Electron-phonon mass-enhancement parameter and the Fermi-line eccentricity at the Be($10\bar{1}0$) surface from angle-resolved photoemission

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We report angle-resolved photoemission measurements of the dispersion of the shallow surface state around $\bar{A}$ and the surface electron-phonon mass-enhancement parameter λ_s at the Be($10\bar{1}0$) surface. The eccentricity of the elliptical Fermi line formed by the surface state is found to be $\epsilon = 0.684$. We obtain $\lambda_s = 0.672 \pm 0.027$ along the major axis and $\lambda_s = 0.642 \pm 0.031$ along the minor axis of the Fermi line. The λ_s values are about three times larger than the bulk $\lambda_b = 0.24$.

Electron-phonon interaction plays an important role in understanding various properties of a metal such as its specifc heat, resistivity, and thermal expansion. The strength of this interaction is given in terms of a dimensionless parameter λ called the electron-phonon mass-enhancement or the electron-phonon coupling parameter. λ is proportional to the electron density of states (DOS) at the Fermi level (E_F) and the electron-phonon matrix elements.[1,2] Typically λ is measured using techniques such as tunneling, electrical resistivity, and specific heat. These techniques are essentially bulk sensitive and hence give the bulk value of λ, λ_b. Furthermore, the very nature of these techniques implies that the resulting λ_b is averaged over all momenta on the Fermi surface. In general, the surface electron DOS at E_F and the electron-phonon matrix elements at the surface could be very different from those in the bulk. This implies that the surface value of λ, λ_s, could be very different from λ_b. Hence an experimental determination of λ_s is needed. It has been shown[3] that one can measure λ_s at a crystalline metallic surface by angle-resolved photoemission (ARPES). The ideas and the conditions under which this can be done are clearly presented in Ref. 3. One important point to notice is that unlike the bulk techniques, ARPES measurement of λ_s is not averaged over the Fermi line and hence one can measure λ_s in any momentum direction on the Fermi line.

The main ideas for the measurement of λ_s by ARPES can be summarized as follows. For ARPES from a two-dimensional band state of a perfect crystalline surface, the photohole (which will henceforth be referred to as hole) lifetime τ is related to the width W observed in the ARPES spectra by $W = \hbar/\tau$. The hole lifetime arises from electron-electron, electron-impurity, and electron-phonon interactions. For hole energies close to E_F, the electron-electron contribution to the hole lifetime and its temperature dependence are negligible. In the dilute impurity/defect limit, the contribution from the electron-impurity interaction is independent of temperature. However, the electron-phonon contribution is not negligible and can be shown to be the dominant contribution to the lifetime and its temperature dependence. The electron-phonon interaction contribution to the lifetime at any temperature can be calculated using the following formula:[1]

$$W_{ep}(\omega) = \hbar/\tau_{ep}(\omega) = 2\pi\hbar \int_0^{\omega_m} d\omega' \alpha^2F(\omega')[1 - f(\omega - \omega') + 2n(\omega') + f(\omega + \omega')], \quad (1)$$

where $\alpha^2F(\omega)$ is the Eliashberg coupling function, ω_m is the maximum phonon frequency, and $f(\omega)$ and $n(\omega)$ are the Fermi and Bose-Einstein distributions. The electron-phonon mass-enhancement parameter λ_s is related to $\alpha^2F(\omega)$ by $\lambda_s = 2\int_0^{\omega_m} d\omega' \alpha^2F(\omega')/\omega'$. For temperatures larger than the Debye temperature (T_D) and for hole energies close to E_F, Eq. (1) can be shown to lead to a simple form[1] $W_{ep} = 2\pi\lambda_s kT + \text{const}$. This linear form is independent of the shape and dimensionality of the phonon spectrum[1,4] and can be shown to be valid to within 20% down to temperatures one-third of T_D. Hence in this high temperature limit λ_s can be determined[3] from the slope of the width versus temperature data. However, because of the high bulk Debye temperature ($T_D = 1000$ K) and high vapor pressure (10^{-7} torr at 900 K) of Be, one cannot perform the experiments at $T \geqslant T_D$. Another way to determine λ_s is to fit the experimental width versus temperature data directly using Eq. (1) by assuming a model for the phonon density of states. This requires one to assume a shape for the phonon spectrum and thus introduces additional uncertainties. Hence, the determination of λ_s at the Be surface cannot be expected to be as accurate as that on low T_D materials like Cu.[3,6]

Be is a semimetal with a very low DOS at E_F. The surface DOS's at E_F at the Be($10\bar{1}0$) and Be(0001) surfaces are much higher[7–9] than the bulk DOS at E_F. One of the main differences between the surface electronic structure of these two surfaces is the shape of the Fermi line formed by the surface state. At the Be(0001) surface, the surface state Fermi line is centered in the gap around $\bar{\Gamma}$ and is almost circular.[10,11] At Be($10\bar{1}0$), the surface state Fermi line is centered in the gap around $\bar{A}$ and is elliptical.[8,9,11] Three surface core-level shifted components[13,14] corresponding to layers 1 to 3 and anisotropic Friedel oscillations[12] have been observed earlier at this surface and attributed to the large surface to bulk DOS at E_F and to the anisotropic shape of the Fermi line.

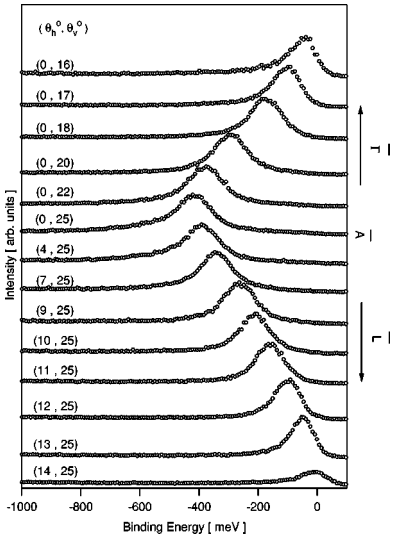

FIG. 1. Room temperature surface state spectra along $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ at various angles. The angles θ_h and θ_v are the analyzer angles in the horizontal and vertical planes. The sample was oriented such that $\bar{\Gamma}$-$\bar{M}$ is in the horizontal plane and $\bar{\Gamma}$-$\bar{A}$ in the vertical plane. The photon energy is 21.2 eV and the angular resolution is $\pm 0.2°$.

A recent measurement[5,6] of λ_s at the Be(0001) surface reported $\lambda_s = 0.7 \pm 0.1$. The bulk value for Be is $\lambda_b = 0.24$. If one assumes the surface and bulk electron-phonon matrix elements to be similar, the close scaling of λ_s/λ_b with the ratio of the surface to bulk DOS at E_F is not surprising. However, this assumption is not obvious for Be, especially if one takes into account that the bulk Fermi surface of Be is far from free-electron-like and that λ_b measured by bulk techniques is averaged over all momenta on the Fermi surface. The high surface to bulk DOS ratio at E_F and the anisotropic shape of the Fermi line at the Be$(10\bar{1}0)$ surface make it a good candidate to check for the dependence of λ_s on the DOS at E_F and the electron-phonon matrix elements.

The experiments were performed at beamline 33, at the MAX-I synchrotron radiation facility in Lund, Sweden. The beamline is equipped with a SGM monochromator[15] and a VG end station equipped with a variable angular resolution VG 75 mm electron analyzer.[16] A photon energy of 21.2 eV and an incident angle of 45° were chosen for the experiments. The combined energy resolution of the photons and the analyzer was set to 35 meV. An angular resolution of $\pm 0.2°$ was selected. The Be$(10\bar{1}0)$ single crystal was mounted on a 0.2 mm tungsten wire. This wire was also used for heating the crystal. For the temperature dependent study, the heating current was pulsed at 1 kHz and the electron counting was disabled when the heating current was on. During the temperature dependent studies, the temperature of the sample was stable to within 5 °C. The crystal was cleaned by repeated Ne^+ sputter and anneal cycles. The surface order was checked with low-energy electron diffraction, which showed a rectangular 1×1 pattern typical of the Be$(10\bar{1}0)$ surface. The cleanliness of the surface was monitored by the Be 1*s* spectrum and the width of the shallow surface state around $\bar{A}$. There was no oxide component in the Be 1*s* spectrum and the surface state width decreased as it dispersed toward the Fermi level.

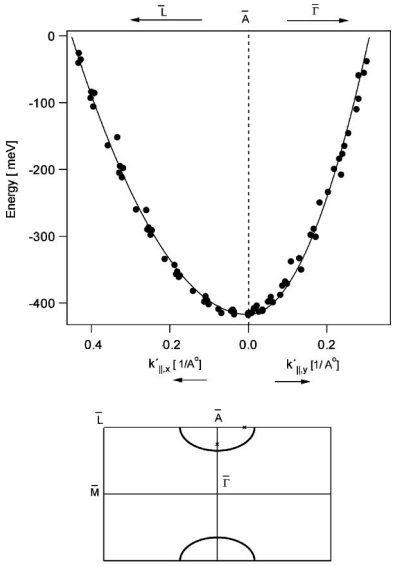

FIG. 2. The top part of the figure shows the dispersion of the surface state along the $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ directions. The filled circles are the derived peak positions and the lines represent the fits to these data. The fit along $\bar{A}$-$\bar{L}$ is $E = 2048 k'^{\,2}_{\parallel,x} - 415$ and $E = 4382\ k'^{\,2}_{\parallel,y} - 415$ along $\bar{A}$-$\bar{\Gamma}$, where E is measured in meV and $k'_\parallel$ in Å^{-1}. The bottom part of the figure is a picture of the first Brillouin zone. The thick line is the surface state Fermi line. The crosses indicate the points at which the temperature dependent studies were performed (see text for details). The Fermi momenta along $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ are 0.450 Å^{-1} and 0.308 Å^{-1}, respectively. The eccentricity of the Fermi line is $\epsilon = 0.684$. The Brillioun zone dimensions are $\bar{A}$-$\bar{L} = 1.375$ Å^{-1} and $\bar{A}$-$\bar{\Gamma} = 0.877$ Å^{-1}.

A detailed mapping of the surface states at the Be$(10\bar{1}0)$ surface has been reported earlier.[9] There are two surface states located in the gap around $\bar{A}$.[9] Here we concentrate only on the lower binding energy surface state. This surface state has a binding energy of 415 meV at $\bar{A}$ and disperses toward E_F when moving away from $\bar{A}$. A series of spectra taken at room temperature along $\bar{A}-\bar{\Gamma}$ and $\bar{A}$-$\bar{L}$ are shown in Fig. 1. In order to determine the location of the surface state peak, these and other similar spectra were fitted to a Lorentzian plus a linear background times a Fermi function. The resulting dispersion is shown in Fig. 2. For convenience we use $\bar{A}$ as the origin for measuring the value of the parallel component of the electron wave vector. We use the notation $k''_{\parallel,x}$ along $\bar{A}$-$\bar{L}$ and $k'_{\parallel,y}$ along $\bar{A}$-$\bar{\Gamma}$. At $\bar{A}$, $k'_{\parallel,x} = 0$ Å^{-1} and $k'_{\parallel,y} = 0$ Å^{-1}.

One can clearly see from Fig. 2 that the dispersion of the surface state in the $\bar{A}$-$\bar{L}$ direction is slower than the dispersion along $\bar{A}$-$\bar{\Gamma}$. Fitting these dispersions to a quadratic function in $k'_\parallel$, we obtain $E = 2048 k'^{\,2}_{\parallel,x} - 415$ along $\bar{A}$-$\bar{L}$ and $E = 4382 k'^{\,2}_{\parallel,y} - 415$ along $\bar{A}$-$\bar{\Gamma}$, where E is measured in meV and $k'_\parallel$ in Å^{-1}. The effective masses along $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ are 1.15 and 0.537, respectively. The Fermi momenta measured from $\bar{A}$ along $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ are 0.450 Å^{-1} and 0.308 Å^{-1}, respectively. We thus obtain the eccentricity of the elliptical Fermi line, $\epsilon = 0.684$. This is in contrast to the previous photoemission study,[9] which reported $\epsilon = 0.75$. We believe that

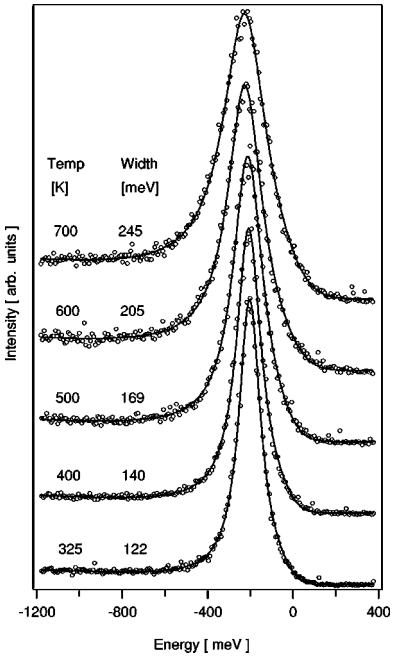

FIG. 3. Surface state spectra at various temperatures. The hole momentum is 0.324 Å $^{-1}$ along $\overline{A}$-$\overline{L}$. The filled circles are the experimental data and the line is a fit using a Lorentzian plus a linear background times a Fermi function. The photon energy is 21.2 eV. The angular resolution is $\pm 0.2°$ and the corresponding momentum resolution is ± 0.003 Å $^{-1}$.

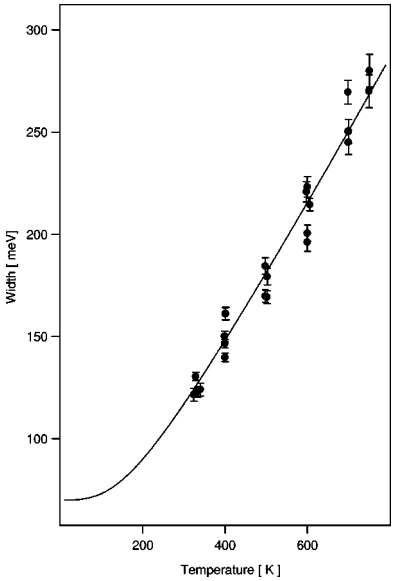

FIG. 4. Surface state width versus temperature plots at $k'_{\parallel,x} = 0.324$ Å $^{-1}$ (see text for the definition of $k'_{\parallel,x}$). The filled circles are the widths obtained by fitting spectra similar to the ones shown in Fig. 3 using a Lorentzian plus a linear background times a Fermi function. The line is a fit using Eq. (1) with the Debye model for phonons and yields $\lambda_s = 0.737 \pm 0.033$. Applying the correction factor to the widths (see text for details) and refitting the data yields $\lambda_s = 0.672 \pm 0.027$.

this discrepancy is due to a better surface quality of our sample and to our better energy and momentum resolution. Our results compare well with the scanning tunneling microscopy results where $\epsilon = 0.69$ was reported.[11,12] The theoretical value[11] for the eccentricity is $\epsilon = 0.67$.

The temperature dependent study was performed on the above mentioned surface state. From the spectra shown in Fig. 1, it is seen that the background is almost constant and also the intensity at E_F is small, as long as the surface state is not close to E_F. The room temperature width of the surface state at $\overline{A}$ is about 170 meV and decreases as the surface state disperses toward E_F. These observations suggest that the impurity/defect contribution to the spectra is small.[3,17] Hence one is justified in assuming that the temperature dependence of the impurity contribution to the width is negligible and that all the temperature dependence of the width for hole energies close to E_F can be attributed the contribution from the electron-phonon interaction.

The temperature dependent study was performed at $k'_{\parallel,y} = 0.222$ Å $^{-1}$ and $k'_{\parallel,x} = 0.324$ Å $^{-1}$. These correspond to a binding energy of about 200 meV along both the axes. A typical set of spectra for $k'_{\parallel,x} = 0.324$ Å $^{-1}$ is shown in Fig. 3. The $\pm 0.2°$ angular resolution used for collecting the spectra corresponds to a momentum resolution of ± 0.003 Å $^{-1}$. It is clearly seen in Fig. 3 that the width of the peak increases with temperature. These and other similar spectra were fitted to a Lorentzian plus a linear background times a Fermi function. The resulting width versus temperature plot together with the fitted curve are shown in Fig. 4. The fit was done using Eq. (1) with the Debye model for phonons. In the Debye model for phonons, $\alpha^2 F(\omega) = \lambda_s (\omega/\omega_m)^2$. We used the experimentally determined[18] maximum surface phonon energy $\hbar\omega_m = 60$ meV. The fit yields $\lambda_s = 0.737 \pm 0.033$ for the $\overline{A}$-$\overline{L}$ direction. The results of the temperature study at $k'_{\parallel,y} = 0.222$ Å $^{-1}$ are shown in Fig. 5. The Debye model fit yields $\lambda_s = 0.749 \pm 0.038$ for the $\overline{A}$-$\overline{\Gamma}$ direction.

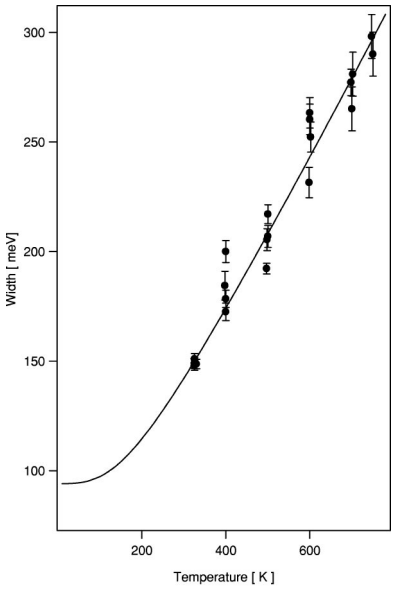

FIG. 5. Surface state width versus temperature plots at $k'_{\parallel,y} = 0.222$ Å $^{-1}$ (see text for the definition of $k'_{\parallel,y}$). The filled circles are the widths obtained by fitting experimental spectra at various temperatures (not shown). The line is a fit using Eq. (1) with the Debye model for phonons and yields $\lambda_s = 0.749 \pm 0.038$. Applying the correction factor to the widths (see text for details) and refitting the data yields $\lambda_s = 0.642 \pm 0.031$.

It was recently pointed out[5] that a correction needs to be applied to the data analysis described above. It stems from the fact that when one takes data in the energy distribution mode, i.e., by fixing the angle and photon energy and scanning the kinetic energy, the variation of $k_\parallel$ within the peak makes the peaks appear broader by a factor $[1-(\partial E/\partial k_\parallel)(m/\hbar^2)(\sin^2\theta/k_\parallel)]^{-1}$, where m is the free electron mass. This correction factor reduces the widths along $\bar{A}$-$\bar{L}$ and $\bar{A}$-$\bar{\Gamma}$ by about 9% and 12%, respectively. Applying the correction factor and refitting the temperature versus width data, we obtain $\lambda_s = 0.672 \pm 0.027$ for the $\bar{A}$-$\bar{L}$ direction, and $\lambda_s = 0.642 \pm 0.031$ for the $\bar{A}$-$\bar{\Gamma}$ direction. Since the ratio of the surface state DOS to the bulk DOS at E_F for the Be$(10\bar{1}0)$ surface is about 3,[8] our results suggest that λ_s/λ_b roughly scales with the ratio of surface to bulk DOS's at E_F. Our results also suggest that the electron-phonon matrix elements do not vary significantly on the surface Fermi line.

One interesting aspect to consider due to the enhanced electron-phonon interaction at the surface is the possibility that the Be$(10\bar{1}0)$ surface could superconduct at a much higher temperature than its bulk.[6] A detailed discussion of this possibility for the Be(0001) surface is given in Ref. 6. The main ideas are the following. In conventional superconductors, which are driven by the electron-phonon interaction, larger values of λ lead to higher superconducting transition temperatures (T_C). The relationship between λ and T_C is given by McMillan's equation, $T_C = (T_D/1.45)e^{-1.04(1+\lambda)/[\lambda-\mu^\star(1+0.62\lambda)]}$, where $\mu^\star$ represents the electron-electron interaction and is[1,2] typically 0.1. If we use $T_D = 700$ K and $\lambda_s = 0.66$, we obtain $T_C \approx 17$ K. Here we have implicitly assumed that the surface state electrons do not scatter into the bulk.[6] It can be argued that in the case of negligible density of impurity/defect at the surface, the scattering of the surface state electrons into the bulk is negligible.[6] In this limit, it is conceivable that the T_C at the surface of Be$(10\bar{1}0)$ is as much as 600 times higher than in the bulk. It is known that amorphous Be films of about 100 Å thickness have $T_C = 10$ K, about 400 times higher than the $T_C = 0.026$ K in bulk Be.[19] It is believed that the enhanced T_C in these films is related to the enhanced DOS at E_F compared to that in bulk Be.[19]

In conclusion, we have mapped the shallow surface state around $\bar{A}$ and obtained the eccentricity of the elliptical Fermi line to be $\epsilon = 0.684$. We measured the electron-phonon mass-enhancement parameter $\lambda_s = 0.672 \pm 0.027$ along the $\bar{A}$-$\bar{L}$ direction and $\lambda_s = 0.642 \pm 0.031$ along the $\bar{A}$-$\bar{\Gamma}$ direction. The λ_s values are about 3 times larger than the bulk value $\lambda_b = 0.24$. From these observations we conclude that for Be$(10\bar{1}0)$, λ_s/λ_b roughly scales with the ratio of the surface to bulk DOS's at E_F. We also conclude that the electron-phonon matrix elements do not vary significantly on the surface Fermi line. Based on $\lambda_s = 0.66$, we speculate that the superconducting transition temperature at the surface of Be$(10\bar{1}0)$ could be as high as 17 K, about 600 times higher than its bulk T_C.

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