

# Electron–phonon interaction in a free standing beryllium monolayer

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## Abstract

We report ab initio study of the electron–phonon coupling in a free standing Beryllium monolayer. The calculations were carried out using a linear–response approach in the plane–wave pseudopotential representation. The Eliashberg spectral function  $\alpha^2F(\omega)$  and the electron–phonon coupling parameter  $\lambda$  are evaluated at the Fermi level. The obtained results show a large contribution to the electron–phonon coupling from the low-energy transverse mode scattering.

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## 1. Introduction

Systems with two dimensional translation symmetries have been extensively studied during the last decades for a variety of different phenomena such as: surface states, surface reconstructions, surface magnetism or metal non-metal transitions. Today it is well known that the effect of reducing the dimensionality of a system can change dramatically its properties, this is why a better understanding of surfaces and, in particular, of monolayers, may be very helpful whenever we describe materials with a clear layered structure such as graphite or the MgB<sub>2</sub> superconductor.

In the present work, we study for the first time the role of the electron–phonon (e–ph) coupling in a metal monolayer, Be(0001). The electron–phonon interactions produce a finite phonon lifetime as well as contribute to final lifetimes of excited electrons and holes. They are responsible for the enhancement of the effective electron mass as it is measured in experiments of electronic heat capacity [1]. Moreover, in the framework of the Migdal–Eliashberg theory of superconductivity, the transition temperature to the

superconducting state is determined by the Eliashberg spectral function which reflects the effectiveness of a certain phonon with energy  $\hbar\omega$  to scatter an electron at the Fermi surface to another place of the same surface. A lot of work has been done for the e–ph coupling in bulk metals [1–3]. Recently, few calculations of the e–ph interaction on metal surfaces have been published [4], where the important role of surface phonon modes was emphasized. These vibrations are normally much softer than the bulk ones and couple in a very efficient way to electrons, giving a strong contribution the spectral function  $\alpha^2F(\omega)$  and the e–ph coupling parameter  $\lambda$ . For example, in the case of Be, there is a factor of two between the bulk value of  $\lambda_{\text{bulk}} = 0.21\text{--}0.24$  [1,3] and  $\lambda$  at the Fermi level ( $E_F$ ) calculated for the Be(0001) surface [4].

Here, for the first time we have tackled the limit case of a single layer in the study of the e–ph interaction. In such systems the contribution of soft phonons polarized perpendicular to the surface is bigger than in any of the above cases, so it can results in the value of  $\lambda$ .

## 2. Theory

E–ph coupling is described by the matrix elements that relate the electron transition from an initial electronic state

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(*i*) to a final state (*f*) through the absorption (emission) of a phonon. These matrix elements are given by (in atomic units) [1]:

$$g_{\mathbf{q}\nu}(\mathbf{k}, i, f) = \sqrt{\frac{\hbar}{2M\omega_{\mathbf{q}\nu}}} \langle \psi_{f, \mathbf{k}+\mathbf{q}}^0 | \varepsilon_{\mathbf{q}, \nu} \cdot \delta V_{\mathbf{q}}^{scf} | \psi_{i, \mathbf{k}}^0 \rangle \quad (1)$$

Here,  $\mathbf{k}$  and  $\mathbf{q}$  are momenta of electrons and phonons, respectively. The Fermi golden rule allows us to define phonon lifetimes due to the e–ph interaction.

$$\gamma_{\mathbf{q}\nu} = 2\pi\omega_{\mathbf{q}\nu} \sum_{i,f} \int \frac{d^3k}{\Omega_{\text{BZ}}} |g_{\mathbf{q}\nu}(\mathbf{k}, i, f)|^2 \times \delta(\epsilon_{\mathbf{k}, i} - \epsilon_F) \delta(\epsilon_{\mathbf{k}+\mathbf{q}, f} - \epsilon_F) \quad (2)$$

Note that this expression has been obtained under the quasielastic approximation where  $\delta(\epsilon_{\mathbf{k}, i} - \epsilon_F \pm \omega_{\mathbf{q}\nu}) \approx \delta(\epsilon_{\mathbf{k}, i} - \epsilon_F)$ . Finally, we are able to obtain the Eliashberg spectral function averaged at the Fermi level and the dimensionless mass enhancement parameter [5]:

$$\alpha^2 F(\omega) = \frac{1}{2\pi N(\epsilon_F)} \sum_{\mathbf{q}, \nu} \delta(\omega - \omega_{\mathbf{q}\nu}) \frac{\gamma_{\mathbf{q}\nu}}{\omega_{\mathbf{q}\nu}}, \quad (3)$$

$$\lambda = 2 \int d\omega \alpha^2 F(\omega) / \omega = \frac{1}{\pi N(\epsilon_F)} \sum_{\mathbf{q}, \nu} \frac{\gamma_{\mathbf{q}\nu}}{\omega_{\mathbf{q}\nu}^2}. \quad (4)$$

### 3. Results and discussion

All calculations have been performed using the density-functional perturbation theory [6] and the PWSCF code [7]. To describe the electron–ion interaction in Be atoms we used a non-local norm-conserving pseudopotential with non-linear core corrections [8] and a plane-wave basis. The basis set was restricted by a kinetic energy cut-off of 32 Ry which was found to be sufficient for the convergence criteria. We have considered Be(0001) monolayers separated by a  $\sim 28$  a.u. thick vacuum region. Atomic positions in the monolayer were fully relaxed to find an equilibrium lattice parameter. In our case of hexagonal geometry, the obtained value of  $a$  is 3.95 a.u. In the Brillouin zone (BZ) integrations we used 154 special points in the irreducible wedge of the BZ and the first-order Hermite–Gaussian smearing technique [9] with a width of 0.02. The computed band structure and density of states (DOS) are shown in Fig. 1. All the energies are referred to the Fermi level. As follows from the figure, the electronic properties of the monolayer are very distinct from those of the bulk Be. In particular, the bulk electron density of states has a very deep minimum at  $E_F$  making this material nearly semiconducting [10] whereas for the monolayer a relatively large DOS near  $E_F$  is obtained. The evaluated phonon spectrum along the high symmetry directions is shown in Fig. 2. As one can see, unlike the phonon modes with in-plane displacements of atoms the lowest transverse mode corresponding to the motion along the normal to the monolayer ( $z$ -polarized) is softened especially in the zone center where it is very shallow. Such a behavior results from the broken bonds in this direction because the dynamical properties

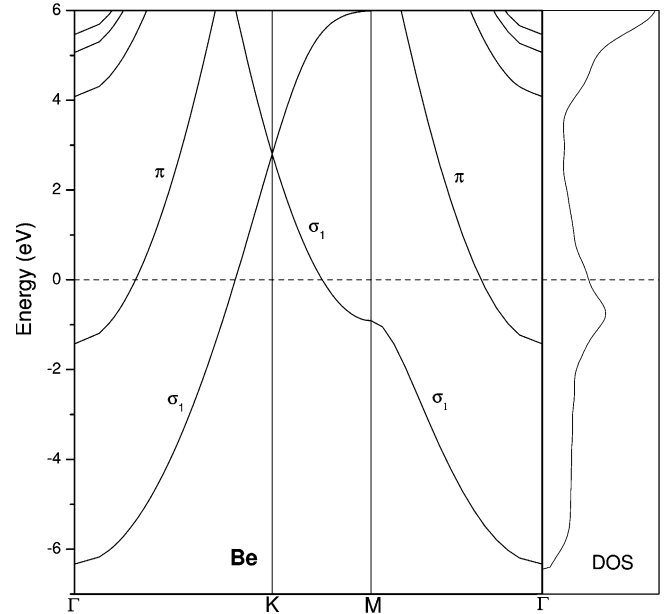


Fig. 1. Electronic band structure of a fully relaxed Be(0001) monolayer.

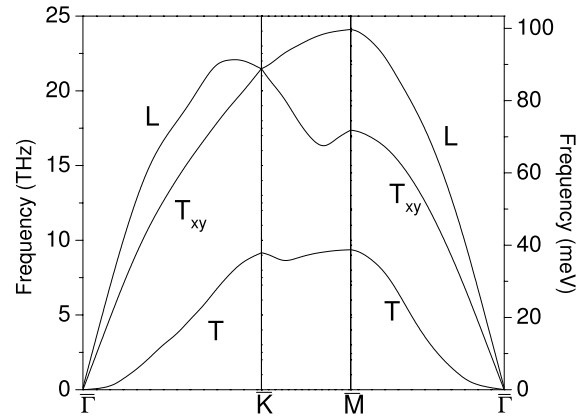


Fig. 2. Calculated phonon dispersion curves along the high symmetry directions for a monolayer of Be(0001).

of atoms depend strongly on their bonding environment. On the other hand, the maximum phonon frequency for the monolayer is somewhat larger than that of the bulk spectrum [3,11] due to the smaller (by  $\sim 9\%$ ) lattice parameter and, as a result, the stronger in-plane interactions between Be atoms. The distinct character of the electronic structure and dynamical properties results in different e–ph interactions in the bulk and in the monolayer.

To calculate the spectral function the sum over the phonons ( $\mathbf{q}, \nu$ ) in Eq. (3) was performed with more than 110 points in the irreducible part of the BZ. For the double Fermi sums in Eq. (2) we used a denser mesh of up to 330  $\mathbf{k}$  points. The delta functions were approximated by the first-order Hermite–Gaussian function with a smearing width in the range of 0.01–0.03 Ry. In Fig. 3 we show the spectral function  $\alpha^2 F(\omega)$  and the phonon density of states  $F(\omega)$ . In spite of the fact that the main features of  $\alpha^2 F(\omega)$

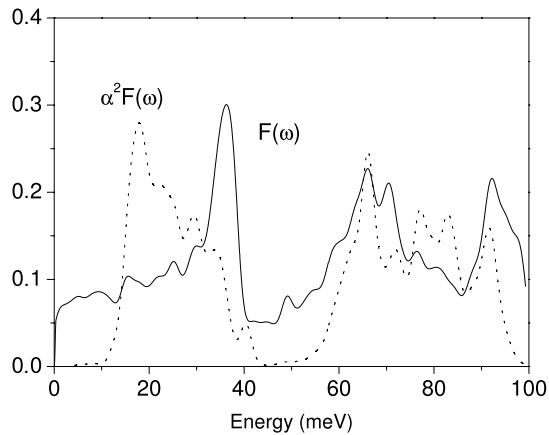


Fig. 3. Phonon density of states  $F(\omega)$  (solid line) and e-ph spectral function  $\alpha^2 F(\omega)$  (dashed line) for a monolayer of Be(0001).

are determined to a large extent by the  $F(\omega)$ , the two functions are rather different especially in the low-energy region. Unlike the bulk Be, where the high-frequency modes contribute mostly to the e-ph interaction [3], in the case of the Be(0001) monolayer, both low-energy and high-energy phonon modes participate in the e-ph coupling. As one can see, these contributions are well separated from each other. The lower-frequency contribution corresponds mainly to the scattering processes of the low-energy  $z$ -polarized transverse phonons, the other is determined by the scattering of the high-energy phonons with in-plane displacements of Be atoms. A rather broad small peak in the density of states at low frequencies related with

the zone center  $z$ -polarized transverse phonons is completely suppressed by the e-ph matrix elements and is not observed for the spectral function. The e-ph mass enhancement parameter,  $\lambda$ , was found to be equal to 0.51 that is significantly larger than  $\lambda = 0.21$ – $0.24$  evaluated at  $E_F$  for bulk Be [1,3].

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