Electron-phonon mass enhancement parameter of the $\bar{\Gamma}$ surface state on Au(111) measured by photoemission spectroscopy

S. LaShell*
Physics Department, Işık University, Maslak, Istanbul, Turkey

B. A. McDougall
ECFI Division, Applied Materials, 974 East Arques Avenue M/S 81301, Sunnyvale, California 94086, USA

E. Jensen†
Physics Department, Brandeis University, Waltham, Massachusetts 02454, USA
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We report the measurement of λ, the electron-phonon mass enhancement parameter, for the spin-orbit-split $\bar{\Gamma}$ surface state on Au(111). λ is determined from the change of the photoemission linewidth as a function of temperature. The difference between the normal emission $\lambda=0.34\pm0.01$ and midband $\lambda=0.30\pm0.01$ is explained as increasing bulk penetration of the surface state as it approaches the Fermi level.

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Low-energy excitations in solids are fundamental to life as we know it. They determine quantities such as conduction and specific heat, which are important properties for things as common as how high the electric bill is. One type of low-energy excitation is the electron-phonon interaction. Understanding the electron-phonon interaction helped unlock the door to the description of traditional superconductivity and may be fundamental to understanding the mechanism of the more technologically exciting high-T_c superconductors.

As electromechanical miniaturization progresses and the number of surface atoms becomes comparable to the number of bulk atoms for a given sample or device, surface properties are becoming more and more important. The combination of the increasing importance of surface properties and an interest in the electron-phonon interaction has led to a significant increase in research in this area. See the reviews by Plummer *et al.*[1] and Kevan and Rotenberg[2] and references therein.

In 1995 McDougall *et al.*[3] published a seminal paper on the use of photoemission spectroscopy to measure λ, the electron-phonon mass enhancement parameter. The relevant theory is as follows. The contributions to the hole lifetime and therefore to the total photoemission linewidth, are electron-electron, electron-phonon, and electron-impurity scattering. Electron-impurity scattering is not temperature dependent and the temperature dependence of electron-electron scattering is negligible. For temperatures T with k_bT greater than phonon energies the temperature dependence of the photoemission linewidth W should be almost entirely due to the electron-phonon interaction which has the temperature-dependent linewidth

$$W_{e\text{-}p} = 2\pi\lambda k_b T. \tag{1}$$

Thus, λ can be measured by plotting W vs T and measuring the slope. λ is formally defined right at the Fermi level (E_F);[4] therefore, the term λ is used somewhat loosely here. Nevertheless, for the reasons given above the present data do in fact provide a direct indication of the strength of the electron-phonon interaction near E_F.

λ has been measured on the (111) surfaces of the other noble metals copper[3,5,6] and silver;[6] however, we are not aware of any measurements of λ on Au(111). We present here data from the $\bar{\Gamma}$ surface state on Au(111).

The Au(111) surface has been the subject of much research due to its well-known herringbone reconstruction[7–13] and the more recent discovery of the spin-orbit splitting of the $\bar{\Gamma}$ surface state.[14–18] The dispersion of the spin-orbit-split surface state can be described as a pair of parabolas offset from each other in momentum. According to the present work, at room temperature the two parabolas along $\bar{\Gamma}$-$\bar{K}$ are $E_1(k)=13.6(k+0.0132)^2-0.412$ and $E_2(k)=13.7(k-0.0135)^2-0.413$ with energies E in eV, momenta k in Å^{-1} and dispersion in $\text{eV}/\text{Å}^{-2}$.

The data were acquired with an energy resolution of ~28 meV and angular resolution of 5×22 mrad^2. The sample temperature was varied between ~120 and ~680 K by a closed-cycle helium refrigerator run continuously in conjunction with a pulsed heater mounted behind the sample. The temperature was varied by adjusting the duty cycle of the heater and data were taken only during the "off" part of the heater cycle.

Normal emission data are shown in Fig. 1. The higher-energy peaks are satellites due to the Ar doublet from the resonance lamp used in the experiment. The lines are fits to the data: (a Lorentzian on a linear background) (Fermi function)+(the same for the Ar I satellite peak). Note the obvious increase in peak width with temperature.

The peak width as a function of temperature is plotted in Fig. 2. (The peak widths are derived from the data in Fig. 1 combined with another similar data set.) The line is a linear fit to the data and has a slope of 0.177 meV/K which yields $\lambda=0.33\pm0.01$. The uncertainty is from the fit. If the measured linewidths are corrected for the energy resolution of the analyzer, the derived value is $\lambda=0.34\pm0.01$.

Also visible in Fig. 1 is the change in peak energy E_0

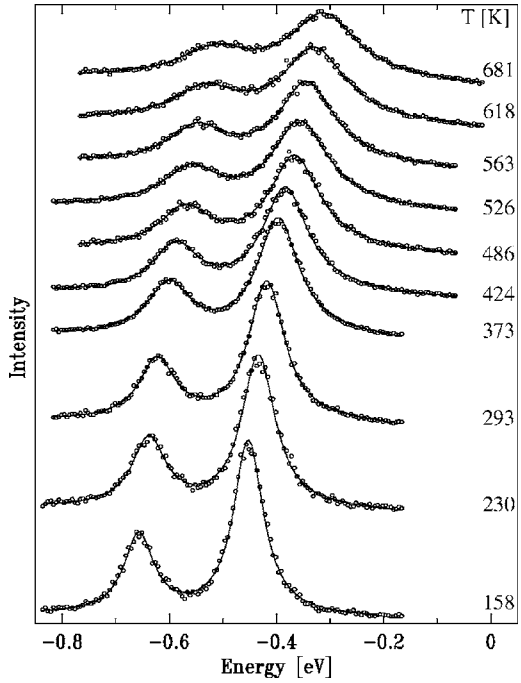

FIG. 1. Normal emission spectra showing the temperature dependence of the photoemission linewidth of the $\bar{\Gamma}$ surface state on Au(111). The circles are the data and the lines are fits to the data (see text for details). The higher-binding-energy satellite is from the Ar satellite.

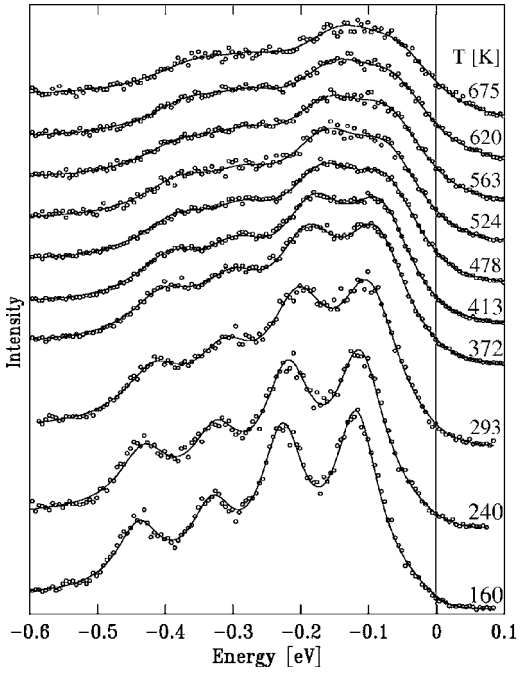

FIG. 3. Midband spectra showing the temperature dependence of the photoemission linewidth of the $\bar{\Gamma}$ surface state on Au(111). The circles are the data and the lines are fits to the data (see text for details). The two higher-binding-energy satellites are from the Ar satellite.

with temperature, which is $dE_0/dT=0.27$ meV/K. This effect has been explained on Cu(111) as due to the thermal expansion of the lattice.[19] Paniago *et al.* measure $dE_0/dT=0.18$ meV/K for the Au(111) surface state.[20] We measure a normal emission peak width of 80 meV at 293 K. Paniago *et al.* show a normal emission peak width of ~220 meV at 355 K.[20] This is indicative that the present work is from a much higher-quality surface and this is probably the reason for the discrepancy in values of dE_0/dT. Extrapolation of our measured E_0 to 30 K gives $E_0(30\ \mathrm{K})=-0.489$ eV in good agreement with the $E_0=-0.487$ eV reported by Reinert *et al.*[21] at 30 K.

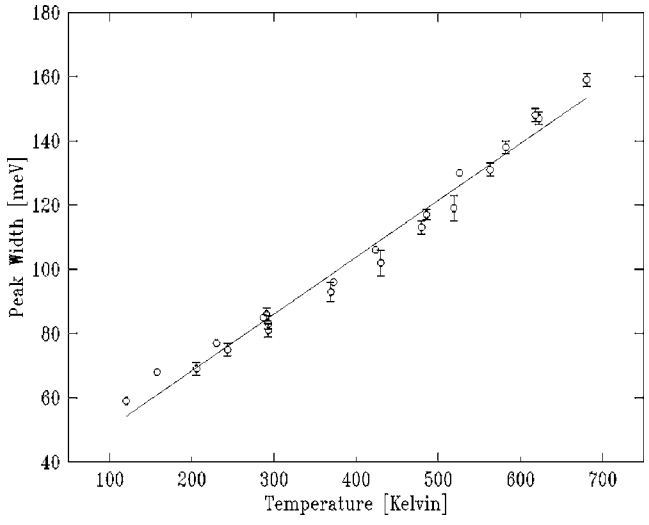

FIG. 2. Peak width vs temperature for normal emission from the $\bar{\Gamma}$ surface state on Au(111). The line is a linear fit to the data and has a slope of 0.177 meV/K which yields $\lambda=0.33\pm0.01$. The error bars on the data show uncertainties in the fitting of the peak widths. If the measured linewidths are corrected for the energy resolution of the analyzer, the derived value is $\lambda=0.34\pm0.01$.

Temperature-dependent spectra acquired midband along

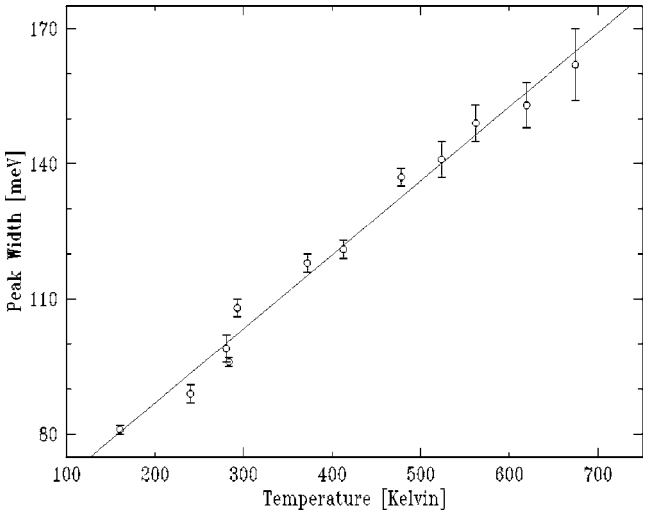

FIG. 4. Peak width vs temperature for midband spectra from the $\bar{\Gamma}$ surface state on Au(111). The line is a fit to the data and yields $\lambda=0.30\pm0.01$. Note that the two peaks were forced to have the same width as each other in fitting the original spectra. The error bars on the data show uncertainties in the fitting of the peak widths.

$\bar{\Gamma}$-$\bar{K}$ on Au(111) are shown in Fig. 3. The lines are fits to the data: (two Lorentzians)×(Fermi function)+(the same for the Ar I satellite peak) all on a linear background. The Lorentzians all have the same width to force sensible fits at high temperatures when the peaks are not clearly resolved. These data also display increasing width and shallower binding energy as the temperature increases. The peak energy changes with temperature as $dE/dT=0.14$ meV/K for the shallower peak and $dE/dT=0.17$meV/K for the deeper peak.

The peak width as a function of temperature is plotted in Fig. 4. The fit results give $\lambda=0.30\pm0.01$.[27] The uncertainty is from the fit.

Scanning tunneling microscopy (STM) results give a linewidth of 18 meV at a temperature of 4.6 K.[22] If the present data were extrapolated to that temperature, the linewidth would be 45 meV. Since STM offers the opportunity to take data as far as possible from defects, it is likely that the discrepancy between the values is due to defect scattering. Note that because defect scattering is independent of temperature the primary result of this paper is unaffected.

Fermi surface average measurements of λ for gold range from 0.05 using specific heat[23] to 0.15 using resistivity.[23] The difference between Fermi surface average measurements and the present (momentum-localized, surface-sensitive) measurement is not surprising for at least two reasons. First, bulk measurements show significant variation with location on the Fermi surface: for the (111) belly, $\lambda=0.13$,[24] while for the (111) neck, $\lambda=0.2$.[24] Thus, a momentum-localized measurement is expected to be different from a Fermi surface average measurement. Second, for the $\bar{\Gamma}$ surface states on Ag(111) and Cu(111) the Rayleigh mode is expected to be responsible for about 40% of the electron-phonon contribution to the lifetime.[6] If a similar result holds for Au(111) one would expect surface and bulk values for λ to be different. Eiguren *et al.* calculate $\lambda=0.11$ for the $\bar{\Gamma}$ surface state on Au(111).[25] While their calculations agree with the STM data point (linewidth 18 meV at temperature 4.6 K), their projected increase in linewidth with temperature (and consequent value of λ) is approximately one-third of that found in the present paper. The reason for the discrepancy is not clear.

Variation of λ in momentum space has been observed on other surfaces[26] and attributed to the degree of surface localization of the surface state. This explanation is likely to hold here as well. As the surface state approaches the Fermi level it also approaches the bulk bands and therefore its surface localization decreases. This explains the decrease in surface state λ from a more surface-localized value at $\bar{\Gamma}$ toward the lower bulk value at midband.

In summary, we report measurement of the electron-phonon mass enhancement parameter for the spin-orbit-split $\bar{\Gamma}$ surface state on Au(111). At the bottom of the band, $\lambda=0.34\pm0.01$ and at midband $\lambda=0.30\pm0.01$.

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*Corresponding author. Email address: lashell@securenym.net
†Deceased.

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[27] Correcting for energy and angular resolution raises λ to 0.32. Correcting for broadening due to taking data at fixed angle rather than fixed momentum brings the value back down to $\lambda=0.30\pm0.01$.