEG model.

Recently first-principles calculations based on many-body theory have been performed for electron lifetimes in magnesium and beryllium [21], aluminium [21, 22] and noble metals [21–25]. The hole lifetimes have been evaluated in copper [25, 26], silver [25] and gold [25, 26]. These calculations have been performed within the GW approximation for the self-energy by using the LDA pseudo-potential approach together with the plane wave Bloch basis set and also by using the LMTO approach [25], which employs a set of numerical *muffin-tin* orbitals to construct the basis Bloch functions. The *ab initio* calculations in general correctly reproduce the experimental trends, although some discrepancies between the experimental and theoretical data still remain [24, 25].

One more approach used to study the hot-electron de-excitations in solids is the scattering theory approximation (STA). In its rigorous form, [27], STA has the disadvantage of very large computational efforts to evaluate the transition matrix elements. After averaging the transition probabilities over wavevectors [28] and neglecting the exchange part of the matrix elements [29], the scattering rate (inverse lifetime) can be reduced to a simple equation which contains the convoluted density of states available for scattering and the unique energy-dependent matrix element (hereafter we call this the STA–DOS model). Within this model the scattering rates were evaluated for the first time by Kane [28] for bulk silicon. Passek *et al* [30] measured the spin-dependent lifetimes of the $n = 1$ image-potential state on Fe(110) and interpreted them by invoking the convolution of the first-principles DOS. Drouhin [31, 32] has developed a model similar to STA–DOS to evaluate the scattering cross-section and spin-dependent inelastic mean free path and applied it to some 3d- and 5d-transition metals. Zarate *et al* [33] have proposed simple approximations to the density of states to obtain analytical expressions for the electron lifetimes in transition metals. In [10] an approach proposed before by Penn *et al* [29] has been modified to include the generation of secondary electrons and applied to lifetimes in ferromagnetic metals.

Due to the physical transparency, the STA–DOS model represents an attractive alternative to the more elaborate *ab initio* approaches in the studies of momentum-averaged quasi-particle lifetimes. The greatest problem of the STA–DOS model is connected with the proper choice of the transition matrix element. In all the above-cited references the matrix elements of the model were evaluated semi-empirically from the comparison between the calculated and available experimental lifetimes. The energy dependence of the matrix elements was either neglected [31–33] or estimated by using experimental data [29]. To our knowledge, there were no attempts to justify theoretically the neglecting of the energy dependence of matrix elements. On the other hand, the evaluation of the energy dependence based on experimental data is a risky procedure in view of the differences in the experimental data derived in different research (see [23]). Besides, in many cases the quasi-particle relaxation times derived from experimental data are determined not only by the electron–electron scattering, but also by some additional processes: electron–phonon scattering, transport effects, cascade processes etc [10]. The goal of our paper is therefore to analyse the possibility of correct description of the momentum-averaged lifetimes within the STA–DOS model by choosing the value of the transition matrix element from comparisons with the results of FEG theory and of the *ab initio* LMTO–GW lifetime calculations. We do this by applying the STA–DOS model to two different metallic systems: to aluminum, which represents free-electron-like metals, and to niobium, which is an example of a metal with non-localized d electrons at the Fermi level. Electron lifetimes in Al have been calculated before using the pseudo-potential GW method [21, 22]. It was found that the evaluated lifetimes do not practically show dependence on the direction of

momentum vector. Here we discuss the energy dependence of the STA–DOS transition matrix elements that follow from the comparison between the STA–DOS model and LMTO–GW calculations. For both electrons and holes we derive some conclusions on the validity of the STA–DOS model. For Nb we show more detailed data on the momentum-resolved lifetimes and demonstrate the importance of band-structure effects, which are completely neglected in the FEG model and partially included in the STA–DOS model.

2. The methods of evaluating the hot-electron lifetimes

In the FEG theory the scattering rate of an excited electron in the initial state at energy E_i, with momentum q and velocity v_q, is calculated by using the self-energy formalism of many-body theory as [15, 16]

$$\tau^{-1} = \frac{1}{2\pi^2 q}\int_0^{(E_i-E_F)} \mathrm{d}\,\omega \int_{q^-}^{q^+} \mathrm{d}\,q\,q\,v_q \mathrm{Im}\,[-\epsilon^{-1}(q,\omega)] \tag{1}$$

where $q^{\pm} = \sqrt{2mE_i} \pm \sqrt{2m(E_i-\omega)}$ are the minimum and maximum values of momentum that can be transferred from the scattered electron to the Fermi sea, and ϵ is the Lindhard RPA dielectric function of non-interacting electrons. (We use the atomic units throughout, i.e. $e^2 = \hbar = m_e = 1$.) In the limit of a small electron density parameter r_s and a small excitation energy $E_i - E_F$ the lifetime is reduced to the simple expression [15]

$$\tau = 263 r_s^{-\frac{5}{2}}(E_i - E_F)^{-2}\ (\mathrm{fs}\times \mathrm{eV}^2) \tag{2}$$

which assumes that the so-called scaled lifetime $\tau \times (E - E_F)^2$ is energy independent and determined only by the density parameter r_s. An energy scaling qualitatively similar to that of equation (2) has been observed for electrons in the free-electron-like band-states of noble metals [23, 24].

In the STA no limitations are imposed on the shape of charge density, and the decay rate of an electron in the initial state $\phi_i(\boldsymbol{r})$ at energy E_i is determined by the probability of this primary electron scattering into a final state $\phi_f(\boldsymbol{r})$ at energy E_f. It is accompanied by a secondary electron excitation from an occupied initial state $\phi_{i'}(\boldsymbol{r})$ at energy E_i' into an unoccupied state $\phi_{f'}(\boldsymbol{r})$ at energy $E_{f'}$. In the first order of the time-dependent perturbation theory and by using the 'golden rule' this probability is written as [27]

$$P_{i,i'}^{f,f'} = 2\pi \left|[M(E_i - E_f)]_{i,i'}^{f,f'}\right|^2 \delta(E_i - E_f + E_{i'} - E_{f'}) \tag{3}$$

where M is the matrix element of the dynamically screened interaction:

$$[M(\omega)]_{i,i'}^{f,f'} = \int \mathrm{d}\boldsymbol{r}\,\mathrm{d}\boldsymbol{r}'\,\phi_i^*(\boldsymbol{r})\phi_{i'}^*(\boldsymbol{r}')M(\boldsymbol{r}-\boldsymbol{r}',\omega)\phi_f(\boldsymbol{r})\phi_{f'}(\boldsymbol{r}'). \tag{4}$$

After neglecting the exchange terms contained in equation (3) [29], performing angular averaging and summation over all the possible scatterings of primary and secondary electrons this equation is reduced to the following expression for the scattering rate of a hot electron characterized by energy E and spin coordinate σ (with $\overline{\sigma}$ being the opposite spin direction):

$$\frac{1}{\tau_\sigma(E)} = 2\pi \int_{E_F}^{E} \mathrm{d}E'\,\rho_\sigma^{>}(E') \int_{E_F-\omega}^{E_F} \mathrm{d}\varepsilon\,[\rho_\sigma^{<}(\varepsilon)\rho_\sigma^{>}(\varepsilon+\omega) + \rho_{\overline{\sigma}}^{<}(\varepsilon)\rho_{\overline{\sigma}}^{>}(\varepsilon+\omega)]|M(\omega)|^2 \tag{5}$$

where $\omega = E - E'$ is the energy loss in the primary electron de-excitation, $\rho^{>}(E) = [1 - f(E)]\rho(E)$, $\rho^{<}(E) = f(E)\rho(E)$ where $f(E)$ is the Fermi–Dirac occupation function and $\rho(E)$ is the density of states. One can then suppose that within a small energy interval the matrix element M is fairly constant [30–33]. The most drastic simplification of the STA is

achieved when one assumes that not only the matrix element but also the DOS takes a constant value ρ_S [34]:

$$\tau_\sigma(E)^{-1} = \pi\rho_S^3|M|^2(E - E_F)^2. \tag{6}$$

The similarity between equations (2) and (6) allows us to express the matrix element $|M|^2$ in terms of the FEG theory [15].

In this paper we evaluate the transition matrix elements of the STA–DOS theory by fitting the STA–DOS lifetimes to those obtained from the *ab initio* LMTO–GW method. In the LMTO–GW method [12, 35–40] the polarization function of a solid is evaluated within the RPA approximation [12]

$$\boldsymbol{P}_{i,j}(\boldsymbol{q},\omega) = \sum_{\sigma,t,\boldsymbol{k}} \sum_{n}^{occ} \sum_{n'}^{unocc} \frac{1}{t\omega - \epsilon_{\boldsymbol{k}+\boldsymbol{q},n'} + \epsilon_{\boldsymbol{k},n} + \mathrm{i}\delta} \langle B_{\boldsymbol{q},i}\psi_{\boldsymbol{k},n}|\psi_{\boldsymbol{k}+\boldsymbol{q},n'}\rangle\langle\psi_{\boldsymbol{k}+\boldsymbol{q},n'}|\psi_{\boldsymbol{k},n}B_{\boldsymbol{q},j}\rangle. \tag{7}$$

The summation includes terms with $t = \pm 1$ (electrons and holes) and spin value σ. To calculate the LDA single-particle states of a solid $\psi_{\boldsymbol{k},n}$ we employ the tight-binding version of the LMTO [36]. The basis Bloch functions $B_{\boldsymbol{q},i}$ of the polarization matrix are composed from the products of the *muffin-tin* orbitals by using the procedures of orthogonalization described in [38]. Once the polarization matrix is obtained, we evaluate the density–density response function matrix $\boldsymbol{R}$, dielectric and inverse dielectric matrices, $\boldsymbol{\epsilon}$ and $\boldsymbol{\epsilon}^{-1}$, and calculate the matrix of the screened Coulomb interaction $\boldsymbol{W}$

$$\boldsymbol{R} = \boldsymbol{P} + \boldsymbol{P}\boldsymbol{V}\boldsymbol{R} \tag{8}$$

$$\boldsymbol{\epsilon} = \boldsymbol{1} - \boldsymbol{V}\boldsymbol{P} \tag{9}$$

$$\boldsymbol{\epsilon}^{-1} = \boldsymbol{1} + \boldsymbol{V}\boldsymbol{R} \tag{10}$$

$$\boldsymbol{W} = \boldsymbol{\epsilon}^{-1}\boldsymbol{V}. \tag{11}$$

The Coulomb potential matrix $\boldsymbol{V}$ is computed by the prescriptions of [38]. We calculate the self-energy within the GW approximation of many-body theory [13]:

$$\Sigma(\boldsymbol{r},\boldsymbol{r}',\omega) = \frac{\mathrm{i}}{2\pi}\int \mathrm{d}\omega'\, G(\boldsymbol{r},\boldsymbol{r}',\omega+\omega')W(\boldsymbol{r},\boldsymbol{r}',\omega'). \tag{12}$$

In the GW method the self-energy is usually obtained by replacing the full Green function by the Green function of non-interacting electrons. The imaginary part of the correlation term in the self-energy is then expressed as [12]

$$\begin{aligned}\mathrm{Im}\,\Sigma_{\boldsymbol{q},n}(\omega) = &\sum_{\boldsymbol{k}} \sum_{n'}^{occ} \sum_{i,j} \mathrm{Im}\, W^c_{i,j}(\boldsymbol{k}, \epsilon_{\boldsymbol{k}-\boldsymbol{q},n'} - \omega) \\ &\times \langle\psi_{\boldsymbol{q},n}\psi_{\boldsymbol{k}-\boldsymbol{q},n'}|B_{\boldsymbol{k},i}\rangle\langle B_{\boldsymbol{k},j}|\psi_{\boldsymbol{k}-\boldsymbol{q},n'}\psi_{\boldsymbol{q},n}\rangle\Theta(\epsilon_{\boldsymbol{k}-\boldsymbol{q},n'} - \omega)\end{aligned} \tag{13}$$

when $\omega \leqslant \mu$, and

$$\begin{aligned}\mathrm{Im}\,\Sigma_{\boldsymbol{q},n}(\omega) = &-\sum_{\boldsymbol{k}} \sum_{n'}^{unocc} \sum_{i,j} \mathrm{Im}\, W^c_{i,j}(\boldsymbol{k}, \omega - \epsilon_{\boldsymbol{k}-\boldsymbol{q},n'}) \\ &\times \langle\psi_{\boldsymbol{q},n}\psi_{\boldsymbol{k}-\boldsymbol{q},n'}|B_{\boldsymbol{k},i}\rangle\langle B_{\boldsymbol{k},j}|\psi_{\boldsymbol{k}-\boldsymbol{q},n'}\psi_{\boldsymbol{q},n}\rangle\Theta(\omega - \epsilon_{\boldsymbol{k}-\boldsymbol{q},n'})\end{aligned} \tag{14}$$

when $\omega > \mu$.

$W^c = W - V$ is the correlation part of the screened potential. The real part of the self-energy is calculated by the Hilbert transform. The many-body self-energy corrections to the LDA eigenvalues $\epsilon_{\boldsymbol{q},i}$ are determined by the expectation values of the operator $\Delta\Sigma(\omega) = \Sigma(\omega) - V^{xc}_{LDA}$, where V^{xc}_{LDA} is the LDA exchange–correlation potential.

Table 1. The calculated dependence of the squared STA–DOS transition matrix element on the electron density parameter r_s at an excitation energy of 1 eV.

r_s	1.0	1.5	1.75	2.0	2.25	2.5	2.75	3.0	3.25	3.50	3.75	4.0
M^2 (eV^2) (electrons)	0.013	0.120	0.28	0.57	1.12	1.84	3.22	5.02	7.12	10.08	13.62	17.17
M^2 (eV^2) (holes)	0.013	0.120	0.28	0.57	1.14	2.32	3.92	5.76	8.64	13.20	21.66	30.43

Namely, from the first-order perturbation theory we have the Dyson equation for the complex quasiparticle energy

$$E_{q,i}(\omega) = \epsilon_{q,i} + \langle \psi_{q,i} | \Delta\Sigma_{q,i}(\omega) | \psi_{q,i} \rangle. \tag{15}$$

We solve this equation retaining only the linear part of the dependence of Re $\Delta\Sigma$ on ω near the LDA eigenvalue and neglecting the change of Im $\Delta\Sigma$. In this approximation the self-energy corrections to the LDA eigenvalues are

$$\Delta\epsilon_{q,i} = E_{q,i} - \epsilon_{q,i} = Z_{q,i}\Delta\Sigma_{q,i}(\epsilon_{q,i}) \tag{16}$$

where

$$Z_{q,i} = \left[1 - \frac{\partial \mathrm{Re}\,\Delta\Sigma_{q,i}(\omega)}{\partial\omega}\right]^{-1}_{\omega=\epsilon_{q,i}} \tag{17}$$

is the so-called re-normalization factor. The imaginary part of the self-energy correction gives then the line-width of the excitation, and the inverse value determines the lifetime of excitation [14]

$$\tau^{-1}_{q,i} = 2|\mathrm{Im}\,\Delta\epsilon_{q,i}|. \tag{18}$$

For a given excitation energy we average the calculated lifetimes over $\boldsymbol{q}$, i, taking into account the degeneracy of q-vectors in the Brillouin zone. Then substituting the *ab initio* densities of states and averaged lifetimes into equation (5) we evaluate the STA energy-dependent matrix element and choose the energy-independent matrix element.

3. The lifetimes of excited electrons in a free-electron gas, aluminum and niobium

In figure 1 we present some of the typical results of our FEG calculations. The inset in (*a*) shows the energy dependence of the STA–DOS matrix element M^2 calculated at the electron density parameter $r_s = 2.0$, which is close to the value $r_s = 2.06$ of aluminum. The density of states in the FEG was normalized to the 'unit-cell' volume equal to 100 au^3. In the energy range of interest, from -5 to 5 eV, the change of matrix element does not exceed 30%. With the M^2 value fixed in the interval between 0.4 and 0.6 eV^2 the energy variation of the STA–DOS lifetimes agrees well with the results of rigorous FEG theory, so we define the energy argument of the matrix element as equal to 1 eV, and show in (*a*) the dependence of matrix element on the density parameter. The numerical values of M^2 are given in table 1. Using these data one can calculate lifetimes for any r_s straightforwardly from equation (5). The quality of such calculations is characterized by (*b*) and (*c*), where the results of the FEG theory and STA–DOS approach are compared at $r_s = 2$. In the whole energy range of interest the agreement is very good, except for a $\sim$10% difference at an energy of about 0.5 eV.

In figures 2 and 3 we present the data on aluminum that demonstrate the possibility of using the STA–DOS approach with fixed transition probability for the lifetime calculations in

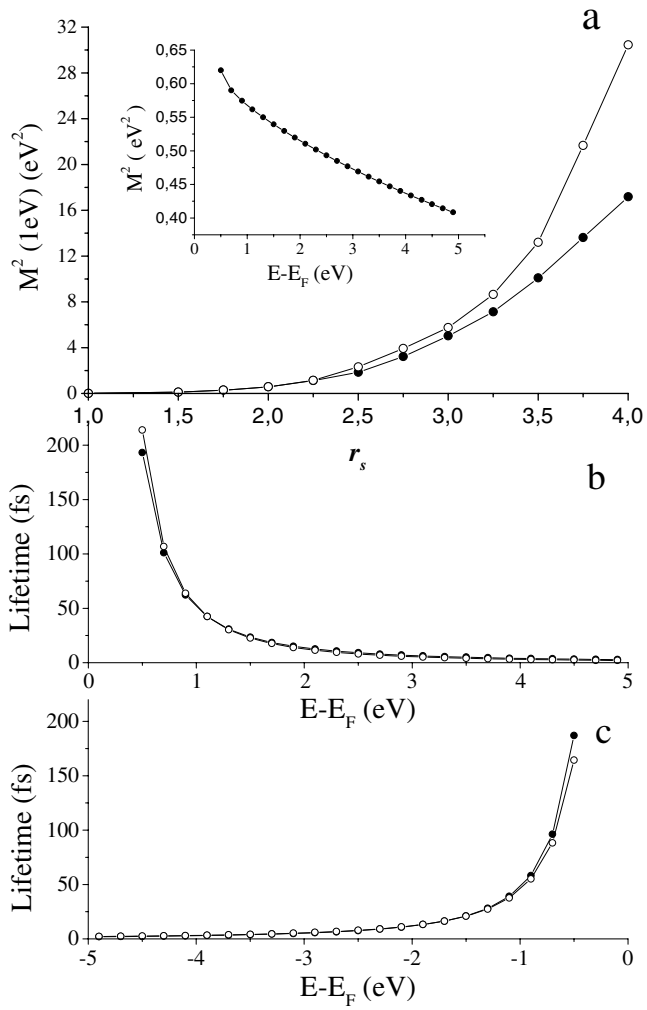

Figure 1. The lifetimes of electrons and holes in a FEG. (*a*) The calculated dependence of the STA–DOS transition matrix elements on the electron density parameter r_s for an excitation energy of 1 eV. Solid and open circles correspond to electrons and holes, respectively. The inset shows the energy dependence of the transition matrix element for $r_s = 2.0$. (*b*) The calculated energy dependence of the electron lifetimes in a FEG with $r_s = 2.0$. Solid circles indicate the results of a rigorous FEG calculation; open circles represent the results of the STA–DOS calculation carried out with a fixed transition matrix element. (*c*) The computed energy dependence of the hole lifetimes in a FEG with $r_s = 2.0$. The notations are the same as in (*b*).

real free-electron-like metals. Figure 2 shows that at energy from -12 to -5 eV the density of states in Al is close to that of a FEG with $r_s = 2.06$, whereas some deviations from the free-electron behaviour are observed at higher energy. Panel (*a*) of figure 3 presents the energy dependence of the matrix element of STA–DOS method as calculated from the comparison with the LMTO–GW lifetimes. The convolution of the DOS sweeps out the DOS variations near the Fermi energy and the change of M^2 appears to be rather smooth, thus indicating the possibility of using a fixed transition probability. In particular, variations in M^2 of electrons do not exceed 15%. In order to use the fixed M^2 values of table 1, normalized to the unit-cell

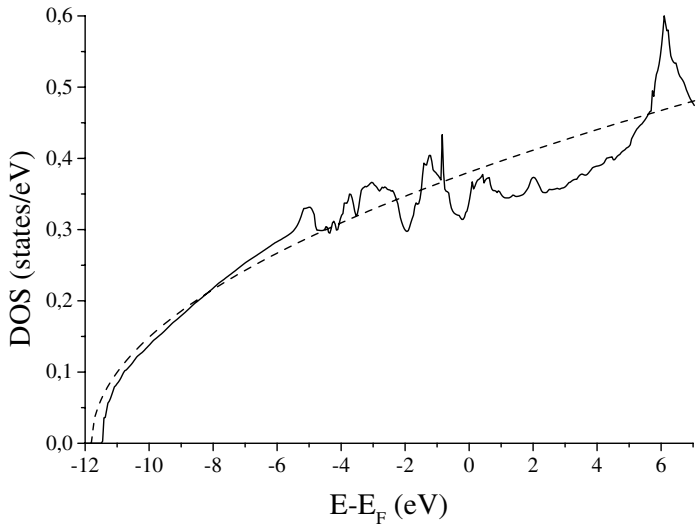

Figure 2. The total density of states in Al. The solid curve shows the LMTO calculation results; the dashed curve represents the FEG DOS for $r_s = 2.06$.

volume $V_0 = 100$ au^3, we recalculate them in accordance with the real unit-cell volume V as $M^2 = M(V_0)(V_0/V)^2$. The value $M^2 = 0.58$ eV^2 obtained in this way is very close to that of figure 3(a) at an energy of 1 eV. The comparison between the electron and hole lifetimes calculated by the LMTO–GW method and by the STA–DOS approach with this value of the matrix element shows almost perfect agreement (see figures 3(b) and (c)).

Hence, our calculations show that the STA–DOS model with fixed transition matrix element, determined from comparisons between STA–DOS and FEG theory and presented in table 1, provides a simple method of evaluating the lifetimes in real free-electron-like metals with the precision comparable to that of the *ab initio* LMTO–GW method.

In figure 4 we show the density of states of body-centred-cubic (bcc) Nb, that differs drastically from that of free-electron-like metals. From this DOS one may suppose that the band-structure effects in Nb lifetimes can be very important. In figure 5 we present both energy- and momentum-resolved (diamonds) and momentum-averaged (thick curve) electron lifetimes calculated by the LMTO–GW method. The averaged lifetime is determined mainly by the lifetimes of the big number of low-symmetry q-points that are far from the Γ–H direction. The lifetimes of states belonging to the Γ–H direction (in figure 5 connected by the dashed curve) are much higher then the averaged values. The lifetimes of the states with q-vectors close to the Γ–H direction also deviate from the averaged curve. Strong momentum dependence is well seen in the energy- and momentum-resolved scaled lifetimes $\tau(E) \times (E - E_F)^2$ shown in the inset in figure 5.

So the *ab initio* LMTO calculations reveal some deviations of the energy- and momentum-resolved electron lifetimes in Nb from the predictions of FEG theory. Nevertheless, the analysis of averaged lifetimes even in this case finds reminiscences of the free-electron-like properties. This can be followed by figure 6, where we present the averaged electron and hole lifetimes and, in the insets, the matrix elements of the STA–DOS theory evaluated by equating the LMTO and STA–DOS lifetimes. In spite of great variations of DOSs near the Fermi energy, the changes of the M^2 values with energy appear to be rather smooth, which makes it possible to choose relevant M^2 averaged values equal to 0.055 eV^2 for electrons and 0.065 eV^2 for holes.

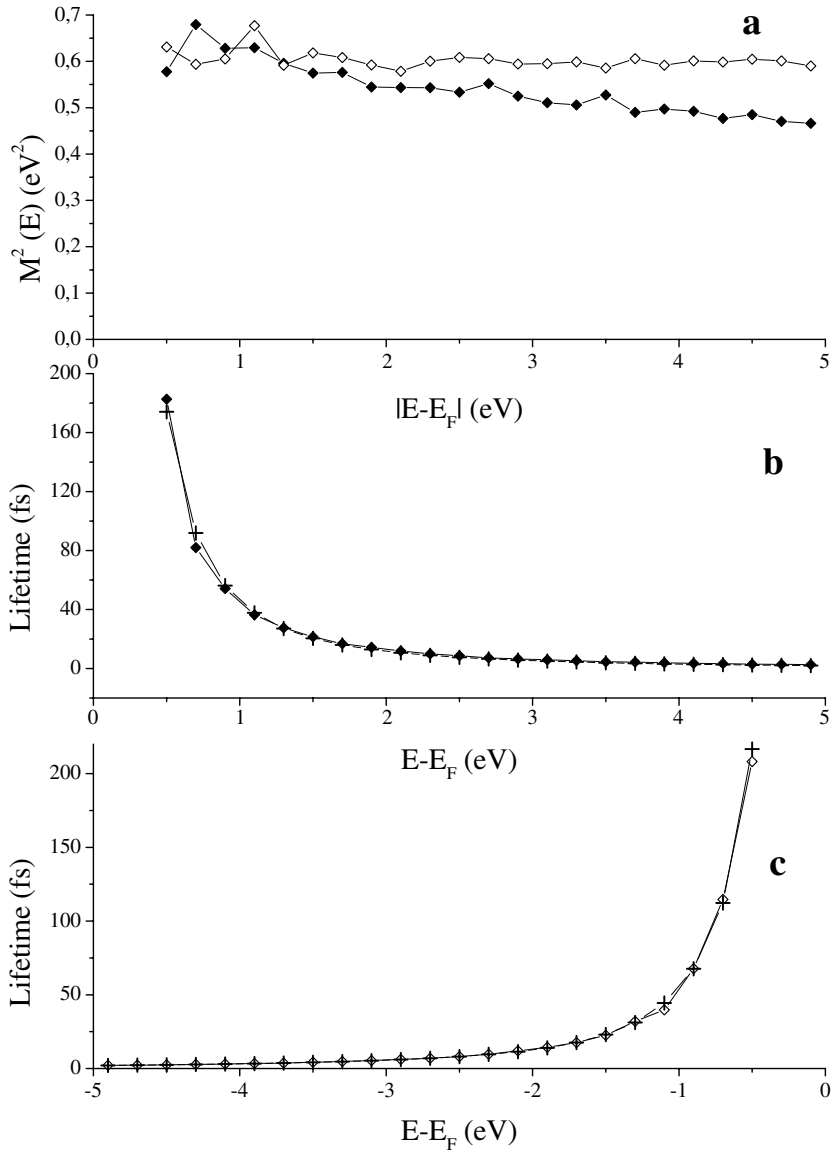

Figure 3. The calculated quasiparticle lifetimes in Al. (*a*) The energy dependence of the STA–DOS transition matrix element. Solid and open diamonds correspond to electron and hole excitations, respectively. (*b*) The calculated energy dependence of the electron lifetimes. Solid diamonds represent the results of the LMTO–GW calculation; crosses show the results of the STA–DOS calculation with a fixed transition matrix element (see text). (*c*) The computed energy dependence of the hole lifetimes. The LMTO–GW calculation results are denoted by open diamonds and the STA–DOS data evaluated with a fixed matrix element are indicated by crosses.

These values are much lower than the corresponding FEG transition probabilities evaluated from table 1 at the formal electron density parameter of Nb, $r_s = 1.78$. Nevertheless, with these averaged M^2 values the correspondence between the LMTO and STA–DOS lifetimes is very good for both electrons and holes.

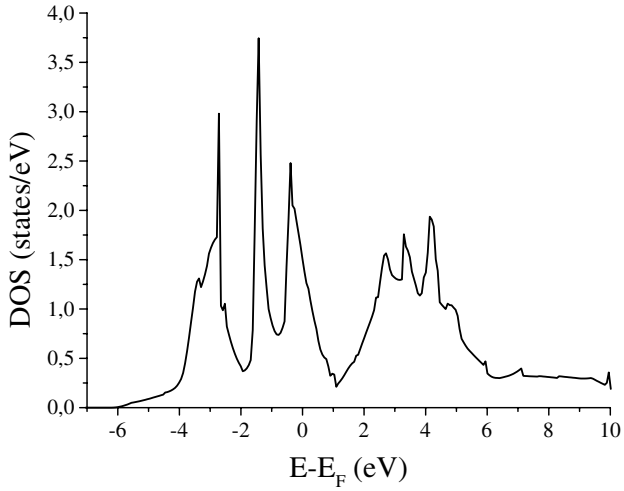

Figure 4. The total density of states in Nb as calculated by the LMTO tight-binding method.

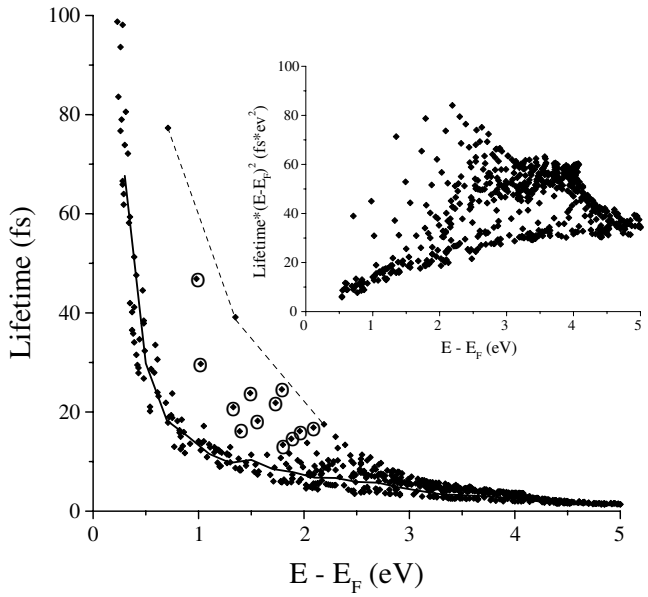

Figure 5. Electron lifetimes in Nb as calculated by the LMTO–GW method. Solid diamonds represent the energy- and momentum-resolved lifetimes. The solid curve shows the hot-electron lifetimes averaged over momenta. By the dashed curve are connected the lifetimes of the band-states belonging to the Γ–H direction of the Brillouin zone, whereas the lifetimes of some states with momentum vectors close to the Γ–H direction are surrounded by circles. Scaled lifetimes are shown in the inset.

4. Conclusions

The main objective of our work was to assess the feasibility of evaluating the lifetimes of excited electrons in free-electron-like metals and d-electron metals by employing the simple DOS convolution model of the scattering theory. We did this based on the FEG lifetime calculations and on the *ab initio* LMTO–GW calculations for aluminum and niobium.

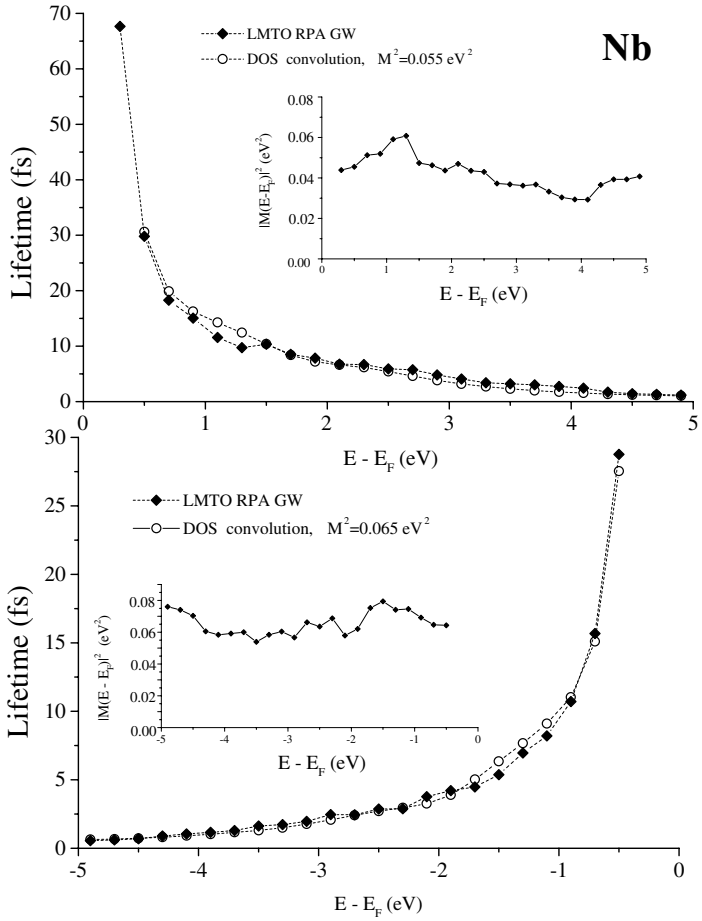

Figure 6. The LMTO and STA–DOS calculated quasiparticle lifetimes in Nb. Upper panel: electron lifetimes. Solid diamonds show the energy-resolved (averaged over momenta) lifetimes computed by the LMTO–GW method; open circles indicate the lifetimes evaluated by using the STA–DOS approach with a fixed transition matrix element. The inset represents the energy dependence of the STA–DOS transition matrix element. Lower panel: hole lifetimes. The notations are the same as in the upper panel.

The performed evaluations show that the approximation of constant transition matrix element of the STA–DOS approach is good for the lifetimes of excited states in FEG. Moreover, the calculations for Al testify that the STA–DOS approach can be used to calculate the momentum-averaged lifetimes in real free-electron-like metals in good agreement with the LMTO–GW theory, employing the tabulated values of transition matrix element.

By contrast, the hot-electron lifetimes in Nb show great dispersion with respect to the momentum-averaged values. The calculated lifetimes appear to be far from the predictions of the FEG theory. Nevertheless, the approximation of energy-independent transition matrix element of the STA–DOS approach appears to be also good, and with a proper choice of the averaged transition probability the STA–DOS lifetimes are in good agreement with the momentum-averaged *ab initio* LMTO–GW values.

The calculations for some free-electron-like and transition metals that can confirm these conclusions are in progress now.

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