Unusually weak electron-phonon coupling in the Shockley surface state on Pd(111)

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Electron-phonon (*e-ph*) coupling in the $\bar{\Gamma}$ unoccupied surface state on Pd(111) is studied using density-functional perturbation-theory calculation and two-photon photoemission measurements. Also, an *ab initio* GW calculation is performed to combine it with the *e-ph* coupling evaluation in the study of the surface-state linewidth. We show that the *e-ph* coupling in the surface state is unusually weak. It is smaller by a factor of 5 than that at the Fermi surface of bulk Pd. Temperature-dependent two-photon photoemission measurements confirm this result indicating an important role of interband scattering from surface to bulk states.

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I. INTRODUCTION

Dynamics of excited electrons on metal surfaces are of paramount importance for molecular motion induced by femtosecond laser pulses,[1] for energy transfer in photochemical reactions,[2] for catalytical reactions,[3] and for charge and spin transfer across surfaces and interfaces.[4] Excited electrons interact with other electrons (*e-e*), phonons (*e-ph*), and defects (*e-d*).[5] The associated scattering processes contribute to the total linewidth $\Gamma_{tot}=\Gamma_{e\text{-}e}+\Gamma_{e\text{-}ph}+\Gamma_{e\text{-}d}$ observed in spectroscopy. In time-resolved spectroscopy the decay of the population in a particular state can be followed directly and is described by the lifetime τ. The lifetime broadening $\hbar/\tau$ is included in the total linewidth and describes the scattering of the excited electron into other states associated with a change in energy or/and momentum. Electron-electron scattering is predominantly inelastic and $\Gamma_{e\text{-}e}$ is contained in $\hbar/\tau$.[5] In *e-ph* and *e-d* scattering the energy exchange is small compared to the experimental resolution. Therefore most scattering events leave the population of the observed state apparently unchanged. Contributions from $\Gamma_{e\text{-}ph}$ and $\Gamma_{e\text{-}d}$ to $\hbar/\tau$ are limited to scattering events with large momentum transfer, e. g., from surface to bulk bands.[6]

An estimate of $\Gamma_{e\text{-}ph}$ is normally performed by using a Debye model with the experimental *e-ph* coupling parameter λ measured at E_F of bulk metal. For surfaces studied up to now including noble-metal surfaces,[5,7–10] Mo(110),[11,12] as well as simple and semimetal surfaces[13,14] this picture works quite well. Probably the only exception is beryllium whose surfaces show density of states (DOS) at E_F much higher than that in bulk Be due to the appearance of strong surface electronic states at E_F.[15] In this work we show an example when the *e-ph* coupling in a Shockley surface state is very distinct from that at E_F of bulk metal despite that the bulk DOS at E_F is not very different from the surface DOS. This distinction being important at low temperature essentially affects the linewidth at elevated temperatures when $\Gamma_{e\text{-}ph}$ can significantly exceed $\hbar/\tau$. By using time-resolved two-photon photoemission Schäfer *et al.*[16] measured the lifetime broadening of the $\bar{\Gamma}$ Shockley surface state on Pd(111), $\hbar/\tau=54$ meV at $T=450$ K and the total linewidth $\Gamma_{tot}=100$ meV. The difference between $\Gamma_{e\text{-}e}$ and Γ_{tot} was attributed to the quasielastic scattering due to phonons. The theoretical estimation of the *e-e* inelastic scattering with a model that combines one-dimensional potential and many-body effects[16] gave $\Gamma_{e\text{-}e}=37$ meV which is slightly smaller than the experimental values for $\hbar/\tau$. The Debye model with *e-ph* coupling parameter $\lambda=0.40$ taken from *ab initio* calculations[17] of bulk Pd gives $\Gamma_{e\text{-}ph}=60$ meV at $T=450$ K. This leads to theoretical $\hbar/\tau+\Gamma_{e\text{-}ph}=97$ meV in good agreement with the measured linewidth Γ_{tot} but not with the measured $\hbar/\tau$.

Here we show by performing *ab initio* calculations that in the unoccupied $\bar{\Gamma}$ surface state on Pd(111) the *e-ph* coupling parameter is very small, $\lambda=0.08$, i. e., by a factor of 5 smaller than λ obtained at the Fermi energy of bulk Pd.[17] This reduces the calculated $\Gamma_{e\text{-}ph}$ to 19 meV and cannot explain the large difference between the experimental values for $\hbar/\tau$ and Γ_{tot} at $T=450$ K. In order to clarify this discrepancy we performed temperature-dependent linewidth measurements by time-resolved two-photon photoemission. We also carried out an *ab initio* evaluation of the *e-e* contribution to the lifetime broadening of the $\bar{\Gamma}$ surface state.

II. DETAILS OF THE CALCULATION

The *e-ph* calculations were performed using density-functional theory and the local-density approximation for the exchange-correlation functional. Phonon frequencies and polarization vectors were obtained within the mixed-basis density-functional perturbation theory[18,19] using a norm-conserving scalar-relativistic pseudopotential.[20] The plane-wave energy cutoff was 20 Ry and, additionally, one *d*-type localized wave function at each atomic site of Pd was employed. Integrations over the surface Brillouin zone (SBZ)

were performed with a uniform mesh of 576 special points and a Gaussian energy smearing scheme with a width of 0.2 eV. The surface is presented by nine-layer Pd slabs separated by five layers of vacuum. This thickness is quite sufficient to avoid a strong interaction between the two surfaces of a slab: the splitting of the $\bar{\Gamma}$ surface state consists of only 0.25 eV. For comparison with experimental data we average the energies of these two states. Atomic positions inside the Pd(111) planes are fixed at the theoretical lattice parameter, a =7.34 a.u., which is close to the experimental value.[21] The calculated relaxation of the Pd(111) layers shows a very small contraction of the outermost interlayer spacing (about 0.15%) relative to the bulk distance, that is, consistent with the experimental expansion of $0.9 \pm 1.3\%$.[22]

The phonon-induced lifetime broadening of an electron state with momentum $\mathbf{k}_\nu$ and energy $\epsilon_{\mathbf{k}_\nu}$ is related to the Eliashberg spectral function α^2F through the integral over all the scattering events that conserve energy and momentum[23] (we use atomic units, i.e., $e^2=\hbar=m_e=1$)

$$\Gamma_{e\text{-}ph}(\mathbf{k}_\nu) = 2\pi \int_0^{\omega_m} \alpha^2F^{E}(\mathbf{k}_\nu;\omega)[1+n(\omega)-f(\epsilon_{\mathbf{k}_\nu}-\omega)] + \alpha^2F^{A}(\mathbf{k}_\nu;\omega)[n(\omega)+f(\epsilon_{\mathbf{k}_\nu}+\omega)]d\omega. \quad (1)$$

Here, f and n are the Fermi and Bose distribution functions, and ω_m is the maximum phonon frequency. $\alpha^2F^{E(A)}(\mathbf{k}_\nu;\omega)$ is the electron state-dependent Eliashberg spectral function corresponding to phonon emission (E) and absorption (A) processes. The state-dependent *e-ph* coupling parameter is just the first reciprocal moment of the Eliashberg function

$$\lambda(\mathbf{k}_\nu) = \int_0^{\omega_m} \frac{\alpha^2F^{E}(\mathbf{k}_\nu;\omega)+\alpha^2F^{A}(\mathbf{k}_\nu;\omega)}{\omega} d\omega. \quad (2)$$

The evaluation of the *e-e* scattering contribution to the linewidth, $\Gamma_{e\text{-}e}$, was performed within the first-principles GW self-energy formalism. Using the calculated ground-state electronic structure we evaluate $\Gamma_{e\text{-}e}$ of an electron (hole) in the state $\psi_{\mathbf{k}_\nu}(\mathbf{r})$ as

$$\Gamma_{e\text{-}e}(\mathbf{k}_\nu) = -2 \sum_{\nu',\mathbf{k},\mathbf{q}}{}' \sum_{\mathbf{G},\mathbf{G}'} B_{\mathbf{k}_\nu,\mathbf{k}_{\nu'}}(\mathbf{q}+\mathbf{G}) \times \mathrm{Im}\, W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},|\epsilon_{\mathbf{k}_\nu}-\epsilon_{\mathbf{k}_{\nu'}}|) B^*_{\mathbf{k}_\nu,\mathbf{k}_{\nu'}}(\mathbf{q}+\mathbf{G}'). \quad (3)$$

Here $\mathbf{G}$ and $\mathbf{G}'$ are the reciprocal-lattice vectors, $W_{\mathbf{G},\mathbf{G}'}(\mathbf{q},\omega)$ is the Fourier transform of the screened interaction $W(\mathbf{r},\mathbf{r}',\omega)$, and $B_{\mathbf{k}_\nu,\mathbf{k}_\nu}(\mathbf{q}+\mathbf{G})$ are coefficients

$$B_{\mathbf{k}_\nu,\mathbf{k}_{\nu'}}(\mathbf{q}+\mathbf{G}) = \int \psi^*_{\mathbf{k}_\nu}(\mathbf{r}) e^{i(\mathbf{q}+\mathbf{G})\mathbf{r}} \psi_{\mathbf{k}_{\nu'}}(\mathbf{r}) d\mathbf{r}. \quad (4)$$

More details of the GW calculation can be found in Ref. 5.

III. CALCULATION RESULTS AND DISCUSSION

The calculated energy of the unoccupied surface state at $\bar{\Gamma}$ is 1.21 eV above E_F (Fig. 1). Our measured value at 450 K is 1.31 eV with a temperature-dependent shift of 0.12 meV/K

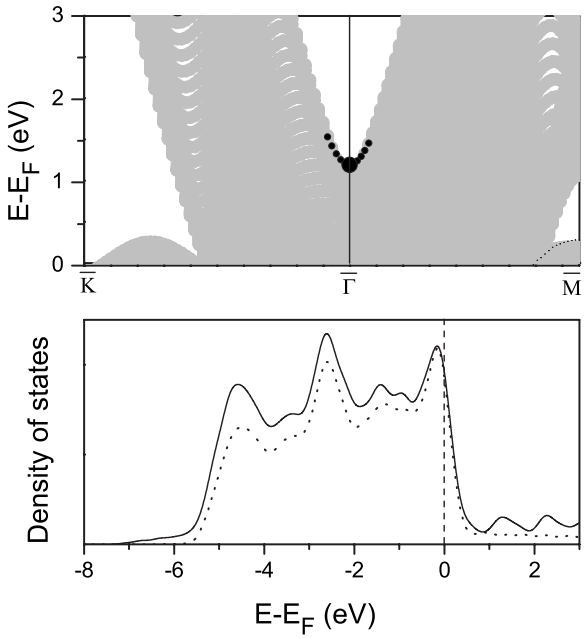

FIG. 1. (Upper panel) The Shockley surface electronic state (black circles) on Pd(111). The gray background represents bulk Pd bands projected onto the two-dimensional Brillouin zone. (Lower panel) The calculated total density of electronic states, DOS (solid line) and DOS of d states only (dotted line) for a nine-layer Pd slab.

(see also Fig. 4). This yields at T=0 a value of 1.26 eV in agreement with the calculation and previous results.[16] First, we calculated exactly the electron-phonon matrix elements using 576 wave vectors $\mathbf{q}$ in the SBZ. Then, to check the convergence the summation was carried out on a denser mesh of 2304 $\mathbf{q}$ points. For the additional $\mathbf{q}$ points, the matrix elements were calculated using a Fourier interpolation scheme for the change in the self-consistent potential with respect to atomic displacements as well as for the dynamical matrices.

Figure 2 shows $\alpha^2F(\mathbf{k}_\nu;\omega)$ for the unoccupied $\bar{\Gamma}$ surface state. Since the contributions from phonon emission and adsorption processes nearly coincide, only the average

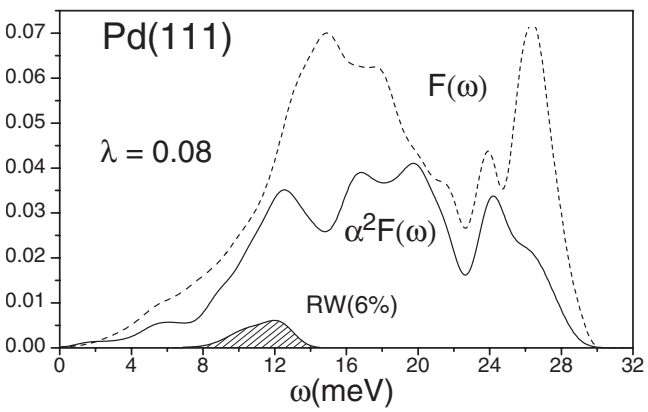

FIG. 2. Electron-phonon Eliashberg spectral function $\alpha^2F(\omega)$ for the $\bar{\Gamma}$ unoccupied surface state. The contribution from the Rayleigh surface mode is indicated by hatched area. Phonon density of states for a nine-layer Pd slab, $F(\omega)$, is shown by dashed line.

TABLE I. Electron-phonon coupling parameters for surface electronic states at $\bar{\Gamma}$ (Refs. 24–27). The surface-state energies E are shown with respect to the Fermi level. Also λ averaged over momentum at E_F of bulk Al, Mg, Pd (Ref. 17), and noble metals (Ref. 23) are presented.

	Ag(111)	Cu(111)	Au(111)	Al(001)	Mg(0001)	Pd(111)
E (eV)	−0.04	−0.44	−0.5	−2.8	−1.7	1.26
λ	0.12	0.16	0.11	0.51	0.28	0.08
$\lambda(E_F)$	0.10	0.14	0.14	0.44	0.30	0.4

$\alpha^2F(\mathbf{k}_\nu;\omega)$ is shown. We calculated λ for both split surface states at $\bar{\Gamma}$ and obtained $\lambda_{\bar{\Gamma}}=0.07$ for the lower state and $\lambda_{\bar{\Gamma}}=0.09$ for the upper state. Extrapolating these results to the thick films (semi-infinite crystal) we take the average value of $\lambda_{\bar{\Gamma}}=0.08$. The obtained $\lambda_{\bar{\Gamma}}$ is very small and differs drastically from the *e-ph* coupling parameter averaged over momenta at the Fermi energy of the nine-layer film of Pd(111) and of bulk Pd, $\lambda_{E_F}=0.4$.[17]

As a rule, the strength of the *e-ph* interaction in a Shockley surface state is close to λ at the Fermi energy of the corresponding bulk material (see Table I). On the (111) surface of noble metals, the Shockley states lie just below E_F and well inside the surface-projected band gap. As a result, their wave functions are mostly localized near the surface and the contribution to the *e-ph* coupling coming from surface-phonon modes is important.[26] The Shockley state at Pd(111) resembles much the $\bar{\Gamma}$ surface state on Al(001).[25] Both states lying very close to the bottom of the band gap at $\bar{\Gamma}$ are characterized by a deep penetration into the bulk. In both cases, the *e-ph* coupling is determined by bulk phonons and the contribution coming from the surface Raleigh modes is very small. It does not exceed 6% for the surface state on Pd(111) (see Fig. 2). However, like in the case of noble-metal (111) surfaces, $\lambda_{\bar{\Gamma}}$ for the Al(001) surface state is close to that at E_F of bulk Al though the state is much deeper in energy.[25] The strength of the *e-ph* coupling for the Shockley state on Pd(111) is closer to that of image-potential states, especially, when the latter lies close to the band edge, e.g., on the Cu(111) surface.[28] Such negligible values of λ for the image states were attributed to a small penetration of the states into the bulk, e.g., for Pd(111) the penetration of the first image-potential state is 4.6%.[16] However, the situation with the unoccupied surface state on Pd(111) is quite different. It is located almost completely (90%) inside the bulk. A plausible reason could be an abrupt decrease in the density of states above E_F and, correspondingly, the number of electronic states which may participate in the *e-ph* coupling (see Fig. 1). Though such a relation is not evident. The values of DOS at the energies of the Pd(111) surface state and the $\bar{\Gamma}$ surface electronic states on Al(001) and Mg(0001) do not differ substantially (~2, 2.4, and 3.4 states/Ry/atom/spin, respectively) unlike the values of λ: 0.08, 0.51, and 0.30, respectively.[24,25] On the other hand, the calculations for the Al(001) surface showed that there was no direct relationship between the value of DOS and λ, e.g., the density of states at the energy of the surface state at the $\bar{X}$ point is half as large than that at the $\bar{\Gamma}$ point while $\lambda_{\bar{X}}=0.78$.

The evaluation of the *e-e* scattering contribution to the linewidth gives $\Gamma_{e\text{-}e}=29$ meV for the surface state. That is smaller than 37 meV obtained from the one-dimensional calculation.[16] This difference can be attributed to use of *ab initio* electronic structure that includes *d* states just above E_F in the electron transitions to final states and as well as in the screening.

Figure 3 shows the calculated linewidth of the unoccupied surface state as a function of temperature by a solid line. The temperature-independent linewidth, $\Gamma_{e\text{-}e}=29$ meV, has been added and is indicated by the dashed line. We also show in Fig. 3 two data sets for the intrinsic linewidth derived from two-photon photoemission. The data were obtained by exciting the unoccupied surface state by a photon with energy $h\nu=1.55$ eV from occupied states below the Fermi energy E_F (see inset of Fig. 4and Ref. 16). A second photon with energy $3h\nu=4.65$ eV lifts the energy above the vacuum level E_{vac}. Electrons emitted along the surface normal are detected by a hemispherical energy analyzer.[16] The kinetic-energy scale in Fig. 4 refers to the analyzer and the work function can be obtained by adding the analyzer work function of 4.32 eV to the low-energy cutoff of the spectra. The decrease in −0.11 meV/K is similar to values for other surfaces.[29] The spectra in Fig. 4 show an intensity decrease and linewidth increase with temperature for the peak assigned to the Shockley surface state.[16] Spectra were fitted using a Lorentzian for the intrinsic linewidth convoluted with a Gaussian accounting for the experimental resolution

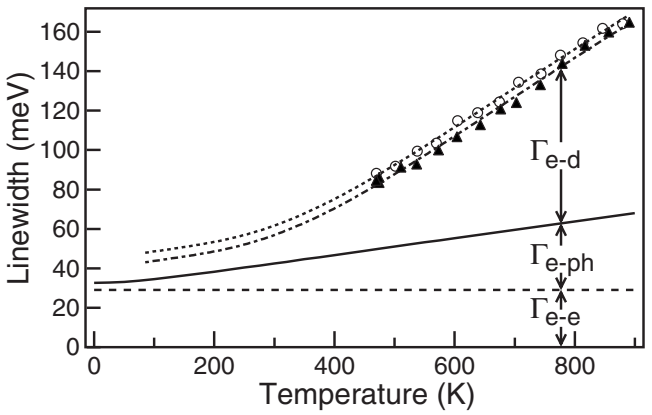

FIG. 3. Temperature dependence of the lifetime broadening for the unoccupied surface state at $\bar{\Gamma}$. The solid curve shows the calculated electron-phonon contribution plus the electron-electron contribution (dashed line). The symbols present two experimental data sets with the corresponding fits including the contribution by thermally generated defects.

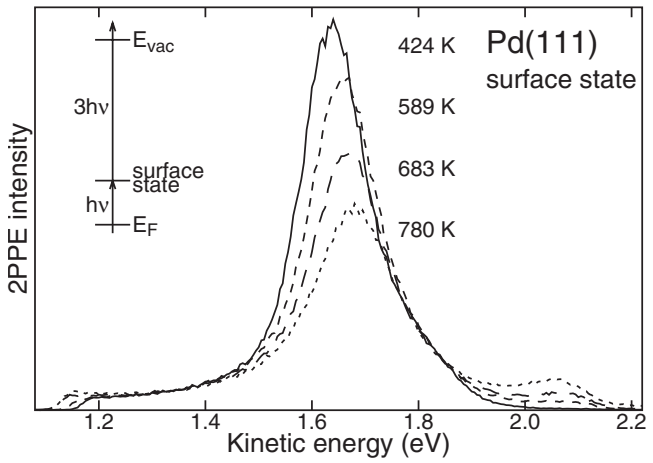

FIG. 4. Two-photon photoemission spectra for the unoccupied surface state at the $\bar{\Gamma}$ symmetry point for different temperatures. The kinetic energy is relative to the vacuum level of the analyzer. The inset shows the energy diagram of the two-photon photoemission process.

of the analyzer and the bandwidth of the laser pulses. The experimental data in Fig. 3 can be fitted using the high-temperature approximation $\Gamma_{e\text{-}ph}=2\pi\lambda kT$ (Refs. 23 and 30) with $\lambda=0.38\pm0.05$. This value is much larger than the calculated one and would extrapolate the linewidth to negative values for $T=0$. These variances can be resolved by including the electron scattering due to thermally activated defects following Ref. 30. This contribution is modeled by an added term $\Gamma_{e\text{-}d}=C\exp(-E_a/kT)$ to the expression for the temperature-dependent linewidth. The activation energy E_a and λ cannot be fitted simultaneously in the available temperature range, so we used the calculated value $\lambda=0.08$. The resulting fits are shown as dotted and dash-dotted lines in Fig. 3. The obtained activation energy, 115 ± 13 meV is in the range of the values for Au(111) (81 meV) and Al(100) (170 meV).[30] The value of the prefactor $C=390\pm20$ meV compares similarly. When the exponential factor is interpreted as defect concentration the obtained value corresponds to 4 meV linewidth increase for 1% defects. This value is similar to the linewidth increase due to adatoms for image-potential states on Cu(100).[31]

Measurements of the linewidth for the image-potential state on Pd(111) as a function of temperature using a straight-line fit give also a rather high value for $\lambda=0.14$. For the image-potential state on Cu(111), $\lambda=0.06$ has been measured which is attributed to a rather strong coupling to bulk bands at an energy near the band edge[28] due to the significant overlap of the image-potential state and bulk states wave functions. For Ag(100) and Cu(100) which have band gaps similar to Pd(111) $\lambda=0.01$ has been calculated[32] and no temperature dependence of the linewidth has been observed,[33] respectively. A consistent fit of the data for the image-potential state on Pd(111) assuming $\lambda=0$ can be obtained using the thermally induced defect model with an activation energy $E_a=74\pm15$ meV and a prefactor $C=135\pm12$ meV. Because the image-potential state is measured with the available photon energy close to the Fermi edge the linewidths might be underestimated somewhat. This would lead in turn to a larger value for E_a and explains the deviation to the value obtained for the Shockley surface state.

The linewidth extrapolated to $T=0$ for the best sample preparations is 39 ± 5 meV which has to be compared to the calculated contribution from electron-electron scattering, $\Gamma_{e\text{-}e}=29$ meV. Adding the contribution from the electron-phonon scattering, $\Gamma_{e\text{-}ph}=4$ meV at $T=0$, to the calculated $\Gamma_{e\text{-}e}$ yields a reasonable agreement between the experiment and calculation. For the image-potential state a similar agreement is reached with a calculated value of 27 meV (Ref. 16) compared to the experimental value of 24 ± 6 meV for the linewidth extrapolated to $T=0$. Time-resolved measurements at 450 K (Ref. 16) gave for the surface state $\hbar/\tau=54\pm13$ meV which includes besides $\Gamma_{e\text{-}e}$ also contributions from phonon- and possible defect-induced interband scattering from the surface state to bulk bands. The measured value is in good agreement with the calculated $\Gamma_{e\text{-}e}+\Gamma_{e\text{-}ph}=29+19$ meV result. The measured lifetime broadening $\hbar/\tau$ for the surface state increases with increasing temperature. This observation as well as the comparison of the different linewidth contributions at 450 K indicate that phonon- and defect-induced scattering to bulk bands is about a factor of 5 smaller than the corresponding elastic intraband scattering.

IV. SUMMARY

We have presented the results of an *ab initio* study and time-resolved two-photon photoemission measurements of the electron linewidths for the Shockley surface state on Pd(111). The calculations show that the *e-ph* interaction is mostly determined by coupling of bulk electronic states to bulk-phonon modes. This interaction results in an unusually small *e-ph* coupling parameter λ at the $\bar{\Gamma}$ surface state due to a low density of bulk electron states at the surface-state energy. Time-resolved two-photon photoemission measurements taking into account thermally created defects confirm the calculated results.

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