PHYSICAL REVIEW B **72**, 075422 (2005)

Electron-phonon coupling on the Mg(0001) surface

T. K. Kim,[1] T. S. Sørensen,[1] E. Wolfring,[1] H. Li,[1,2] E. V. Chulkov,[3,4,5] and Ph. Hofmann[1,*]
[1]*Institute for Storage Ring Facilities, University of Aarhus, DK-8000 Aarhus C, Denmark*
[2]*Department of Physics, Zhejiang University, Hangzhou 310027, China*
[3]*Donostia International Physics Center (DIPC), 20018 San Sebastián, Basque Country, Spain*
[4]*Departamento de Física de Materiales and Centro Mixto CSIC-UPV/EHU, Facultad de Ciencias Químicas, UPV/EHU, Apdo. 1072, 20080 San Sebastián, Basque Country, Spain*
[5]*Laboratoire des Collisions Atomiques et Moléculaire, UMR CNRS-Université Paris-Sud 8625, Bat. 351, Université Paris-Sud, 91405 Orsay Cedex, France*

(Received 28 March 2005; revised manuscript received 15 June 2005; published 12 August 2005)

We have studied the $\bar{\Gamma}$ surface state on the Mg(0001) surface by angle-resolved photoemission spectroscopy. An analysis of the temperature-dependent linewidth of this state within the Debye model yields a value of $\lambda = 0.27(2)$ for the electron-phonon coupling constant which is in good agreement with available data for bulk Mg. The electron-electron+electron-defect scattering contribution is found by subtracting the electron-phonon contribution from the measured hole linewidth. Its value compares well with the computed result. The analysis of the role of two- and three-dimensional effects in the hole dynamics shows that interband transitions from bulk states to the hole are the dominant mechanism of the hole decay.

DOI: 10.1103/PhysRevB.72.075422 PACS number(s): 79.60.Bm, 73.20.−r, 71.38.−k

I. INTRODUCTION

Angle-resolved photoemission spectroscopy (ARPES) is a widely used experimental technique to study the electronic structure of metallic surfaces[1,2] and the dynamics (decay) of holes in surface states.[3] One of the most interesting mechanisms of the hole (electron) decay is provided by the electron-phonon (*e-ph*) interaction. ARPES allows one to deduce the momentum- and energy-resolved *e-ph* coupling constant λ from the temperature dependence of the linewidth of a quantum state of interest. In contrast, traditional methods measure λ as averaged over momenta at the Fermi surface only.[4] Photoemission studies of λ have recently been reported on electronic states of, among others, the noble metal's (111) face,[5–7] Be(0001),[8–10] Be($10\bar{1}0$),[11–13] Bi(111),[14,15] Bi(100),[16] Bi(110),[17] α-Ga(010),[18,19] and Mo(110).[20] For reviews see Refs. 3, 21, and 22. First scanning tunneling spectroscopy measurements of λ were also reported recently for ferromagnetic Gd(0001).[23]

Here, we present an ARPES study of *e-ph* coupling for the $\bar{\Gamma}$ surface state on the Mg(0001) surface. This state is quite different from the examples given above: while it shows a free electronlike dispersion and thereby resembles the noble metal (111) or the Be(0001) surface state, it penetrates much deeper into the bulk of the crystal. Of particular interest is the comparison with Be(0001): Like Be, magnesium is an alkaline-earth metal with a close-packed hexagonal crystal structure. However, both bulk band structure and (0001) surface electronic structure of magnesium are very different from those of beryllium.[24] A similar $\bar{\Gamma}$ surface state can be found on both Mg(0001) and Be(0001). On Be(0001) it is located mostly in the first two surface layers but on Mg(0001) it is not.[24] This can be expected to lead to different *e-ph* coupling on these surfaces.

We have determined the electron-phonon coupling parameter λ from an analysis of the temperature-dependent linewidth of the $\bar{\Gamma}$ surface state on Mg(0001) using a three-dimensional Debye model. For a surface state with a slow decay into the bulk such a model should be quite appropriate.[21] Indeed, the agreement between the model and the experimental data is very good and the resulting value of λ compares well to the bulk value for Mg.

The measured surface-state linewidth Γ_{exp} includes three components: inelastic *e-ph*, $\Gamma_{e\text{-}ph}$, and electron-electron, $\Gamma_{e\text{-}e}$, contributions as well as the contribution from elastic scattering of a surface-state hole on defects, $\Gamma_{e\text{-def}}$. As mentioned above, we have determined the *e-ph* contribution by using the Debye model, the rest was obtained by subtracting this contribution from the measured linewidth. To discriminate the *e-e* and *e*-def contributions, we have performed calculations of $\Gamma_{e\text{-}e}$ based on the self-energy formalism of many-body theory.[3]

II. METHODS

The Mg(0001) sample was mechanically polished and cleaned *in situ* by several 30-min cycles of sputtering with Ar ions (1 keV, 10 μA/cm^2) followed by 5-min annealing at 220 °C. Surface cleanliness was monitored with Auger electron spectroscopy (AES) and photoemission. In the initial stages of cleaning a clear oxygen peak was found in the valence band even though AES indicated a clean surface. This oxygen could only be removed by a "hot" sputtering at 150 °C and annealing at 220 °C.[25] Later, the surface quality was judged by the shape and intensity of the surface states. The line shape of the surface states was not found to change within about 6 h after cleaning. Surface order was checked by low-energy electron diffraction (LEED). Our Mg(0001) crystal showed a good quality, sixfold symmetric LEED pattern. Angle-resolved photoemission experiments were performed at the SGM-3 beamline of the synchrotron radiation

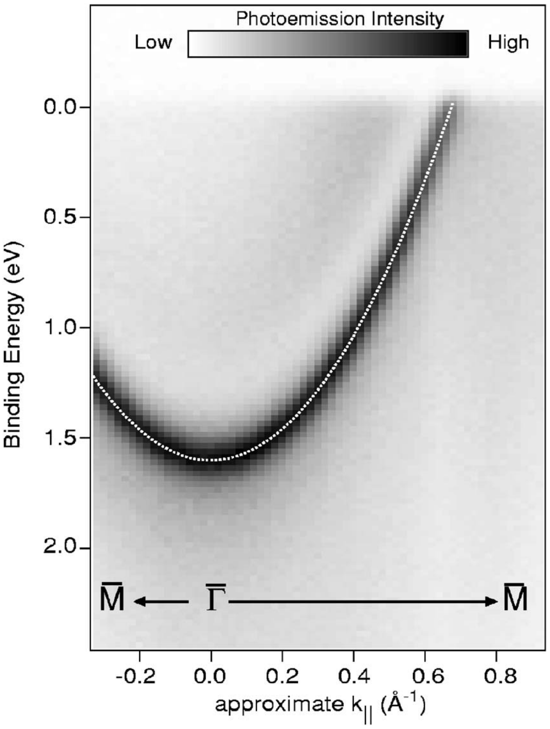

FIG. 1. Dispersion of the Mg(0001) surface state around the center of the surface Brillouin zone. The grey-scale image shows the photoemission intensity as a function of binding energy and momentum parallel to the surface ($h\nu$=44 eV, T=73 K). The horizontal axis is the crystal momentum parallel to the surface calculated for a binding energy of 0 eV. The white dotted line shows the result of a parabolic fit of the surface state dispersion (see text for details).

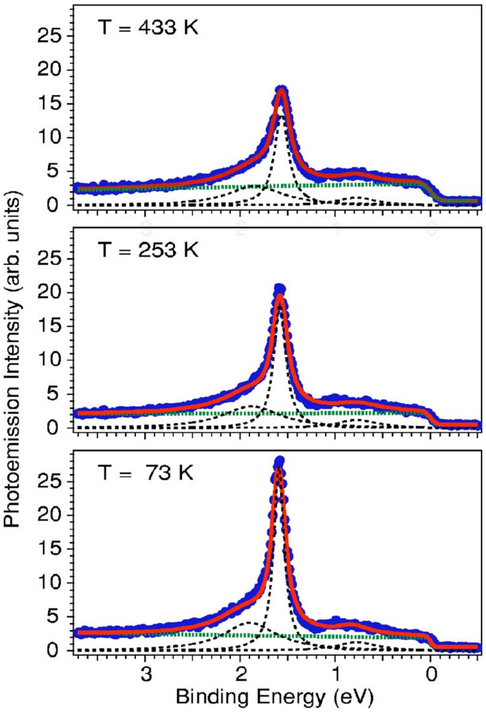

FIG. 2. (Color online) EDCs at $\bar{\Gamma}$ for three different temperatures ($h\nu$=44 eV). The blue circles are the experimental data points; the red solid line is a result of the fit; dashed lines give the fit Lorentzians and the green dotted line is a background multiplied on a Fermi function.

source ASTRID in Aarhus. A detailed description of the instrument is given elsewhere.[26] The sample could be cooled to approximately 50 K with a closed-cycle He cryostat. The pressure during the experiments was in the mid-10^{-11}-mbar range. The overall energy resolution used in this work was 71 meV, as determined from a Fermi edge of polycrystalline copper at 53 K. The overall angular resolution was around ±0.5°.

We have evaluated $\Gamma_{e\text{-}e}$ within *GW* approximation[3] for the quasiparticle self-energy by using eigenvalues and eigenfunctions of a model potential of Ref. 27. Details of the calculation method for the self-energy can be found in Refs. 3 and 28. The parameters of the model potential were fitted to reproduce the bulk $\Gamma_3^+-\Gamma_4^-$ energy gap measured recently[29] and the binding energy of the surface state at $\bar{\Gamma}$ as measured in the present work.

III. RESULTS

The dispersion of the surface state around the $\bar{\Gamma}$ point is shown in Fig. 1. The figure is a grey-scale plot constructed from a series of energy distribution curves (EDCs) taken in the $\bar{\Gamma}-\bar{M}-\bar{\Gamma}$ direction of the surface Brillouin zone, at a photon energy of $h\nu$=44 eV. The horizontal axis represents the crystal momentum parallel to the surface, $k_{\|}$, calculated for electrons emitted at the Fermi level. For electrons emitted off-normal from higher binding energy states, the crystal momentum is lower but the difference is very small due to the high photon energy and the small binding-energy range.

At $h\nu$=44 eV the emission from the surface state is resonantly enhanced. The reason for this enhancement lies in the similarity of the surface-state wave function and the wave functions of the bulk states it is derived from.[30] The enhancement is very pronounced for surface states located in narrow gaps.[31] In the present case, a very intense surface state is desirable because it permits relatively quick data collection and it facilitates the curve fitting of the actual surface state peak. However, the vicinity of the bulk photoemission peaks also means that these have to be taken into account in the curve fitting of the spectra (see below).

The surface state reaches its highest binding energy of 1.60(1) eV at $\bar{\Gamma}$ and its dispersion is well described by a free electronlike parabola with an effective mass of m^*/m_e =1.07(02). This parabola is indicated as a white dashed line in Fig. 1. Actually, the parabola has not been fitted directly to the data in the figure but a correction for the binding-energy dependence of $k_{\|}$ has been applied before the fit. This correction is very small, as pointed out above. The binding energy and dispersion of the surface state are in good agreement with earlier results.[25,29,32]

Figure 2 shows photoemission spectra of the surface state at the $\bar{\Gamma}$ point at three different temperatures. The energy distribution curves were fitted using the following function:

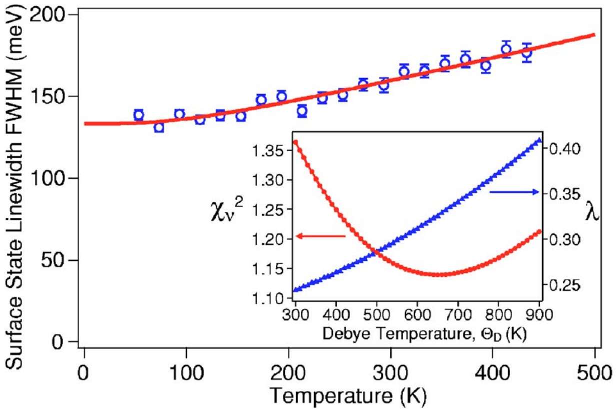

FIG. 3. (Color online) Temperature dependence of the surface state linewidth at $\bar{\Gamma}$. The open circles give the experimental results. The solid line is the result of the three-dimensional (3D) Debye model fit (see text for details). The inset shows the reduced χ^2 value χ_ν^2 and the coupling constant λ as a function of the Debye temperature used in the fit.

$$I(\omega,T) = [p_{SS}(\omega) + p_{B1}(\omega) + p_{B2}(\omega) + b(\omega)]f(\omega,T) \otimes G_R,$$

where $b(\omega)$ is a linear background and p_{SS}, p_{B1}, and p_{B2} are Lorentzians, describing the pronounced surface-state peak and two bulk states discussed below. $f(\omega,T)$ is the Fermi function and G_R is a Gaussian line representing the experimental energy resolution. The angular (momentum) resolution of the spectrometer is sufficiently good to be ignored here.

The two peaks which are required in the fit in addition to the surface-state peaks are found at binding energies of 1.84(2) and 0.78(2) eV at the lowest temperature. They are are assigned to transitions from bulk states close to the Γ_3^+ and Γ_4^- points, respectively. This is fully consistent with the resonant enhancement of the surface state which is expected to take place for at a photon energy where emission from these states is observed.[25]

From such fits we can extract the surface-state linewidth as a function of temperature, as shown in Fig. 3. Under certain conditions, the linewidth can be interpreted as the inverse lifetime of the hole state or, equivalently, as the twice the imaginary part of the self-energy. These conditions are (i) that the state has only a two-dimensional dispersion, (ii) that the dispersion is locally flat, i.e., that we are in a minimum or maximum of the dispersion curve,[33] and (iii) that the peak in the EDC is far away from the Fermi energy compared with typical phonon energies in the material.[17] In the present case, all these conditions are fulfilled.

There are three contributions limiting the hole lifetime and determining the linewidth of the surface state. These are the electron-electron scattering, the electron-defect scattering, and the electron-phonon scattering. The first two are generally assumed to be temperature independent or at least to have a very small temperature dependence.[5] We can write

$$\Gamma_{\exp}(T) = \Gamma_{e-e} + \Gamma_{e-\mathrm{def}} + \Gamma_{e-p}(T). \tag{1}$$

Therefore the temperature-dependence of the linewidth in Fig. 3 is solely due to the electron-phonon coupling.

This contribution can be expressed by

$$\Gamma_{e\text{-}p} = 2\pi\hbar \int_0^{\omega_{\max}} \alpha^2F(\omega')[1 - f(\omega-\omega') + 2n(\omega') + f(\omega+\omega')]d\omega', \tag{2}$$

where ω is the hole energy, ω' is the phonon energy, $\alpha^2F(\omega')$ is the Eliashberg coupling function, and $f(\omega)$ and $n(\omega')$ are the Fermi and Bose-Einstein distribution functions, respectively. The integral extends over all phonon frequencies in the material. Thus the data in Fig. 3 can be fitted by combining Eqs. (1) and (2), i.e., by using Eq. (2) plus a temperature-independent offset $\Delta\Gamma = \Gamma_{e\text{-}e} + \Gamma_{e\text{-def}}$ to account for electron-electron and electron-defect scattering.

Apart from the known Fermi and Bose functions, Eq. (2) contains the Eliashberg function which describes the actual coupling. For the present situation of a deeply penetrating surface state, a three-dimensional Debye model for the Eliashberg function can be expected to work well. We take $\alpha^2F(\omega') = \lambda(\omega'/\omega_D)^2$, for $\omega' < \omega_D$ and zero elsewhere.[21]

A critical parameter in the fit is the Debye energy $\hbar\omega_D$ or Debye temperature Θ_D of the solid since its choice has an influence of the resulting λ. Θ_D is not a well-defined parameter: different values can be found in the literature and the result depends on the type of measurement and on the sample temperature. For example, one finds values of 318 K (Ref. 34) and 400 K (Ref. 35) for bulk Mg. The problem is illustrated in the inset of Fig. 3 which shows the reduced χ^2 value χ_ν^2 (Ref. 36) and the coupling constant λ as a function of the Debye temperature used in the fit. The fits over the whole temperature range are of similar excellent quality, expressed by a small χ_ν^2 with a very shallow minimum around 660 K. From a statistical point of view, it cannot be decided which Debye temperature should be chosen but from a physical point of view the highest values of this range can be excluded. The Debye temperature is, after all, a rough measure of the highest phonon energies in a material and it is highly unlikely that these can be higher at the surface than in the bulk by more than a factor of 2 or so. The resulting λ depends on the choice of Θ_D but for physical sensible values of Θ_D, λ lies around 0.3. Note that the problem with the unknown Debye temperature can be avoided in the high-temperature limit, where Eq. (2) reduces to a simple linear relation which is independent of the chosen phonon model. This approach has been used in several works[5,37] but it cannot be applied for Mg because the high vapor pressure at elevated temperature renders photoemission experiments impossible.

An experimental technique which provides information about the vibrations of the surface atoms is dynamic low-energy electron diffraction (LEED) because the mean-square vibrational amplitudes are needed for a quantitative description of the diffraction intensities. In the present case, we can use information from a recent LEED study of Mg(0001).[38] We have calculated Debye temperatures from the root-mean-square displacements using a well-known formula.[35] This gives Debye temperatures values equal to 260, 380, and 500 K for the first, second, and lower (i.e., bulk) layers of Mg(0001), respectively. This result can be combined with the

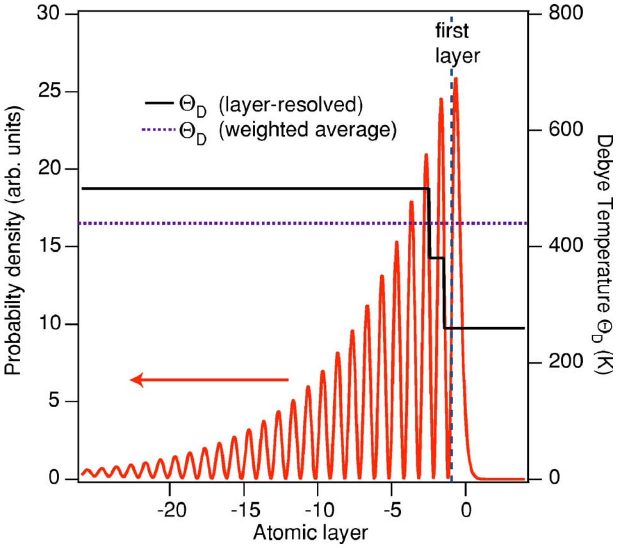

FIG. 4. (Color online) Left axis: Calculated probability density for the surface-state wave function as a function of distance from the surface (in units of atomic layers, layer 1 being the surface layer). Right axis: Layer-resolved Debye temperature from a dynamical LEED study (Ref. 38).

probability density $|\Psi|^2$ for the surface state, as found from first-principles calculations, to obtain an effective weighted Debye temperature for the fit. This calculated probability density is shown together with the layer-resolved Debye temperature in Fig. 4. The very slow decay of the surface-state wave function into bulk results in a weighted average of Θ_D=440 K.

With this value of Θ_D, we can fit the experimental linewidth to obtain λ. The fit is shown as a solid line in Fig. 3. It gives $\lambda=0.27(2)$ and an additional broadening $\Delta\Gamma=112(2)$ meV for the average Debye temperature $\Theta_D=440$ K. From this fit we find an extrapolated total linewidth at zero *K* of 133 meV, of which 21 meV are due to electron-phonon scattering and the remaining 112 meV are caused by the combined effect of electron-defect and electron-electron scattering.

From this type of experimental data, it is not possible to disentangle the electron-electron and electron-defect contributions to $\Delta\Gamma$. More insight can be gained by comparing the experimental value of $\Delta\Gamma$ with the calculated contribution to the linewidth from inelastic electron-electron scattering.[39] The computed value of $\Gamma_{e\text{-}e}$ is 91 meV. The bigger part of this value, 63 meV, comes from interband transitions to the hole from bulk electron states located between the Fermi energy and the edge of the $\bar{\Gamma}$ surface state. The smaller part, 28 meV, results from intraband transitions within the surface-state band. The difference between the experimental $\Delta\Gamma$ and $\Gamma_{e\text{-}e}$ of 21 meV can be attributed to the elastic electron-defect scattering contribution.

IV. DISCUSSION

The value of electron-phonon coupling constant, $\lambda=0.27(2)$, obtained for the bottom of the $\bar{\Gamma}$ surface-state band is smaller than $\lambda=0.35(4)$ derived from calculations with empirical and model pseudopotentials for bulk Mg at the Fermi energy E_F (for a review see Ref. 4). However, the measured λ is in a good accord with $\lambda=0.30$ recently obtained from an *ab initio* calculation for bulk Mg at E_F.[40] This close agreement between the experimental (surface) and *ab initio* (bulk) *e-ph* coupling constant can be attributed to the very bulklike character of the $\bar{\Gamma}$ surface state on Mg(0001),[24] and to the weak energy dependence of λ in bulk Mg.[40] That the experimental value for λ is slightly lower than the calculated bulk value may well be related to the fact that the state is, after all, a surface state. According to the inset in Fig. 3, a decrease of the average Debye temperature caused by the larger vibrational amplitude at the surface results indeed in a slightly smaller value of λ.

The value of additional (nontemperature dependent) broadening obtained from the fit $\Delta\Gamma$ is 112 meV, the theoretical value for the broadening due to the electron-electron scattering $\Gamma_{e\text{-}e}$ is 91 meV. The 21-meV difference between them can be attributed to electron-defect scattering. This order of magnitude can be expected for a well-prepared crystal surface and it compares well to typical results from Cu(111).[6,41] In the most advanced photoemission experiments on the noble-metal surfaces *L*-gap surface states, however, very narrow lines have been observed which correspond directly to the calculated values of Γ and do not require the inclusion of any defect scattering term.[42] Such a situation is very hard to achieve on Mg(0001) which is chemically far more reactive than the noble metals and therefore prone to adsorption of rest-gas atoms in the vacuum system.

We can compare our value of the room-temperature linewidth of the surface state of 160(5) meV to the results of earlier investigations of Mg(0001). From the figures in the papers of Karlsson *et al.*[32] and Bartynski *et al.*,[25] we obtain values of $\approx$250 meV and $\approx$ 500 meV, respectively. These large widths were probably caused by the limited energy resolution in these early works which have been focused on the position of the spectral features and not on their line shape. In the recent work of Schiller *et al.*, however, the room-temperature linewidth is of the order of 175 meV,[43] and compares very well with our result. Those data have been taken from a high quality epitaxial film of Mg on W(110).

Having obtained the results for the electron-phonon coupling, it is interesting to re-address the important assumption that we can neglect the temperature dependence of the electron-electron scattering $\Gamma_{e\text{-}e}$ in Eq. (1). We have analyzed two possible sources of this dependence. First, at finite temperature $\Gamma_{e\text{-}e}$ is given by the change of the Fermi distribution function (see Ref. 44. This leads to quadratic dependence of $\Gamma_{e\text{-}e}$ on temperature and it is important for energies in the k_BT interval around the Fermi level only.[44] In the case of Mg(0001) the binding energy of the surface state at the $\bar{\Gamma}$ point is much bigger than thermal energies and therefore this mechanism does not produce any contribution to the temperature dependence of $\Gamma_{e\text{-}e}$. Another possible mechanism is based on the possible change of binding energy of the surface state with temperature. The temperature-induced shift of binding energy can lead to a change of phase space and through this to a temperature dependence of $\Gamma_{e\text{-}e}$. However, over the whole temperature range used in the present experiments the surface-state binding energy shifts by less than 30 meV. Our calculations show that this energy shift changes $\Gamma_{e\text{-}e}$ by less than 2 meV. This value is very small compared to the variation of the electron-phonon contribution with temperature.

Finally, it is interesting to compare the electron-phonon coupling on Mg(0001) to the situation on Be(0001). As pointed out in the introduction, the dispersion of the surface state on Be(0001) is quite similar to that on Mg(0001), only that the projected band gap is much wider. Upon a more detailed inspection, there are pronounced differences, mostly caused by the different bulk character of Mg and Be. Whereas Mg is a free-electron-like metal, Be is not. In fact, bulk Be shows a pronounced minimum in the density of states (DOS) near E_F. At the surface, this DOS minimum is removed due to the presence of the $\bar{\Gamma}$ surface state (Ref. 24, for a review see also Ref. 45). This surface state penetrates much less into the bulk because it is situated in a much wider gap. In view of this, it is not surprising that entirely different considerations apply for the lifetime of the Be surfaces states: intraband scattering is much more important than on Mg,[46,47] at E_F the surface state λ (Refs. 8–10 and 48) is much higher than the bulk value[4,49] and it is also energy dependent.[48,50] Finally, the bulk Debye temperature for Be is much higher than for Mg. This, together with the strong coupling, leads to a pronounced kink in the dispersion close to the Fermi level.[9] In our work such a kink cannot be observed. Indeed, from λ and the Debye temperature used here we can estimate the deviation from the parabolic dispersion to be very small, less than 10 meV at very low temperatures.

V. SUMMARY

We have presented experimental and theoretical results of the lifetime broadening of the Mg(0001) $\bar{\Gamma}$ surface state. The temperature-dependent electron-phonon contribution to the linewidth was modeled using a three-dimensional Debye model. This results in very good agreement with the experimental data. However, it is difficult to determine both the Debye temperature and the coupling strength λ with high accuracy because these parameters are strongly correlated in the fit function. We have therefore constructed an effective Debye temperature as input parameter, which was obtained from the layer-resolved mean-square vibrational amplitudes found by LEED and the calculated probability density of the surface state. With this we have obtained a value of $\lambda = 0.27(2)$ and an extrapolated 0-K linewidth of 133 meV. This linewidth was found to have the following contributions: 21 meV are due to electron-phonon scattering, 21 meV are caused by electron-defect scattering, and 91 meV by electron-electron scattering. The latter value has two contributions: interband scattering from bulk states (63 meV) and intraband scattering from other electrons in the surface state (28 meV). The strong interband contribution is caused by the very bulklike nature of the surface state.

ACKNOWLEDGMENTS

E.V.C. would like to thank A. G. Borisov, P. M. Echenique, J. P. Gauyacq, F. Schiller, and V. M. Silkin for discussions. We acknowledge partial support by the Danish National Science Foundation, Spanish MCyT (Grant No. MAT 2001-0946), by the European FP6 Network of Excellence [FP6-NoE NANOQUANTA (Grant No. 500198-2)], and by the NSFC (Grant No. 10374080), and by the Danish Rector's Conference.

---

*Electronic address philip@phys.au.dk

[1] *Angle-resolved Photoemission*, Studies in Surface Chemistry and Catalysis No. 74, edited by S. D. Kevan (Elsevier, Amsterdam, 1992).

[2] R. Matzdorf, Surf. Sci. Rep. **30**, 153 (1998).

[3] P. M. Echenique, R. Berndt, E. V. Chulkov, T. Fauster, A. Goldmann, and U. Höfer, Surf. Sci. Rep. **52**, 219 (2004).

[4] G. Grimvall, *The Electron-phonon Interaction in Metals* (North-Holland, Amsterdam, 1981).

[5] B. A. McDougall, T. Balasubramanian, and E. Jensen, Phys. Rev. B **51**, R13891 (1995).

[6] M. Matzdorf, Appl. Phys. A: Mater. Sci. Process. **63**, 549 (1996).

[7] A. Eiguren, B. Hellsing, F. Reinert, G. Nicolay, E. V. Chulkov, V. M. Silkin, S. Hüfner, and P. M. Echenique, Phys. Rev. Lett. **88**, 066805 (2002).

[8] T. Balasubramanian, E. Jensen, X. L. Wu, and S. L. Hulbert, Phys. Rev. B **57**, R6866 (1998).

[9] M. Hengsberger, D. Purdie, P. Segovia, M. Garnier, and Y. Baer, Phys. Rev. Lett. **83**, 592 (1999).

[10] S. LaShell, E. Jensen, and T. Balasubramanian, Phys. Rev. B **61**, 2371 (2000).

[11] T. Balasubramanian, P.-A. Glans, and L. I. Johansson, Phys. Rev. B **61**, 12709 (2000).

[12] S. J. Tang, Ismail, P. T. Sprunger, and E. W. Plummer, Phys. Rev. B **65**, 235428 (2002).

[13] J. Shi, S.-J. Tang, B. Wu, P. T. Sprunger, W. L. Yang, V. Brouet, X. J. Zhou, Z. Hussain, Z.-X. Shen, Z. Zhang, and E. W. Plummer, Phys. Rev. Lett. **92**, 186401 (2004).

[14] C. R. Ast and H. Höchst, Phys. Rev. B **66**, 125103 (2002).

[15] J. E. Gayone, C. Kirkegaard, J. W. Wells, S. V. Hoffmann, Z. Li, and Ph. Hofmann, Appl. Phys. A: Mater. Sci. Process. **80**, 943 (2005).

[16] J. E. Gayone, S. V. Hoffmann, Z. Li, and Ph. Hofmann, Phys. Rev. Lett. **91**, 127601 (2003).

[17] C. Kirkegaard, T. K. Kim, and Ph. Hofmann, New J. Phys. **7**, 99 (2005).

[18] Ph. Hofmann, Y. Q. Cai, C. Grütter, and J. H. Bilgram, Phys. Rev. Lett. **81**, 1670 (1998).

[19] C. Søndergaard, C. Schultz, S. Agergaard, S. V. Hoffmann, Z. Li, P. Hofmann, H. Li, C. Grütter, and J. H. Bilgram, Phys. Rev. B **67**, 165422 (2003).

[20] T. Valla, A. V. Fedorov, P. D. Johnson, B. O. Wells, S. L. Hulbert,

Q. Li, G. D. Gu, and N. Koshizuka, Science **285**, 2110 (1999).

[21] B. Hellsing, A. Eiguren, and E. V. Chulkov, J. Phys.: Condens. Matter **14**, 5959 (2002).

[22] E. W. Plummer, J. Shi, S.-J. Tang, E. Rotenberg, and S. D. Kevan, Surf. Sci. Rep. **74**, 251 (2003).

[23] A. Rehbein, D. Wegner, G. Kaindl, and A. Bauer, Phys. Rev. B **67**, 033403 (2003).

[24] E. V. Chulkov, V. M. Silkin, and E. N. Shirykalov, Surf. Sci. **188**, 287 (1987).

[25] R. A. Bartynski, R. H. Gaylord, T. Gustafsson, and E. W. Plummer, Phys. Rev. B **33**, 3644 (1986).

[26] S. V. Hoffmann, C. Søndergaard, C. Schultz, Z. Li, and P. Hofmann, Nucl. Instrum. Methods Phys. Res. A **523**, 441 (2004).

[27] E. V. Chulkov, V. M. Silkin, and P. M. Echenique, Surf. Sci. **437**, 330 (1999).

[28] E. V. Chulkov, I. Sarria, V. M. Silkin, J. M. Pitarke, and P. M. Echenique, Phys. Rev. Lett. **80**, 4947 (1998).

[29] F. Schiller, M. Heber, V. D. P. Servedio, and C. Laubschat, Phys. Rev. B **70**, 125106 (2004).

[30] S. G. Louie, P. Thiry, R. Pinchaux, Y. Pétroff, D. Chandesris, and J. Lecante, Phys. Rev. Lett. **44**, 549 (1980).

[31] Ph. Hofmann, C. Søndergaard, S. Agergaard, S. V. Hoffmann, J. E. Gayone, G. Zampieri, S. Lizzit, and A. Baraldi, Phys. Rev. B **66**, 245422 (2002).

[32] U. O. Karlsson, G. V. Hansson, P. E. S. Persson, and S. A. Flodström, Phys. Rev. B **26**, 1852 (1982).

[33] N. V. Smith, P. Thiry, and Y. Petroff, Phys. Rev. B **47**, 15476 (1993).

[34] N. E. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders College, Philadelphia, 1976).

[35] C. Kittel, *Solid State Physics* (Wiley, New York, 1995).

[36] P. R. Bevington, *Data Reduction and Error Analysis for the Physical Sciences* (McGraw-Hill, New York, 1969).

[37] J. J. Paggel, D.-A. Luh, T. Miller, and T.-C. Chiang, Phys. Rev. Lett. **92**, 186803 (2004).

[38] Ismail, Ph. Hofmann, A. P. Baddorf, and E. W. Plummer, Phys. Rev. B **66**, 245414 (2002).

[39] P. M. Echenique, J. M. Pitarke, E. V. Chulkov, and A. Rubio, Chem. Phys. **251**, 1 (2000).

[40] A. Leonardo I. Yu. Sklyadneva, P. M. Echenique, and E. V. Chulkov (unpublished).

[41] F. Theilmann, R. Matzdorf, G. Meister, and A. Goldmann, Phys. Rev. B **56**, 3632 (1997).

[42] F. Reinert, G. Nicolay, S. Schmidt, D. Ehm, and S. Hüfner, Phys. Rev. B **63**, 115415 (2001).

[43] F. Schiller (private communication).

[44] D. Pines and P. Nozières, *The Theory of Quantum Liquids* (Benjamin, New York, 1966).

[45] E. W. Plummer and J. B. Hannon, Prog. Surf. Sci. **46**, 149 (1994).

[46] E. V. Chulkov, V. M. Silkin, and P. M. Echenique, Surf. Sci. **454-456**, 458 (2000).

[47] V. M. Silkin, T. Balasubramanian, E. V. Chulkov, A. Rubio, and P. M. Echenique, Phys. Rev. B **64**, 085334 (2001).

[48] A. Eiguren, S. de Gironcoli, E. V. Chulkov, P. M. Echenique, and E. Tosatti, Phys. Rev. Lett. **91**, 166803 (2003).

[49] I. Yu. Sklyadneva, E. V. Chulkov, W. -D. Schöne, V. M. Silkin, R. Keyling, and P. M. Echenique, Phys. Rev. B **71**, 174302 (2005).

[50] T. Balasubramanian (private communication).