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# Electron–phonon interaction and hole (electron) lifetimes on Be(0001)

I.Yu. Sklyadneva [a,b,*], E.V. Chulkov [a,c], P.M. Echenique [a,c], A. Eiguren [a]

[a] Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain
[b] Institute of Strength Physics and Materials Science, pr. Academicheski 2/1,634021 Tomsk, Russia
[c] Depto. de Física de Materiales and Centro Mixto CSIC-UPV/EHU, Facultad de Ciencias Químicas, UPV/EHU Apdo. 1072, 20080 San Sebastián/Donostia, Basque Country, Spain

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**Abstract**

We report an ab initio study of electron–phonon interactions on the Be(0001) surface. The calculations based on density-functional theory were carried out using a linear response approach in the plane-wave pseudopotential representation. The phonon-induced contribution to excited hole (electron) lifetime broadening is calculated for the zone center surface state. The obtained results show a rather strong momentum dependence.


*Keywords:* Metal surfaces; Surface dynamics; Electron–phonon coupling

Recently the electron–phonon (e–ph) coupling at metal surfaces has attracted much attention because a variety of physical phenomena appears to be determined by phonons and their interactions with electrons. In particular, it contributes to final lifetimes of excited electrons and holes, being especially important at energies close to the Fermi level ($E_F$) [1–3]. The present study of the phonon-induced decay of electronic surface states is devoted to the Be(0001) surface, which has received a considerable experimental and theoretical attention due to its unusual electronic properties with respect to the bulk Be [4–7]. For instance, a relatively large surface density of states near $E_F$ makes the electron structure of the surface more free-electron like than that of the bulk [4,5] and results in a distinct character of the e–ph interactions. Indeed, photoemission measurements for the zone center surface state on Be(0001) [7–9] give the value of $\lambda$, e–ph coupling parameter, at $E_F$ in the range from 0.65 to 1.25 that is significantly larger than the theoretical $\lambda = 0.21$–$0.24$ obtained at $E_F$ for bulk Be [10,12]. However, there is a rather large scatter between the experimental data. It can be explained by technical errors as well as by using the bulk Debye temperature, which could be quite different from that at the surface [9]. In this situation, valuable information on e–ph coupling can be obtained from ab initio calculations, which can be done for any wave vector in the Brillouin zone (BZ). The first ab initio study of the e–ph coupling on Be(0001) [13] has been performed for the zone center surface state in the binding energy range from the $\overline{\Gamma}$ point to $E_F$. However, the results presented in Ref. [13] including the Eliashberg function and the e–ph contribution to the real and imaginary parts of self-energy as well as the coupling parameter were averaged over momentum.

Here we present a first-principles study of the e–ph coupling and its contribution to the excited hole (electron) lifetime broadening both energy and momentum resolved. We have considered the $\overline{\Gamma}$ point surface state on Be(0001) and calculated the Eliashberg spectral function $\alpha^2F(\omega)$, $\lambda$, and the phonon-induced contribution to the lifetime broadening, $\Gamma_{e-ph}$, as functions of energy and momentum. We show that the energy variation of both $\lambda$ and $\Gamma_{e-ph}$ on going from the $\overline{\Gamma}$ point to the Fermi level depends strongly on momentum.

The phonon-induced lifetime broadening $\Gamma_{e-ph}(\epsilon_{\mathbf{k}_i})$ of an electron state with momentum $\mathbf{k}_i$ and energy $\epsilon_{\mathbf{k}_i}$ is related to

* Corresponding author. Address: Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain.
*E-mail address:* swxskski@sc.ehu.es (I.Yu. Sklyadneva).

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the Eliashberg spectral function [14] through the integral over all the scattering events that conserve energy and momentum [10,11]:

$$\Gamma_{\text{e-ph}}(\epsilon_{\mathbf{k}_i}) = 2\pi\hbar \int_0^{\omega_m} \alpha^2 F_{\mathbf{k}_i}(\omega)[1 - f(\epsilon_{\mathbf{k}_i} - \omega) + f(\epsilon_{\mathbf{k}_i} + \omega) + 2n(\omega)]\mathrm{d}\omega. \quad (1)$$

Here, $f$ and $n$ are the Fermi and Bose distribution functions and $\omega_m$ is the maximum phonon frequency. The Eliashberg spectral function is given by

$$\alpha^2 F_{\mathbf{k}_i}(\omega) = \sum_{\mathbf{q},\nu,f} \delta(\omega - \omega_{\mathbf{q},\nu}) |g(\mathbf{k}_i, \mathbf{k}_f, \mathbf{q}, \nu)|^2 \delta(\epsilon_{\mathbf{k}_i} - \epsilon_{\mathbf{k}_f}), \quad (2)$$

where $g(\mathbf{k}_i, \mathbf{k}_f, \mathbf{q}, \nu)$—the e–ph matrix element which reflects the probability of electron scattering from the initial state $\mathbf{k}_i$ and energy $\epsilon_{\mathbf{k}_i}$ to the final state $\mathbf{k}_f$ with energy $\epsilon_{\mathbf{k}_f}$ by the phonon $(\mathbf{q},\nu)$. We apply in Eq. (2) the usual quasielastic assumption that $\delta(\epsilon_{\mathbf{k}_i} - \epsilon_{\mathbf{k}_f} \pm \omega_{\mathbf{q},\nu}) \approx \delta(\epsilon_{\mathbf{k}_i} - \epsilon_{\mathbf{k}_f})$. The sum in Eq. (2) is carried out over final electron states $\mathbf{k}_f$ and all possible phonon modes. The e–ph coupling constant is defined as [10]

$$\lambda_{\mathbf{k}_i} = 2 \int_0^{\omega_m} \frac{\alpha^2 F_{\mathbf{k}_i}(\omega)}{\omega} \mathrm{d}\omega. \quad (3)$$

The calculations have been performed within the local density approximation using the PWSCF code [15] and the density-functional perturbation theory [16]. A nonlocal norm-conserving pseudopotential with nonlinear core corrections [17] and a plane-wave basis set restricted by the kinetic energy cutoff of 22 Ry were used. To describe the surface we have considered a fully relaxed 12-layer Be slabs separated by eight atomic layers of vacuum. In the surface BZ (SBZ) integrations we used 30 special points in the irreducible wedge of SBZ (ISBZ) and the first-order Hermite–Gaussian smearing technique [18] with a width of 0.02 Ry. The computed surface band structure is shown in Fig. 1. The surface state is indicated by a bold line. To calculate the Eliashberg spectral function the summation over the phonons $(\mathbf{q}, \nu)$ in Eq. (2) was performed with more than 60 points in the ISBZ. The delta function with electron energies was approximated by the first-order Hermite–Gaussian function with a smearing width in the range of 0.01–0.03 Ry. The estimated numerical error for the surface state broadening is found to be not larger than ~6%.

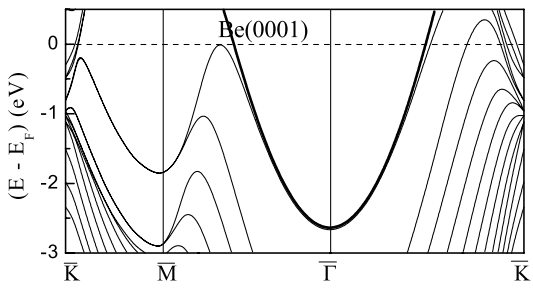


Fig. 1. Electronic band structure of a fully relaxed 12-layer Be(0001) slab. The surface state at the $\bar{\Gamma}$ point is indicated by a bold line.

Let us consider now how the surface electron state couples to phonons and how this coupling varies with momentum and energy. We have calculated the Eliashberg spectral function for a number of states with different energies along the $\overline{\Gamma K}$ and $\overline{\Gamma M}$ symmetry directions. In Fig. 2 we show $\alpha^2 F_{\mathbf{k}_i}(\omega)$ and $\lambda_{\mathbf{k}_i}$ for the surface states at the energy of $(E - E_F) = -1.07$ eV (Fig. 2b) and at $E_F$ (Fig. 2c) as well as for the surface state at the $\bar{\Gamma}$ point (Fig. 2a). As follows from the figure, the Eliashberg spectral functions for the states in the $\overline{\Gamma K}$ direction do not differ substantially on moving to the $E_F$ while for the surface states in the $\overline{\Gamma M}$ direction the e–ph coupling increases strongly. A peak in $\alpha^2 F_{\mathbf{k}_i}(\omega)$ observed at the phonon energies of ~40 meV comes from the Rayleigh mode scattering. Its magnitude is determined both the energy and momentum position of a hole state. As one can see, the largest contribution from the Rayleigh mode scattering is obtained for the states in the $\overline{\Gamma M}$ direction, especially near the Fermi level. At the $\bar{\Gamma}$ point $\lambda_{\mathbf{k}_i}$ is small and in the $\overline{\Gamma K}$ direction becomes twice as much showing a negligible variation with the hole energy on moving to the $E_F$. On the contrary, $\lambda_{\mathbf{k}_i}$ for the states along the $\overline{\Gamma M}$ direction enhances significantly, up to $\lambda_{\overline{\Gamma M}} = 1.17$ at the Fermi level, and exhibits a rather strong energy dependence. Thus, the energy variation of $\lambda$ for the $\bar{\Gamma}$ surface state on Be(0001) depends strongly on the $\mathbf{k}$ position. Having calculated Eliashberg spectral functions we evaluated the e–ph contribution, $\Gamma_{\text{e-ph}}$, to the total hole lifetime broadening as a function of energy and momen-

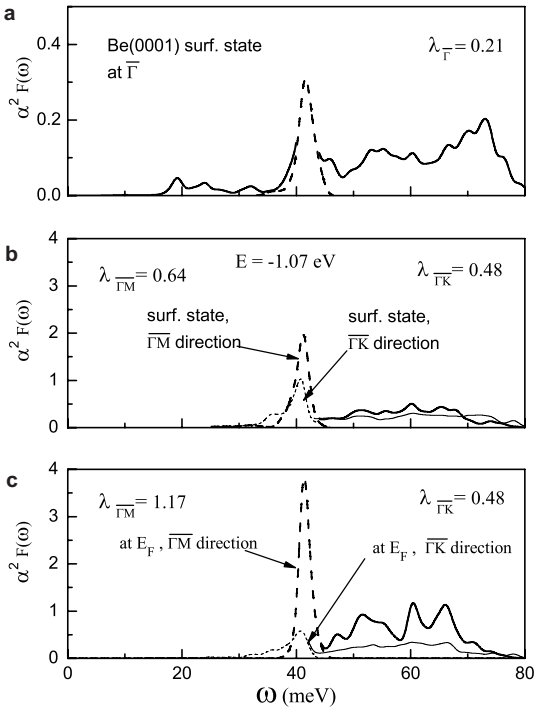


Fig. 2. The electron–phonon spectral function $\alpha^2 F_{\mathbf{k}_i}(\omega)$ is shown for the hole state at the $\bar{\Gamma}$ point (a) and for the hole states at the energy $(E - E_F) = -1.07$ eV (b) as well at $E_F$ (c) in the $\overline{\Gamma K}$ (thin lines) and $\overline{\Gamma M}$ (bold lines) symmetry directions. The contribution from the Rayleigh mode scattering is indicated by a dashed line.

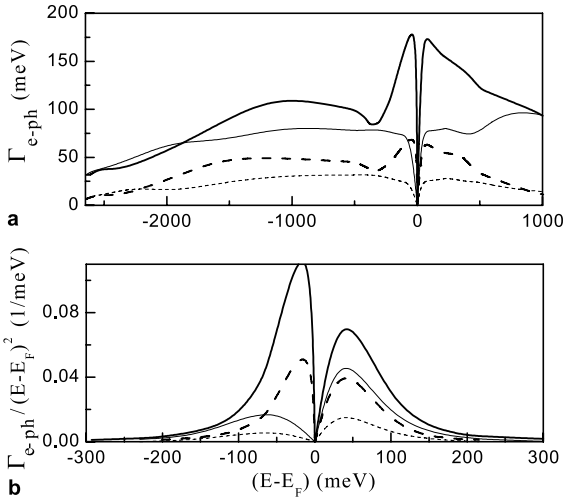


Fig. 3. (a) The $T = 0$ phonon-induced hole (electron) lifetime broadening, $\Gamma_{e-ph}$, as a function of energy for the $\overline{\Gamma}$ surface state along $\overline{\Gamma M}$ (bold line) and $\overline{\Gamma K}$ (thin line) symmetry directions. The contribution from the Rayleigh mode scattering is indicated by a dashed line. (b) $\Gamma_{e-ph}$ divided by $(E - E_F)^2$ as a function of energy. The notations are the same.

tum. The top panel of Fig. 3 gives the energy dependence of $\Gamma_{e-ph}$ at $T = 0$ for the states along the $\overline{\Gamma M}$ and $\overline{\Gamma K}$ directions. $\Gamma_{e-ph}$ averaged over momentum as a function of energy has been evaluated in Ref. [13]. The lower panel shows $\Gamma_{e-ph}$ divided by $(E - E_F)^2$ for the same states. As follows from the figure, the e–ph contribution to the lifetime broadening varies fast around $E_F$ for electron energies smaller than the maximum phonon energy. A notable variation is also observed on moving along the $\overline{\Gamma M}$ symmetry direction to the Fermi level. In the latter case, $\Gamma_{e-ph}$ increases by a factor of 5 near the $E_F$. On the contrary, along the $\overline{\Gamma K}$ symmetry direction as well as in the case of the function averaged over momentum (see Ref. [13]), $\Gamma_{e-ph}$ experiences only slight variations. These results indicate a rather strong momentum dependence of the e–ph coupling.

In summary, we presented a first-principles study of the momentum-resolved electron–phonon contribution to the hole (electron) lifetime broadening for the zone center surface state on the Be(0001) surface. The obtained results for the phonon-induced lifetime broadening $\Gamma_{e-ph}$ and electron–phonon coupling parameter show a strong dependence on the $\mathbf{k}$ position. In particular, $\lambda_{\mathbf{k}_i}$ varies from 0.21 to 1.17 as a function of energy and momentum for the states in the $\overline{\Gamma M}$ direction and remains almost the same along $\overline{\Gamma K}$ up to the Fermi level.

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## References

[1] P.M. Echenique, R. Berndt, E.V. Chulkov, Th. Fauster, A. Goldmann, U. Höfer, Surf. Sci. Rep. 52 (2004) 219.
[2] A. Eiguren, B. Hellsing, F. Reinert, G. Nicolay, E.V. Chulkov, V.M. Silkin, S. Hüfner, P.M. Echenique, Phys. Rev. Lett. 88 (2002) 066805.
[3] J.E. Gayone, S.V. Hoffmann, Z. Li, Ph. Hofmann, Phys. Rev. Lett. 91 (2003) 127601.
[4] R.A. Bartynski, E. Jensen, T. Gustafsson, E.W. Plummer, Phys. Rev. B 32 (1985) 1921.
[5] E.V. Chulkov, V.M. Silkin, E.N. Shirykalov, Surf. Sci. 188 (1987) 287.
[6] E.W. Plummer, J.B. Hannon, Prog. Surf. Sci. 46 (1994) 149.
[7] T. Balasubramanian, E. Jensen, X.L. Wu, S.L. Hulbert, Phys. Rev. B 57 (1998) R6866.
[8] M. Hengsberger, D. Purdie, P. Segovia, M. Garnier, Y. Baer, Phys. Rev. Lett. 83 (1999) 592.
[9] S. LaShell, E. Jensen, T. Balasubramanian, Phys. Rev. B 61 (2000) 2371.
[10] G. Grimvall, The Electron–Phonon Interaction in Metals, North-Holland, Amsterdam, New York, Oxford, 1981.
[11] B. Hellsing, A. Eiguren, E.V. Chulkov, J. Phys.: Condens. Matter 14 (2002) 5959.
[12] I.Yu. Sklyadneva, E.V. Chulkov, W.-D. Schöne, V.M. Silkin, R. Keyling, P.M. Echenique, Phys. Rev. B 71 (2005) 174302.
[13] A. Eiguren, S. de Gironcoli, E.V. Chulkov, P.M. Echenique, E. Tosatti, Phys. Rev. Lett. 91 (2003) 166803.
[14] G.M. Eliashberg, Zh. Eksp. Teor. Fiz. 38 (1960) 966 [Sov. Phys. JETP 11 (1960) 696].
[15] S. Baroni, S. de Gironcoli, A.D. Corso, P. Giannozzi. Available from: <http://www.pwscf.org>.
[16] S. Baroni, S. de Gironcoli, A.D. Corso, P. Giannozzi, Rev. Mod. Phys. 73 (2001) 515.
[17] N. Troullier, J.L. Martins, Phys. Rev. B 43 (1991) 1993.
[18] M. Methfessel, A.T. Paxton, Phys. Rev. B 40 (1989) 3616.