Abstract. The electron–phonon coupling strength for two different surface states on Bi(110) close to the Fermi level is determined by measuring the energy- and temperature-dependent imaginary part of the self-energy and fitting it to different models of the phonon spectrum. For the hole pockets near the \( \bar{\Gamma} \) and \( \bar{\bar{M}} \) points, the electron–phonon mass enhancement parameter \( \lambda \) is found to be 0.19(3) and 0.27(2), respectively.

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1 Author to whom any correspondence should be addressed.
1. Introduction

One of the key advantages of a photoemission experiment is the wealth of information the photoelectron is carrying about the system under investigation. A lot of this information can be extracted, even though the photoemission process is rather complicated and involves both initial- and final-state effects. In the first few decades of angle-resolved photoemission spectroscopy (ARPES) from solids, the experimental objective was mainly to determine the initial- (and final-) state band structure of crystals. As the resolution of photoemission spectrometers improved, it became increasingly possible to analyse the peak shape and intensity of the photoemission spectra also, an approach which was pioneered by Kevan and co-workers. In the last 15 years or so, the focus has entirely shifted away from mere band-structure determination and many experiments are now concerned with details of the photoemission lineshape and their relation to the many-body effects of the solid. This has been driven mainly by the expectation that detailed ARPES investigations will help to understand the origin of high-temperature superconductivity [1, 2]. A fact of particular importance when studying high-temperature superconductors is that their structure can be viewed as quasi-two-dimensional. This greatly simplifies the description of the photoemission process and appears to be a necessary condition for the detailed analysis of photoemission lineshape.

High-temperature superconductors are very complex systems. They do show pronounced signatures of many-body effects in their photoemission spectra [2], but the origin of these spectral features is not easy to pin down and, in fact, highly debated. Therefore, it is also worthwhile to study many-body effects and photoemission line shapes of much simpler systems especially when one particular many-body interaction is dominating all the others and can be singled out experimentally. A lot of physical insight has been gained by studying the properties of electronic surface states on clean and adsorbate-covered metal surfaces [3]–[14]. Here, as in the case of the high-temperature superconductors, the surface-localized electronic structure represents a quasi-two-dimensional system which is therefore well suited for lineshape investigations. This general idea is also the motivation for the present paper in which we present a study of the electron–phonon coupling (epc) on Bi(110).

All the low-index surfaces of Bi studied so far can be viewed as quasi-two-dimensional metals on an almost-insulating substrate, due to the semimetallic character of Bi and the nature of the electronic surface states. Bulk Bi shows a pronounced pseudo-gap at the Fermi level and has a carrier density which is five orders of magnitude smaller than in a typical metal [15, 16]. The surfaces, however, support metallic surface states with relatively small Fermi velocities, thus turning them into much better metals [17]–[19]. These quasi-two-dimensional metals have the rather peculiar property that their band structure is strongly influenced by the spin–orbit coupling which lifts the degeneracy with respect to the electron spin [17, 20]. Bi, being a heavy metal, shows pronounced spin–orbit coupling effects. In the bulk, this interaction is of crucial importance for describing the electronic bands correctly [21] but every band still has two electrons with opposite spin per \( k \) point. This is due to the combination of time-reversal and crystal inversion symmetry. The former ensures (in the absence of a magnetic field) that for every solution of the Schrödinger equation \( \epsilon(k, \uparrow) \) there must also be a solution \( \epsilon(-k, \downarrow) \). The latter states that for every \( \epsilon(k, \uparrow) \) there must also be an \( \epsilon(-k, \uparrow) \). From the combination of the two it is evident that every bulk state has two possible spin directions per \( k \) point. At the surface, the inversion symmetry is broken and the bands are split such that every band contains only
Figure 1. Left: surface Brillouin zone and Fermi surface (schematically, in green). The red lines in the surface Brillouin zone indicate the $k$ range used for the analysis of the epc for the two states. Right: dispersion of the surface states around the $\bar{\Gamma}$ and $\bar{M}$ points. Details of the surface state dispersion are reported in [17].

one electron per $\vec{k}$ point. The effect of the spin–orbit coupling on the surface band structure is a dramatic change of the dispersion and the band structure [20].

Here we treat the Bi(110) surface as a quasi-two-dimensional metal in which we study the electron–phonon interaction. We have to examine carefully the conditions under which this approach is justified. First of all, the picture of Bi surfaces as quasi-two-dimensional is only valid in the immediate vicinity of the Fermi level. For energies outside the pseudo-gap, bulk states can have considerable importance [12]. In addition to this, we have to rule out dominant contributions from other many-body interactions. For a system like Bi, these are the electron–electron and the electron–impurity interactions. The latter is assumed to be constant and the former is negligible as long as the binding energy is sufficiently small. Consequently, we have to concentrate on the immediate vicinity of the Fermi level in our study. This also corresponds to the energy regime in which many-body interactions have the greatest consequences.

The electronic structure of Bi(110) has been discussed elsewhere [17, 22] but the surface Brillouin zone and Fermi surface are given in figure 1. For the investigation reported here, we concentrate on two electronic surfaces states; the hole-pockets close to the $\bar{\Gamma}$ and $\bar{M}$ points in the $\bar{\Gamma} - \bar{X}_2$ and $\bar{M} - \bar{X}_2$ directions, respectively. These states are especially well suited for the type of analysis outlined below, in particular because they are well separated from other states in these particular directions of $k$ space. The dispersion of the states around the high-symmetry points is also given in figure 1.
We present a detailed investigation of the epc for these two states. Such an analysis has to be divided into two distinct parts: the first is the determination of the many-body signature, i.e. the self-energy from the photoemission data. The second is the interpretation of this self-energy in terms of epc. For both steps, we will clearly state which approximations are made. Therefore, this introduction is followed by two sections describing the determination of many-body effects by ARPES and the spectral signature of the epc. After this, the experimental techniques, the practical determination of the self-energy and its interpretation are presented in separate sections. This is followed by a discussion of the results and the conclusions from our work.

2. Angle-resolved photoemission and the spectral function

ARPES is a firmly established experimental technique and many excellent reviews are available, describing both its theoretical and experimental fundamentals (see, e.g. [23]–[26]). In the following, we basically build on the treatment given by Matzdorf [25] and we focus on what is essential to this paper: ARPES from nearly two-dimensional states and the interpretation of the results in terms of the hole spectral function. The main ideas are as follows. Assuming a weak light field, ARPES is treated in the framework of time-dependent perturbation theory. The external field is coupled to the solid’s Hamiltonian, leading to a transition rate which is given by Fermi’s golden rule. As a further simplification, the dipole approximation is used for photoemission at low energies and the surface emission effects are neglected.

The most important kinematic result is that the photoelectron wave-vector parallel to the surface \( \vec{k}_\parallel \) is conserved in the photoemission process (modulo a surface reciprocal lattice vector), whereas the perpendicular component is not. In the following, we omit the index for the parallel component and define \( \vec{k} \) as the two-dimensional wave-vector parallel to the surface and \( k_\perp \) as the perpendicular component. \( \vec{k} \) is completely determined by the emission angles and the kinetic energy of the photoelectron.

For the final photoemission intensity at the detector, one gets [25]

\[
I(E_{\text{kin}}, \vec{k}) \propto |M_f(k_f, \vec{k})|^2 f(h\nu - E_{\text{kin}} - \Phi, T) \int A(h\nu - E_{\text{kin}} - \Phi, \vec{k}) L(k_{f\perp}, k_{f\perp}^0) \, dk_{f\perp}, \tag{1}
\]

where \( f \) is the Fermi distribution, \( A \) is the hole spectral function and \( L \) is a Lorentzian distribution to account for the real-space damping of the outgoing electron wave. \( h\nu \) is the photon energy, \( \Phi \) is the sample work function, \( E_{\text{kin}} \) is the kinetic energy of the photoelectron and \( M_f \) is the matrix element. The integration is over all possible perpendicular wave vector components \( k_{f\perp} \). \( k_{f\perp}^0 \) is the perpendicular wave vector for the undamped final state wave. For a quasi-two-dimensional system, the hole spectral function is given by

\[
A(\omega, \vec{k}, T) = \frac{\pi^{-1} |\Sigma''(\omega, \vec{k}, T)|}{[h\omega - \epsilon(\vec{k}) - \Sigma'(\omega, \vec{k}, T)]^2 + \Sigma''(\omega, \vec{k}, T)^2}, \tag{2}
\]

where \( \epsilon(\vec{k}) \) is the single-particle dispersion, \( \Sigma' \) and \( \Sigma'' \) are the real and imaginary parts of the so-called self-energy. The meaning of the spectral function will be discussed below. The important point here is that \( A \) does not depend in any way on \( k_{f\perp} \) and can thus be taken out of the integral.
\[ \mathcal{L}(k_{f\perp}) = \frac{\sigma_f/\pi}{(k_{f\perp} - k^0_{f\perp})^2 + \sigma_f^2}, \]  

(3)

where \(2\sigma_f\) is the damping-induced width of the Lorentzian distribution. The precise value of \(k^0_{f\perp}\) depends on many parameters, in particular on the nature of the final-state dispersion. If we now consider again the photoemission intensity

\[ I(E_{\text{kin}}, \vec{k}) \propto |M_f(\vec{k}_f, \vec{k}_i)|^2 f(h\nu - E_{\text{kin}} - \Phi, \vec{k}) A(h\nu - E_{\text{kin}} - \Phi, \vec{k}) \int \frac{\sigma_f/\pi}{(k_{f\perp} - k^0_{f\perp})^2 + \sigma_f^2} \, dk_{f\perp}, \]

(4)

then the integral extends merely over a Lorentzian distribution. For \(k^0_{f\perp} \gg \sigma_f\), it is equal to unity. The important question, however, is whether it depends on the wave-vector parallel to the surface \(\vec{k}\). Formally, it does because \(k^0_{f\perp}\) depends on \(\vec{k}\). But again, if \(k^0_{f\perp}\) is not too small, this dependence is very small. In this case, and if we assume the matrix element in (4) to be constant, the photoemission intensity is proportional to the hole spectral function of the sample times the Fermi distribution. This is only correct, however, in the limiting case of infinitely high resolution of the light source and the electron analyser. To account for finite resolution, the intensity from (4) has to be convoluted with the appropriate resolution functions. We shall address the effect of finite resolution on our results later.

We now discuss the physical interpretation of the spectral function \(A\). It is used to describe the electronic structure of a solid in the presence of many-body effects. \(A\) can be viewed as the probability of finding an electron with energy \(\hbar\omega\) and momentum \(\vec{k}\) at a given temperature \(T\). The spectral function is determined by the unrenormalized dispersion \(\epsilon(\vec{k})\) and the self-energy \(\Sigma\) as in (2). This is usually simplified by assuming that the self-energy is independent of \(\vec{k}\), thus

\[ A(\omega, \vec{k}, T) = \frac{\pi^{-1}|\Sigma'(\omega, T)|}{[\hbar\omega - \epsilon(\vec{k}) - \Sigma'(\omega, T)]^2 + \Sigma''(\omega, T)^2}. \]

(5)

The self-energy is a complete description of the many-body processes. \(\Sigma'\) and \(\Sigma''\) are related by a Kramers–Kronig transformation.

In a modern ARPES set-up, the photoemission intensity in (4) can be measured for many values of \((E_{\text{kin}}, \vec{k})\) such that any cut through the spectral function can be extracted. However, we briefly relate the spectral function and the result of equation (4) to the traditional measuring modes of ARPES, energy distribution curves (EDCs) and momentum distribution curves (MDCs).

An EDC is the photoemission intensity as a function of kinetic energy for a fixed photon energy and a fixed emission angle. The fact that the emission angle, not \(\vec{k}\), is constant means that an EDC corresponds to a fairly complicated cut through the spectral function. Under certain conditions, for example for normal emission or for a very small energy range, an EDC is taken at approximately constant \(\vec{k}\). Even then, an EDC calculated from (4) and (5) has a fairly complicated form. This is due to the energy-dependence of \(\Sigma\). A simple scenario arises when we assume that \(\Sigma'(\omega, T) = 0\) and that \(\Sigma''(\omega, T)\) does not depend on \(\omega\). Then we get

\[ A(\omega, \vec{k}, T) = \frac{\pi^{-1}|\Sigma''(T)|}{[\hbar\omega - \epsilon(\vec{k})]^2 + \Sigma''(T)^2}. \]

(6)
which is a Lorentzian with the maximum at \( \epsilon(\vec{k}) \) and a full-width at half-maximum (FWHM) of \( 2|\Sigma''(T)| \). This approximation is relevant in the case of an EPC, as long as the binding energy of the peak is not too small (see figure 2). However, care is necessary when an EDC linewidth is identified with \( 2|\Sigma''(T)| \) because of the above-mentioned problem that an EDC is, strictly speaking, measured at a constant emission angle, not at a constant \( \vec{k} \) [8, 27, 28].

The situation is simpler in the case of MDCs because they are readily represented by (4). The maximum of an MDC is reached when \( \hbar \omega - \epsilon(\vec{k}) - \Sigma'(\omega, T) = 0 \). Based on this, the renormalized dispersion is defined as the self-consistent solution of

\[
E(\vec{k}) = \epsilon(\vec{k}) + \Sigma'(E(\vec{k}), T). \tag{7}
\]

Equation (5) takes on a particularly simple form in the case of a linear dispersion. We consider only one direction in \( \vec{k} \) space and write \( \epsilon(k) = vk \) such that the origin of the co-ordinates is at the Fermi level crossing. Then it is easy to show that (5) is a Lorentzian line in \( k \) for a given \( \omega \) with the maximum at

\[
k_{\text{max}} = (1/v)(\hbar \omega - \Sigma'(\omega)) \tag{8}
\]

and

\[
\text{FWHM} = 2|\Sigma''(\omega)/v|. \tag{9}
\]

Even if all the above assumptions are fulfilled and the spectral function is measured by ARPES, the extraction of the self-energy near the Fermi level is not straightforward. The key problem is that the unrenormalized dispersion \( \epsilon(\vec{k}) \) is not known. Different solutions have been employed to solve this problem. One way is to extrapolate \( \epsilon(\vec{k}) \) from states at higher binding energy where the renormalization is negligible. Another is to take \( \epsilon(\vec{k}) \) from a calculation of the band structure which does not incorporate the many-body effects. Finally, \( \epsilon(\vec{k}) \) and the self-energy can be determined by a self-consistent fitting procedure [29]. In the present paper, we will obtain \( \epsilon(\vec{k}) \) from a measurement of the dispersion at elevated temperatures, where the renormalization due to epc is negligible.

3. The electron–phonon coupling

There are three important many-body interactions which limit the lifetime of the photohole in a simple system like ours: the electron–electron interaction, the electron–impurity interaction and the electron–phonon interaction. Before we discuss the latter in more detail, we summarize the effect of the others and state how they should be taken into consideration. An electron–electron scattering process is basically an Auger transition, in which the photohole is filled by another electron and a third electron is emitted to conserve energy and momentum. In a Fermi liquid, this contributes to \( \Sigma' \) like \( \beta[(\pi k_B T)^2 + E_{\text{bin}}^2] \). \( \beta \) is usually quite small (of the order of \( 10^{-2} \text{ eV}^{-1} \)), [3] such that the temperature-dependence of the electron–electron scattering is negligible for experimentally practical temperatures. The energy dependence of the electron–electron scattering is, however, of considerable importance but, again because of the small \( \beta \), the quadratic increase of \( \Sigma'' \) as a function of binding energy is usually not relevant for energies...
Figure 2. Renormalization of the electronic dispersion close to the Fermi energy (schematic). The dashed line is the bare dispersion and the blue solid line is the renormalized dispersion at $kT = 0.5\hbar\omega_D$, assuming the Debye model for the phonon spectrum. The red line is for $kT = 10\hbar\omega_D$. Inset: real and imaginary parts of the complex self-energy for the epc, $\Sigma'$ and $\Sigma''$, for the two different temperatures marked by the same colours.

very close to the Fermi level (within 50 meV or so). This has been illustrated for the case of Mo(110) by Valla et al [6], where a d-type surface state shows a somewhat higher $\beta$ of 0.28 eV$^{-1}$. The electron–impurity scattering is commonly assumed to be independent of both energy and temperature. Its main effect is a $\vec{k}$ integration, similar to the effect of the angular resolution [30, 31]. We will also assume this here although, in general, it has to be questioned on surfaces at elevated temperatures where thermally excited defects are known to play an important role.

For the epc, the typical situation is shown in figure 2. The epc changes the dispersion and the lifetime of the electronic states. Very close to the Fermi level, within a typical phonon energy $\hbar\omega_D$, the dispersion is renormalized such that it is flatter at the Fermi energy. Consequently, the effective mass of the electrons at the Fermi level and the density of states is increased [32]. The increase of the effective mass is described by the electron–phonon mass enhancement parameter $\lambda$ such that $m^* = m_0(1 + \lambda)$, where $m^*$ and $m_0$ are the effective masses with and without epc, respectively.

As with other many-body interactions, the effect of the epc is described by the self-energy $\Sigma$, which is also shown in figure 2 for two temperatures. The real part $\Sigma'$ is small except for energies very close to the Fermi level. The imaginary part $\Sigma''$ is changing rapidly close to the Fermi level and is almost constant at higher energies. $\Sigma'$ vanishes exactly at $E_F$ such that the location of the Fermi surface is not affected by the interactions. The rapid increase of $\Sigma''$ very close to $E_F$ is reminiscent of the quadratic increase, which would be expected for the electron–electron coupling but the energy scale is much smaller.

Despite the usually small effect on the electronic dispersion, the epc has important consequences since it mostly affects the electrons at the Fermi level. It strongly influences the
normal-state resistivity of metals, it changes the electronic heat capacity and, most spectacularly, it provides the coupling mechanism for conventional BCS-type superconductivity [32]. It may also play an important role in the mechanism of high-temperature superconductivity [33], but this point is a subject of heavy debate (see for example [34]).

Before we discuss how the measured spectral function can be interpreted in terms of epc, we briefly review the theoretical description of the epc and its relation to ARPES (see also [32], [35]–[37]). The basic function for the epc is the so-called Eliashberg coupling function $\alpha^2 F(\omega)$ which describes the transition probability to a state $\epsilon_{\vec{k}f}$ from a state $\epsilon_{\vec{k}i}$ involving a phonon of energy $\hbar \omega$. The expression $\alpha^2 F(\omega)$ suggests that the Eliashberg function is a product of a (squared) matrix element and the phonon density of states. Indeed, in the quasi-elastic approximation, $\alpha^2 F(\omega)$ can be written as [11, 35]

$$\alpha^2 F_{\vec{k}i}(\omega) = \sum_{\vec{q},\nu,f} |g_{\vec{q},\nu,i,f}|^2 \delta(\omega - \omega_{\vec{q},\nu}) \delta(\epsilon_{\vec{k}i} - \epsilon_{\vec{k}f})$$

(10)

which, if we assume a constant matrix element $|g_{\vec{q},\nu,i,f}|$, is simply a sum over the different possibilities to fill a hole state with an electron using a phonon to provide energy and momentum. In the quasi-elastic approximation above, the phonon energy is neglected in the $\delta$-function for the electronic states. This has the advantage that $\alpha^2 F(\omega)$ can be written as an integral over the phonon states. From a known $\alpha^2 F(\omega)$, all the other properties can be calculated. The imaginary part of the self-energy is given by

$$|\Sigma''(\omega, T)| = \pi \hbar \int_0^{\omega_m} d\omega' \alpha^2 F(\omega')[1 - f(\omega - \omega') + 2n(\omega') + f(\omega + \omega')]$$

(11)

(to the lowest order) where $f$ and $n$ are the Fermi and Bose distribution functions, respectively, and $\omega_m$ is the maximum phonon frequency. The real part of the self-energy can be obtained from the imaginary part by a Kramers–Kronig transformation. In the high-temperature limit ($T \gg \hbar \omega_m / k$), a very useful approximation of (11) is

$$\Sigma'' = \pi \lambda k_B T$$

(12)

which no longer depends on the characteristics of the phonon spectrum.

The mass-enhancement parameter is given by

$$\lambda = 2 \int_0^{\omega_m} d\omega' \alpha^2 F(\omega') / \omega'.$$

(13)

Note that the discussion of figure 2 implicitly suggests that $\lambda$ should be defined by the renormalization of the bands near the Fermi energy. This is, in fact, also possible leading to

$$\lambda = \frac{d\Sigma'}{d\epsilon}_{\epsilon_F,T=0K}.$$  

(14)

For $T = 0$, the definitions in (13) and (14) are identical but for increasing temperatures, the real part of the self-energy is flattening out and $\lambda$ as defined by (14) gets smaller (see figure 2). Therefore, we shall only use the definition in (13), which is based on the temperature-independent Eliashberg function.

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Assuming that the spectral function and the self-energy have been measured by ARPES, the objective is now to obtain information about the epc. In most cases, one is interested in the mass enhancement parameter $\lambda$ and we shall discuss how to determine $\lambda$ from the self-energy. Very recently, the full Eliashberg function has also been extracted from the experimental data [38], but this is probably only possible for systems where the effect is very strong or for very high resolution. Otherwise, some drastic simplifications are necessary: assuming a constant matrix element in (10) and free-electron like electronic states, an analytic expression for $\alpha^2 F(\omega)$ can be derived. If the phonon spectrum is given by an Einstein model, one obtains

$$\alpha^2 F(\omega) = \frac{1}{2}\lambda\omega_E\delta(\omega - \omega_E),$$

and for a three-dimensional Debye model

$$\alpha^2 F(\omega) = \lambda \left(\frac{\omega}{\omega_D}\right)^2, \quad \omega < \omega_D, \quad \alpha^2 F(\omega) = 0, \quad \omega > \omega_D.$$  

An approach used by many researchers is to obtain $\lambda$ through the temperature dependence of $\Sigma''$ at a finite energy. The temperature dependence of $\Sigma''$ is given by (11). This can be directly compared to the experimental linewidth of an EDC of $2|\Sigma''(T)|$ by adding a temperature-independent off-set $W_0$ to account for electron–electron and electron–defect scattering. Care has to be taken not to violate the conditions under which the EDC linewidth can be identified with $2|\Sigma''(T)|$, as discussed in the preceding section. This approach has led to many results; for a review see [36]. It is especially useful for temperatures much higher than the Debye or Einstein temperature of the system: in this case the imaginary part of the self-energy can be approximated by (12) and thus it becomes independent of the detailed phonon spectrum. The disadvantage of this approach is that it does not work for states close to the Fermi level, i.e. the states for which many-body effects are particularly significant. This is especially important when the energy dependence of the epc strength cannot be neglected, i.e. when the $\lambda$ obtained by this approach is energy-dependent [12, 39].

Another strategy is to directly use the manifestation of the epc near the Fermi level. In this approach, $\Sigma$ is determined from ARPES measurements near the Fermi level and fitting to the simple models outlined above is used to determine $\lambda$. Figure 3 shows both components of $\Sigma$ for a fixed temperature (30 K) close to the Fermi energy, calculated for both the Debye and the Einstein model and rather different parameter sets. The actual choice of parameters is inspired by the surfaces of Bi; the characteristic phonon energies are low in the bulk and probably even lower on the surface [40]. The results of all calculations are very similar. The only clear difference between weak and strong coupling is an approximately constant shift of $\Sigma''$. In an experiment, such a difference could equally be interpreted as a different contribution due to electron–electron or electron–impurity scattering, i.e. a different $W_0$. Given the strong correlation between $\lambda$, $\omega_E$ and $\omega_D$ in (15) and (16), respectively, the difficulty in extracting meaningful information from temperature-independent data is not surprising. The solution is to take data for different temperatures and to capture the most important signature of the epc in this way. An additional problem here is that it is not even simple to distinguish between two very different models for the phonon spectrum, Debye and Einstein. As long as the temperature is not very low, the Einstein model gives almost the same results as the Debye model for $\omega_E \approx 0.7\omega_D$. 

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4. Experimental approach

The Bi(110) sample was mechanically polished and cleaned by cycles of sputtering with Ne ions and annealing to 473 K. This resulted in a surface which was well ordered and clean as judged by low-energy electron diffraction and Auger electron spectroscopy, respectively. Angle-resolved photoemission experiments were performed at the SGM-3 beamline of the synchrotron radiation source ASTRID in Aarhus [41]. The total energy resolution for the data shown here is around 30 meV. The angular resolution of the analyser is about ±0.5°. The sample was cooled to approximately 30 K with a closed-cycle He cryostat. Temperature-dependent data were measured by heating the sample with a filament mounted behind the sample holder. Data were taken for temperatures between 48 and 298 K. The filament can be operated in three modes (1) continuous, (2) pulsed, such that it is only turned on for a very small fraction of data collection time or (3) chopped, such that it is strictly turned off during data collection. We have chosen the second mode and experimentally verified that the influence on the spectra is negligible. Care was also taken to avoid significant changes of the emission angles as the temperature was changed. This was monitored by reflecting a laser from the sample surface to a distant point in the laboratory. The photon energy for all the experiments was 15 eV. The energy of the Fermi level was measured by photoemission from the polycrystalline Cu sample holder.

5. Determination of the self-energy

As stated in the introduction, we analyse data for the hole-pockets close to the $\bar{\Gamma}$ and $\bar{M}$ points, in the $\bar{\Gamma} - \bar{X}_2$ and $\bar{M} - \bar{X}_2$ directions, respectively. The determination of the self-energy proceeds in two steps. In the first step, the MDC linewidth is analysed as a function of energy and temperature. In the second step, the unrenormalized dispersion and therefore also the bare velocity $v$ of the states is determined by considering data taken at high temperatures. Finally, these two results are combined to give the imaginary part of the self-energy as a function of temperature and energy.

Figure 4 shows the dispersion of the hole pocket around $\bar{M}$ along $\bar{X}_2 - \bar{M} - \bar{X}_2$ (see the red line around the $\bar{M}$ point in figure 1). A fit to an MDC extracted from the data, using two
Figure 4. Left: dispersion of the $\bar{M}$ hole pocket close to the Fermi level in the $\bar{X}_2 - \bar{M} - \bar{X}_2$ direction at $T = 48$ K (see the corresponding red line in figure 1). Right: fit to a typical MDC extracted from these data. The scale for the one-dimensional $k$ is set such that the origin corresponds to $\bar{M}$. The fit to two Lorentzians and a linear background is shown.

Lorentzian lines and a linear background, is also shown. Note that the two peaks stem from the same state on both sides of the $\bar{M}$ point which is set to have the one-dimensional $k = 0$. The intensity of the two lines can be different but their FWHM has to be the same, a constraint which is also included in the fits. The separation of the peaks directly gives the renormalized dispersion of the state. Throughout the dataset, the fits are of similar good quality suggesting that most of the conditions we have discussed above (e.g. constant matrix element and $\vec{k}$-independent self-energy) are fulfilled. The analysis of the whole dataset gives the FWHM for both symmetry lines as a function of energy and temperature as well as the corresponding statistical uncertainty. It is important to note that the condition of negligible spectrometer resolution is not met. The $\vec{k}$ resolution of the spectrometer is high enough to be unimportant but the energy resolution clearly is not, and the two are also related [42]. Therefore, a more stringent fitting of the experimental data should proceed such that the entire measured dispersion at any given temperature is fitted to the resolution-convoluted model spectral function. This approach is not feasible for the large dataset used here. We will therefore, in the next section, carefully investigate the consequences of the finite resolution on the results.

The next step in the analysis is the determination of the bare dispersion. Here, the effect of the finite experimental resolution and the effect of the epc have to be taken into account. Given the small relevant energy and $\vec{k}$ range of interest, it is safe to assume that the dispersion is linear. We argue that the most appropriate way to extract the surface-state velocity describing this dispersion is from measurements at elevated temperatures. Figure 5(a) shows the simulated ‘measured’ dispersions for a surface state with experimental parameters similar to the situation here and epc.
in the Debye model (linear dispersion with $v = 1$ eV Å, $\lambda = 2$, $\omega_D = 30$ meV, $W_0 = 40$ meV, $\delta E = 30$ meV and $\delta k_{||} = 0.025$ Å$^{-1}$). More precisely, the figure shows the maximum of simulated MDCs which were obtained from a convolution of a simulated spectral function with the $\vec{k}$ and energy resolution functions of our analyser. Such simulations are described in more detail in [43]. At low temperatures, a clear deviation of the measured dispersion from the true dispersion is seen. This is mainly due to the combination of finite energy resolution and the cut-off of the Fermi function. At high temperatures, however, the measured dispersion faithfully mimics the ideal dispersion, the only difference being a small but almost constant off-set in $\vec{k}$. This off-set is due to a combination of the finite resolution and $\Sigma'$ (note that $\Sigma'$ drops very quickly to zero at the Fermi level but remains appreciably large for binding energies greater than $2\omega_D$, see also figure 2). Figure 5(b) shows the dispersion of the actual surface state in the $\bar{M} - \bar{X}_2$ direction at 298 K with standard deviation error bars and a linear weighted fit to the data. From such fits, we obtain velocities of $0.767(6)$ eV Å and $1.29(3)$ eV Å for the $\bar{M} - \bar{X}_2$ and $\bar{\Gamma} - \bar{X}_2$ directions, respectively. In connection with this, it is worth mentioning that the dispersion could change with temperature due to the thermal expansion of the lattice. Such changes can be quite strong (see for example [14]) and it would represent a problem for the type of analysis we want to employ here. Fortunately, the typical change in the binding energy at a given $\vec{k}$ is less than 5 meV over the whole temperature range investigated here and therefore negligible.

Based on these two steps, we can now obtain the final result, the imaginary part of the self-energy $\Sigma''$. We note that the conditions for the derivation of (9) are fulfilled and we can therefore calculate $\Sigma''$ from $v$ and the FWHM as $\Sigma'' = |v| \text{FWHM}(T, \omega)/2$ for both states as a function of energy and temperature together with the corresponding statistical uncertainties.
6. Interpretation of the self-energy

In this section, we interpret the self-energy in terms of epc and defect scattering. We shall use both a Debye and an Einstein model for the phonon spectrum, and fit $\Sigma''$ calculated within these models to the experimental data. At the end of the section, we estimate the impact of our finite experimental resolution on the parameters obtained in the analysis.

Figures 6–9 show a best-fit to the data taken for both surface states, together with the experimentally determined $\Sigma''$ for both models of the phonon spectrum. The fit proceeds almost the same way as in other investigations of the epc [3], except that the data are two dimensional. The parameters describing the model are the mass-enhancement parameter $\lambda$, the characteristic phonon energies $\omega_D$ or $\omega_E$ and a constant off-set $W_0$ due to electron–impurity scattering. Note

Figure 6. $\Sigma''$ for the surface state along $\overrightarrow{M} - \overrightarrow{X_2}$ fitted to the Debye model. (a) The experimental data, (b) fit to data, (c) difference between the data and the model, and (d) a plot of the reduced $\chi^2$ and $\lambda$. The absolute value of the experimental uncertainty $\sigma$ is of the order of 1.2 meV.
that the electron–electron scattering is negligible when close to the Fermi level. In the fitting functions (15) and (16), these parameters are strongly correlated and meaningful results can be obtained only by keeping either the phonon frequency or \( \lambda \) fixed while varying the other. Figures 6 and 9 therefore also show \( \lambda \) as a function of the characteristic phonon energy as well as the reduced \( \chi^2 \), describing the quality of the fit. The results of all the fits are summarized in table 1. Most importantly, the values of \( \lambda \) for both surface states do not appear to depend on the detailed nature of the phonon spectrum (Einstein or Debye).

A more stringent statistical interpretation of the data can be based on an inspection of the reduced \( \chi^2 \) values for the optimum fit [44]. This type of analysis is meaningful because of the high number of data points describing \( \Sigma'' \) (\( n =143 \) for \( \overline{M} - \overline{X}_2 \) and \( n =130 \) for \( \overline{\Gamma} - \overline{X}_2 \)). For any reasonable fit to our dataset, we expect \( \chi^2 \) values in the order of the number of data points.

**Figure 7.** \( \Sigma'' \) for the surface state along \( \overline{M} - \overline{X}_2 \) fitted to the Einstein model. (a) The experimental data, (b) fit to data, (c) difference between the data and the model, and (d) a plot of the reduced \( \chi^2 \) and \( \lambda \). The absolute value of the experimental uncertainty \( \sigma \) is of the order of 1.2 meV.
Figure 8. $\Sigma''$ for the surface state along $\Gamma - X_2$ fitted to the Debye model. (a) The experimental data, (b) fit to data, (c) difference between the data and the model, and (d) a plot of the reduced $\chi^2$ and $\lambda$. The absolute value of the experimental uncertainty $\sigma$ is of the order of 2.5 meV.

The reduced $\chi^2$, i.e. $\chi^2$ divided by the number of data points minus the degrees of freedom in the fit, can be used to judge the statistical backing of our model. These reduced $\chi^2$ values are also given in table 1. First of all, all fits lead to a reasonable statistical backing of the models and there is no statistical justification to prefer the Debye over the Einstein model even though it leads to slightly better fits for both surface states. The reduced $\chi^2$ values for the state in the $M - X_2$ direction are above unity, while those for the $\Gamma - X_2$ direction are slightly below unity. The smaller $\chi^2$ for the $\Gamma - X_2$ direction is likely to be caused by the larger error bars in the experimental data, which are due to the smaller photoemission intensity for this surface state. Additional structure that is not adequately described by the simple models is washed out by error bars. For the $M$ surface state the intensity is higher, the error bars are smaller and the differences between model and data are seen. Note that, even for a perfect description of the Eliashberg function, which is not to be expected for our simple models, we should not obtain a reduced $\chi^2$.
Figure 9. $\Sigma''$ for the surface state along $\Gamma - X_2$ fitted to the Einstein model. (a) The experimental data, (b) fit to data, (c) difference between the data and the model, and (d) a plot of the reduced $\chi^2$ and $\lambda$. The absolute value of the experimental uncertainty $\sigma$ is of the order of 2.5 meV.

equal to unity because the fitting functions do not include the effect of the experimental resolution which is clearly there.

We conclude this section with a critical assessment of the influence of finite spectral resolution on the results. We wish to understand how much the results are affected by this. As a test, we have simulated spectral functions in the Debye model for different Debye energies and convoluted them with the resolution function corresponding to our experimental situation (for a detailed methodology see [43]; the parameters describing energy and $k$ resolution are conservative estimates). These convoluted spectral functions were then analysed in the same way as the actual experimental data: they were sliced into MDCs and fitted with Lorentzian lines, in order to determine the imaginary part of the self-energy. This was interpreted by fitting to a model spectral function as in the present section. The results of this test are given in table 2.
Table 1. Optimum fit parameters for both measured surface states and both models for the phonon spectrum, Einstein and Debye. The reduced $\chi^2$ values for the best fit are also included. Note that the error bars given in this table are the uncertainties obtained from the fit. The final error bars for $\lambda$ given in the text are larger, so as to account for the effect of the finite energy and angular resolution.

| Parameter | M − $\chi^2_2$ | $\Gamma$ − $\chi^2_2$ |
|-----------|----------------|-----------------|
| $\nu$ (eV Å) | 0.767(6) | 1.29(3) |
| $\lambda_D$ | 0.266(5) | 0.19(2) |
| $\omega_D$ (meV) | 30.7(7) | 32(3) |
| $W_{0,D}$ (meV) | 31.6(2) | 62.1(5) |
| $\chi^2_D$ | 1.37 | 0.91 |
| $\lambda_E$ | 0.264(5) | 0.19(2) |
| $\omega_E$ (meV) | 20.0(4) | 20(1) |
| $W_{0,E}$ (meV) | 31.6(2) | 62.0(5) |
| $\chi^2_E$ | 1.69 | 0.94 |

Table 2. Results of a fit to simulated spectral functions in the Debye model, for different Debye energies and including a convolution with the experimental resolution functions. The simulated temperature and energy range were the same as for the experimental data. Common parameters: $\delta E = 30$ meV, $\delta k = 0.025$ Å$^{-1}$, $\nu = 1$ eV Å, $\lambda = 0.2$, $W_0 = 35$ meV.

| $\omega_D$ (meV) | $\Delta \lambda$ (%) | $\Delta \omega_D$ (%) | $\Delta W_0$ (%) |
|-----------------|----------------------|----------------------|------------------|
| 6               | < +1                 | +128                 | +21              |
| 12              | < −1                 | +33                  | +22              |
| 18              | −2                   | +7                   | +22              |
| 24              | −3                   | −4                   | +22              |
| 30              | −4                   | −9                   | +23              |

The finite resolution has a strong effect on $W_0$ which will be seriously overestimated. This is of no great importance because the absolute magnitude of $W_0$, i.e. the amount of electron–impurity scattering, is not of central interest here. More worrying is the effect on $\omega_D$. For true values of $\omega_D$ that are small compared to the energy resolution, the value of $\omega_D$ resulting from the analysis is seriously overestimated. This is easy to understand; for a small $\omega_D$, the imaginary part of the self-energy increases very steeply close to the Fermi level until it reaches saturation at an energy close to $\omega_D$. If the energy resolution is poor, this steep increase will be broadened, leading to a measured $\Sigma''$, where the saturation is reached at higher binding energies, i.e. to an effectively increased $\omega_D$. The most relevant parameter $\lambda$, however, is essentially not affected by the experimental resolution. This result agrees with naive intuition: at least in the high-temperature limit, $\lambda$ dictates the change of $\Sigma''$ for all states and this effect cannot be mimicked by the other parameters or by the (temperature-independent) resolution. However, guided by these simulations, we increase the size of the final error bars for $\lambda$ such that a systematic error of this order is allowed for as well. Our final results are: $\lambda = 0.19(3)$ and $0.27(2)$, near the $\Gamma$ and $M$ points, respectively.

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7. Discussion

The main results of this work are two-fold: the first and more technical is that we have shown that the electron–phonon mass enhancement parameter $\lambda$ can be determined for states close to the Fermi level by analysing temperature- and energy-dependent MDCs, without the need for extremely high resolution and without any a priori assumption about the characteristic energies of the phonon spectrum. We will be discussing the advantages and limitations of this approach. The second result is the value of $\lambda$ for two different surface states on Bi(110), which we will relate to other Bi surfaces and the bulk.

The most important technical result of this work is that we have been able to determine $\lambda$ for two surface states very close to the Fermi level by analysing energy- and temperature-dependent MDCs. If one is only interested in $\lambda$, this method appears to work well, despite the fact that the energy resolution is low (compared to typical phonon energies in Bi) and that very little is known about the surface-phonon spectrum. Indeed, we have not been able to prefer the Debye model over the Einstein model or vice versa with any reasonable statistical certainty. This may not come as a surprise since neither of these limiting cases represents a good approximation of the physical reality and, moreover, the models are essentially identical for the temperature range considered here (see figure 3). We also see that our assumption of neglecting the influence of the electron–electron scattering is justified, since we can fit the data well when we consider only electron–phonon and electron–defect scattering.

Our technique of determining $\lambda$ has a number of advantages over the simplest way of determining $\lambda$, from the temperature-dependent linewidth of EDCs. In particular, it works for states very close to the Fermi level. For such states, the conditions for writing the spectral function in the form of (6) are not fulfilled. Most importantly, $\Sigma''$ depends strongly on the energy and $\Sigma'$ is not zero. Therefore, $\Sigma''$ cannot be determined from EDCs. Being able to measure close to the Fermi level is especially relevant for systems where the coupling strength can be expected to change strongly with the binding energy of the state. In the simplest picture of a constant epc matrix element in (10), these would be systems with a strongly energy-dependent density of states. Bi is such a system but not in the immediate vicinity of the Fermi level [12]. For other systems, such as free electron metals or noble metals (close to the Fermi level), these problems do not arise and a determination of $\lambda$ from EDCs at finite binding energy can be expected to work reliably.

Another way of determining $\lambda$ is from measurements of the renormalization of the bands close to the Fermi level at low temperature. In the limit of zero temperature, $\lambda$ can be determined directly by using (14), assuming that the unrenormalized dispersion is known. In the case of Bi, this would be difficult for three reasons: firstly, the experimental resolution of the spectrometer would have to be much better than the typical bulk phonon energies of 10 meV or so [45]. Secondly, the renormalization is small because of the small value of $\lambda$ and therefore difficult to observe. Thirdly, because of the low Debye temperature of Bi, the temperature which could be considered a good approximation of 0 K would have to be very low.

A very elegant way to determine not only $\lambda$ but the entire Eliashberg coupling function has recently been proposed by Shi et al [38]. The starting point of their analysis is similar to ours here: the determination of the self-energy from energy-dependent MDCs. However, instead of fitting a simple model to the self-energy, the Eliashberg function is directly extracted using a maximum entropy approach. This gives a much more detailed information about the epc than earlier investigations of the same system [46]. This method is probably only applicable in
favourable cases with large energy scales and strong coupling. Its validity is also conditional to a ‘smooth’ electronic structure in the region where it is to be used, i.e. it must be possible to neglect the binding energy dependence of the Eliashberg function.

Strong renormalization and large energy scales are also found for the high-temperature superconductors [47, 48]. The pronounced kink which is observed in the quasi-particle dispersion has been interpreted in different ways, mainly as an interaction with magnetic modes [49] and also as an interaction with phonons [33]. The application of the method by Shi et al has the potential to give a detailed picture of the character of the particular bosonic mode. It has been noted, however, that not only the interaction with a simple bosonic mode could lead to a kink in the dispersion but also other factors, for example a drastic change in the electronic density of states given by a gap or pseudo-gap [50]. For data taken at just one temperature, it is not clear how to distinguish between a bosonic and non-bosonic scenario or to know if the conditions for the applicability of the Shi et al method are met. On the other hand, temperature-dependent data could help and one could even apply the method of Shi et al to data taken at different temperatures as to check the result for self-consistency. Our approach here can be a complementary way to look at such data. While our fits have been confined to very simple models, they give a firm statistical backing for bosonic (i.e. phonon) scattering.

We now address the particular results on Bi(110) and compare them to other Bi surfaces and bulk Bi. The primary results of this analysis are the two values of $\lambda$ for the two surface states of 0.19(3) and 0.27(2), near the $\bar{\Gamma}$ and $\bar{M}$ points, respectively (see table 1). Essentially the same values have been obtained for both the Einstein and the Debye model and our analysis of the effect introduced by the experimental resolutions suggests that the values are only affected to a very small degree. The coupling for the state near $\bar{M}$ is clearly stronger than for the state near $\bar{\Gamma}$ but within the simple models considered here, it is not possible to pin down the origin of this difference.

The other parameters obtained by the fit of our data have to be treated with less confidence because of the resolution-induced changes. However, the values of $\omega_D \approx 31$ meV obtained for the Debye model are unreasonably high, given a bulk Debye energy of about 10 meV for bulk Bi. The surface phonon spectrum is not known but the surface Debye energy is probably lower than its bulk counterpart, as on most other surfaces including Bi(111) [40, 51]. The tendency of the fit to result in high phonon energies can be attributed to the inadequacy of the Debye model, in particular for a crystal with optical phonons. Indeed, the problem is partly resolved by the Einstein model where the data are fitted best with $\omega_E \approx 20$ meV. This is consistent with figure 3, where we have shown that an Einstein model and a Debye model lead to very similar $\Sigma''$ when $\omega_E \approx 0.7 \omega_D$. Still $\omega_E \approx 20$ meV is higher than the maximum (bulk) phonon energy of 13.8 meV [45]. One possible explanation could be an unusually high contribution of multiple-phonon scattering processes, which would increase the maximum energy transfer. We speculate that the relative importance of multiple-phonon processes could be relevant for the surfaces of Bi, because of the strong spin–orbit splitting which drastically limits the number of possible scattering events to fill a hole (see a more detailed discussion at the end of this section).

No results for the epc have been reported for this particular surface but we can compare the $\lambda$ values to those obtained on other Bi surfaces, Bi(100) and Bi(111). For Bi(100) it has been shown that $\lambda$ as obtained from temperature-dependent EDCs for $340 \text{ meV} > E_{\text{bin}} > 70 \text{ meV}$ is strongly binding-energy dependent [12]. This was explained by the dramatic change in the bulk density of states on the edge of the pseudo-gap around the Fermi level. This effect is thus expected to be present for all Bi surfaces. Nevertheless, the $\lambda$ values obtained for the smallest
For Bi(111) there are two determinations of $\lambda$ for the so-called hole pocket near the $\Gamma$ point, which give very different results: by considering the self-energy near the Fermi level, Ast and Höchst have reported a value of $\lambda = 2.3 \pm 0.2$ [52], assuming a surface Debye energy of $\omega_D = 5$ meV which is in reasonable agreement with experimental data [40, 51]. On the other hand, Gayone et al reported a value of $\lambda = 0.40 \pm 0.05$ based on the analysis of temperature-dependent MDCs near the Fermi level [43]. We can resolve this apparent contradiction by having a closer look at the two different determinations of $\lambda$, keeping in mind the results of the present work. Ast and Höchst have started out with a determination of the unrenormalized dispersion at low temperature and proceeded by extracting the MDC line width as a function of binding energy, in order to obtain $\Sigma''$. $\Sigma''$ was then fitted to the Debye model, assuming $\omega_D = 5$ meV in order to yield $\lambda$. The analysis of the unrenormalized dispersion contains a technical error but this is not expected to have any influence on the resulting $\lambda$ [43]. More importantly, the experimental energy resolution of around 25 meV has been ignored in the analysis. As can be seen from table 2 and the corresponding discussion, ignoring the energy resolution of 30 meV for a value of $\omega_D$ in this order of magnitude (6 meV) leads to a measured value of $\omega_D$ more than twice as high. In other words, assuming a resolution of about 25 meV as in [52], one can estimate the measured value of $\omega_D$ to be $\approx 13$ meV, assuming a true value of $\omega_D \approx 5$ meV. Indeed, fitting the $\Sigma''$ obtained by Ast and Höchst with $\omega_D \approx 13$ meV leads to a $\lambda$ value very similar to that of Gayone et al [43]. Gayone et al, on the other hand, have determined $\lambda$ from temperature-dependent MDCs at 25 meV binding energy over a large temperature range, assuming that (12) holds. They also ignore the effect of the energy resolution which is essentially the same as in the case of Ast and Höchst. However, the resulting error in $\lambda$ induced in this case can be expected to be small. Consequently, $\lambda$ for the hole pocket on Bi(111) is of the order of 0.4 and thereby clearly higher than the values obtained here for Bi(110).

Another semimetal, in a sense, is beryllium. As for bismuth, the bulk density of states near the Fermi level shows a depletion but the relative magnitude of the effect is much smaller. On the surfaces of Be, rather high values of $\lambda$ have been observed ($0.49 < \lambda < 1.18$ [36]), compared to the bulk value of 0.24. A similar situation is found for $\alpha$-Ga [4, 53]. All these systems exhibit metallic surface states which greatly increase the density of states at the Fermi level. Just from (10) one would therefore expect a stronger coupling for the surface states but other explanations are also possible [36]. In crystalline bulk Bi, the density of states at the Fermi level is extremely low and $\lambda$ is small, so small that no reliable values have been reported to the best of our knowledge. Gayone et al have estimated $\lambda = 0.13 (-0.13 + 0.2)$ [12]. The semimetallic nature of Bi is closely linked to its crystalline structure. In the liquid state, the pseudo-gap at the Fermi energy is less pronounced [54] and the same probably also holds for the amorphous state. The epc is very high for amorphous Bi ($\lambda = 2.46$) [55] but there can be other factors contributing to this change besides the change in the density of states. On the surfaces of Bi, we therefore expect to find a similar situation as on Be or $\alpha$-Ga: $\lambda$ should increase with respect to the bulk value, if only for the increased density of states. Our findings are in line with this argument but the actual increase is impossible to quantify because of the large error bars on the estimated bulk $\lambda$.

In connection to this, one has to ask how meaningful is a comparison between bulk and surface in the case of Bi. The different roles of the spin–orbit coupling for bulk and surface should have a drastic influence on the epc. In the bulk, no splitting of the bands occurs but on the surface all the bands are split [20]. If we now consider the lifetime of a hole in a surface state, this
splitting can be expected to have a pronounced effect because it drastically reduces the number of possible electrons which can fill the state by emission or adsorption of a phonon (see (10)). The reason is that only spin-conserving scattering events are possible. The situation is similar to the screening of defects on the surfaces of Bi where also only spin-conserving processes participate [22]. Therefore, a direct comparison of the $\lambda$ values is not too meaningful. The same value of $\lambda$ on the surface as in the bulk can be expected to correspond to a much higher actual coupling strength on the surface.

8. Conclusions

We have determined the electron–phonon mass enhancement parameter $\lambda$ for two surface states on Bi(110) by extracting the energy- and temperature-dependent imaginary part of the self-energy $\Sigma''$ from MDCs close to the Fermi level. The unrenormalized dispersion was obtained by measurements of MDCs at elevated temperature where the real part of the self-energy is so small that it can be ignored. The resulting two-dimensional $\Sigma''$ can be accurately fitted by an Eliashberg function calculated from either the Debye or the Einstein spectrum for the phonons. The obtained values of $\lambda$ are essentially independent of the choice of phonon spectrum. Using simulated data, we have shown that this approach of determining $\lambda$ is very stable, even if the spectrometer resolution is lower than the actual width of the phonon band. The $\lambda$ values obtained are 0.19(3) and 0.27(2), near the $\bar{\Gamma}$ and $\bar{M}$ points, respectively. They are in the same order of magnitude as those found on other Bi surfaces. However, because of the spin–orbit splitting of the surface-state bands, we suggest that the absolute values of $\lambda$ cannot be compared directly to other systems where no such splitting is present. The same numerical value of $\lambda$ should be expected to correspond to a much stronger actual coupling for Bi surfaces than for surfaces where the bands are not split or, indeed, for bulk Bi.

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