Direct Extraction of the Eliashberg Function from High-Resolution Photoemission Data.

This is the Ph.D thesis work of Shu-Jung Tang at UT (the role of Surface States in EPC on the Open Surfaces of Simple Metals). His thesis was co-advised by the PI and Phil Sprunger (LSU) and he is now working with Prof. T.-C. Chiang at the University of Illinois. Shu-Jung measured the dispersion and the temperature dependence of the binding energy and linewidth of the surfaces states in a gap in the projection of the bulk bands at the SBZ boundary for both Be(1010) and Mg(1010). For Be(1010) [74-76], the EPC mass enhancement factor was very different for the two surface states [1]. The data for the deep state S2 with a binding energy of 2.62 eV could be fitted with a Debye model ($\omega_D = 60$ meV) resulting in a mass enhancement of $\lambda(S_2) = 0.491 \pm 0.04$. But the data for the upper surface state S_1 with a binding energy of 0.37 eV could not be fitted using a Debye model for the Eliashberg function. The best fit was achieved using an Einstein model ($\omega_E = 64$ meV) with a significantly larger mass enhancement factor, $\lambda(S_1) = 0.646 \pm 0.02$. It was pointed out in this paper that there is a strong surface optical phonon at this energy at the SBZ boundary in both experiment and theory [2,3]. These observations lead to collaboration with Professor Z.-X. Shen at Stanford and Dr. XingJiang Xhou at ALS to measure the band distortion of the S1 surface state as it crosses the Fermi energy [4].

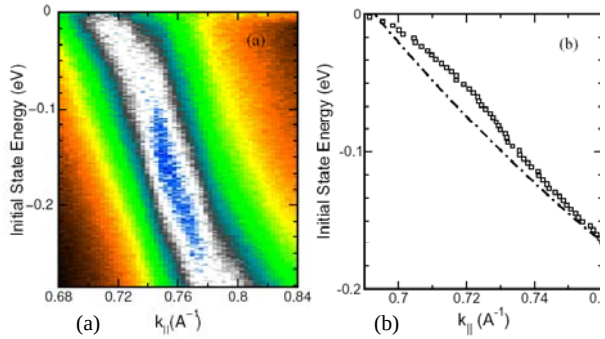

Fig. 1. (a) Photoemission image of the S1 surface state in the $\Gamma \rightarrow A$ direction. (b) Measured quasi-particle dispersion compared to frozen lattice band.

Fig. 1(a) shows the photoemission image of the S1 surface state and 1(b) displays the distortion in the quasi-particle band dispersion $\varepsilon(\mathbf{k})$ determined from a set of momentum distribution curves compared to the calculated or extrapolated [4] dispersion in a frozen lattice $\varepsilon_0(\boldsymbol{\kappa})$. In general, the quasi-particle dispersion can be written as $\varepsilon(\mathbf{k}) = \varepsilon_0(\mathbf{k}) + \mathbf{Re}\Sigma(\mathbf{k},\varepsilon)$, where the self-energy Σ is a result of the screening of the electrons by the lattice. Fig. 2(a) shows the $Re\Sigma(\varepsilon)$ extracted from the data shown in Fig. 2(b). The analysis of this data was accomplished by collaborating with the theory group of Dr. Zhenyu Zhang (ORNL). A technique has been developed by Junren Shi [4] to do the integral inversion to extract the Eliashberg function from the experimentally determined $Re\Sigma(\varepsilon)$ shown in Fig. 2(a). The procedure uses the Maximum Entropy Method, which allows physical constraints to be incorporated into the fitting process. The major constraint used here is that the Eliashberg function must be positive [4]. Fig. 2(b)

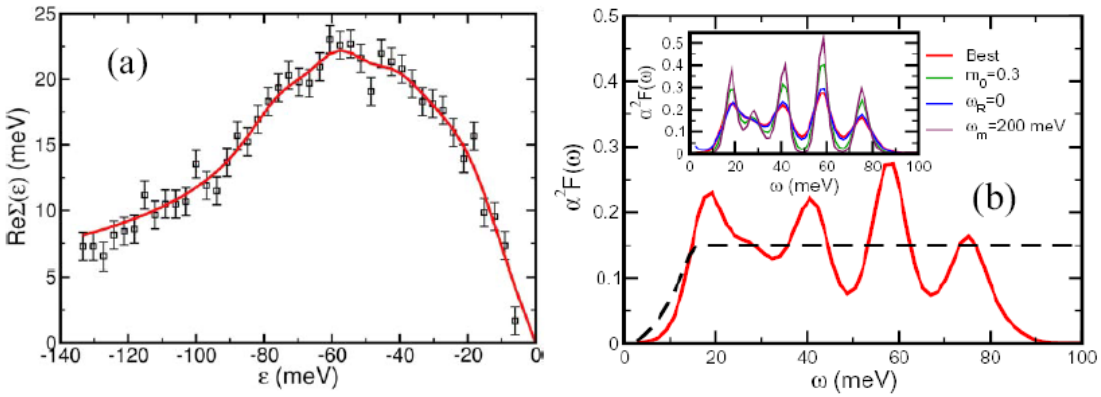

Fig. 2. (a) $Re\Sigma(\varepsilon)$ determined from the data in Fig.4(b). The red line shows the MEM fitting of the data. (b) Eliashberg function extracted from the data in (a). The dashed line is the *constraint* function, and the insert shows the changes resulting from different parameters.[4].

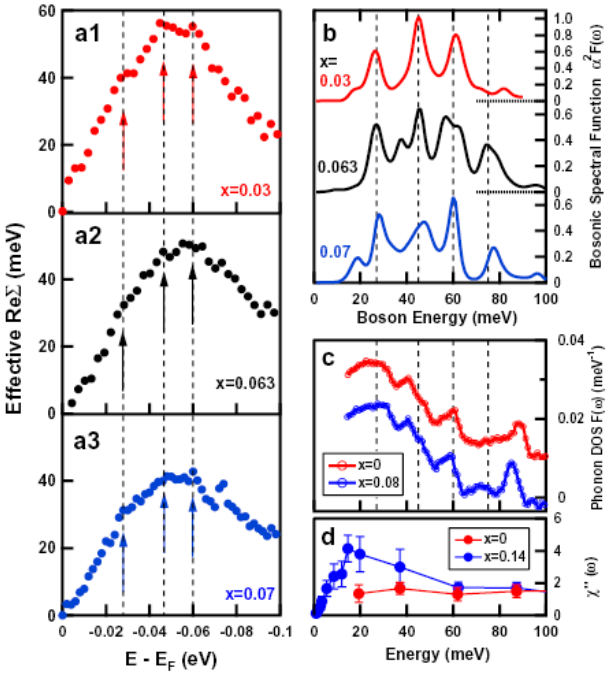

Fig. 3. Real part of the electron self-energy ReΣ(ε) for LSCO x=0.3 (a1), 0.63 (a2) and 0.07 (a3) samples. The arros indicate fine structures in the data. (b) The bosonic spectral functions extracted from the ReΣ(ε) using the maximum entropy method. The for dashed vertical lines, corresponding to energies of 27, 45, 60 and 75 meV, are guides to the eye. (c) The phonon density of states F(ω) for LSCO x=0 (red) and x=0.08 (blue) obtained from neutron scattering. (d) The local magnetic susceptibility $\chi''(\omega)$ for LSCO x=0 at 295 K (red) and LSCO x=0.14 at 17 K (blue).

shows the Eliashberg function extracted from the data. There is an absolutely amazing, almost one-to-one correspondence between the peaks in this function and the measured and calculated surface phonon dispersion [2, 3].

This procedure has now been applied to new and old data for the surface state on Be(0001) [5] and to under doped (normal phase) of the High Tc cuprate, $La_{2-x}Sr_xCuO_4$ (LSCO) [6]. Fig. 3(a) shows the real part of the electron self-energy ReΣ(ε) determined from the high-resolution, angle-resolved photoemission data for three different values of x (0.03, 0.063 and 0.07) at a sample temperature of 20 K. The superconducting temperature for the x=0.063 (0.07) sample is 12 K (14 K). Panel (b) shows the extracted Eliashberg function for the three underdoped samples. The most important observation from both Fig. 2 and Fig. 3 is that there are multiple modes contributing to the Eliashberg function, not just one Debye or Einstein mode.

There is reasonable agreement between the peaks in the Eliashberg functions and the phonon density of states (panel c) measured with neutron scattering. The increase of the coupling to the mode at ~75 meV with increasing x is encouraging. It is known that as x increases there is a phonon softening of the half-breathing mode ~ 75 meV, indicating a stronger coupling of this mode to the electron system.

Once the Eliasberg function has been extracted from the photoemission data it can be used to calculate other quantities related to electron-boson coupling in these systems, such as the mass enhancement factor, the average phonon frequency and the imaginary part of the self-energy. Fig 4 shows ReΣ(ε) ImΣ(ε) for Be(0001) [5] (top) and LSCO (x=0.03) (bottom). The extracted Eliashberg function is shown and the calculated ImΣ(ε) is compared to the data on the right. For Be(0001) there is excellent agreement between the calculated and measured ImΣ(ε). But for LSCO the calculated ImΣ(ε) using the extracted Eliashberg function (shown by the blue curve in (d)) does not explain the shape of the experimentally determined ImΣ(ε) . The green curve is the difference between the measured and calculated ImΣ(ε) . There is some other process present creating an energy dependent lifetime, not represented by the Elisahberg function.

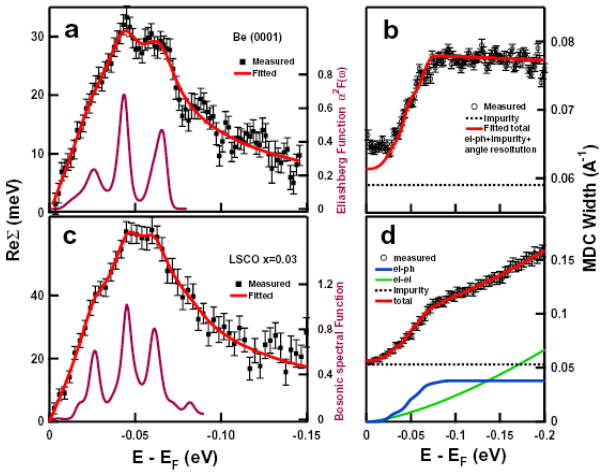

Fig. 4. ReΣ(ε) (a and c) and ImΣ(ε) (b and d) for Be(0001) (top) and LSCO (x=0.03) (bottom).

References:

1. S.-J. Tang, Ismail, P. T. Sprunger, and E. W. Plummer, "Electron-Phonon Coupling and Temperature Dependent Shift of the Surface States on *Be*(10$\bar{1}$0)," *Phys. Rev. B* **65**, 235428 (2002) [.pdf file].
2. Ph. Hofmann and E. W. Plummer, "Lattice Vibrations at the *Be*(10$\bar{1}$0) Surface," *Surf. Sci.* **377–379**, 330 (1997).
3. M. Lazzeri, and S. de Gironcoli, "Ab initio Study of *Be*(10$\bar{1}$0) Surface Dynamical Properties," *Surf. Sci.* **454-456**, 442 (2000).
4. J. Shi, S.-J. Tang, Biao Wu, P. T. Sprunger, W. L. Yang, V. Brouet, X. J. Zhou, Z. Hussain, Z.-X. Shen, Z. Zhang, and E. W. Plummer, "Direct Extraction of the Eliashberg Function for Electron-Phonon Coupling: A Case Study of *Be*(10$\bar{1}$0)," *Phy. Rev. Lett.* **92**, 186401 (2004) [pdf file].
5. S.-J. Tang, Junren Shi, Biao Wu, P. T. Sprunger, W. L. Yang, V. Brouet, X. J. Zhou, Z. Hussain, Z.-X. Shen, Zhenyu Zhang, and E. W. Plummer, A Spectroscopic View of Electron-Phonon Coupling, *Phys. Stat. Sol. (b)* **241**, 2345 (2004) [.pdf file].
6. J. Zhou, Junren Shi, T. Yoshida, T. Cuk, W. L. Yang, V. Brouet, J. Nakamura, N. Mannela, S. Koviya, Y. Ando, F. Zhou, W. X. Ti, J. W. Xiong, Z. X. Zhao, T. Sasagawa, T. Kakeshita, H. Eisaki, S. Uchida, A. Fugimori, Zhenyu Zhang, E. W. Plummer, R. B. Laughlin, Z. Hussain, and Z.-X. Shen, Multiple Bosonic Mode Coupling in Electron Self-Energy of ($La_{2-x}Sr_x$), submitted to PRL, arXiv:cond-mat/0405130 [.pdf file].