

High-resolution photoemission study of electron-phonon interaction in Pd(110)

Mitsuharu Higashiguchi,^a Kenya Shimada,^b Yuichi Miura,^a Xiaoyu Cui,^a
Naohisa Tobita,^a Yoshihiro Aiura,^c Hirofumi Namatame,^b Masaki Taniguchi,^{a,b}

^aGraduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan

^bHiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

^cNational Institute of Advanced Industrial Science and Technology, Tsukuba, Ibaraki 305-8568, Japan

Abstract

High-resolution angle-resolved photoemission study of Pd(110) single crystal has been done to evaluate the strength of electron-phonon interaction. We found a clear kink structure in the energy-band dispersion at $E \sim 30$ meV, which corresponds well to the energy scale of the Debye temperature. The obtained real part of the self-energy has been explained well by the self-energy due to the electron-phonon interaction. We have evaluated the electron-phonon coupling constant $\lambda = 0.41 \pm 0.03$ for the s-like Fermi surface around the Γ point.

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Recently, high-resolution angle-resolved photoemission spectroscopy (ARPES) has developed drastically in energy and angular resolutions. One can examine fine spectral features quantitatively, and evaluate magnitudes of the many-body interactions such as the electron-phonon and electron-electron interactions near the Fermi level (E_F) [1]. We have obtained characteristic spectral features originated from the electron-phonon interaction (EPI) in the Σ_1 bands of the fcc transition metal, Ni [2] and Cu. In the present paper, we will examine the EPI of fcc Pd, which is located below Ni in the periodic table. We have evaluated the coupling constant λ for a s-like electron Fermi surface (FS) around Γ point.

ARPES experiments were performed on the linear undulator beamline of a compact electron-storage ring (HiSOR) at Hiroshima University with a high-

resolution hemispherical electron-energy analyzer (ESCA200, SCIENTA)[3]. Total energy resolution was set at $\Delta E = 15$ meV and angular resolution at $\Delta\theta = \pm 0.15^\circ$ ($\Delta k_{\parallel} = 0.011 \text{ \AA}^{-1}$). A Pd(110) single crystal (99.999%) was cleaned by repeated cycles of Ar^+ sputtering and subsequent annealing. During measurements, the sample temperature was set at 20 K. We set photon energy at $h\nu = 29.0$ eV, and rotated the polar axis of the sample, parallel to the [001] direction to observe s-like FS around the Γ point. We searched an energy band crossing E_F , which is suitable for the quantitative spectral shape analysis.

Fig. 1(a) shows an intensity plot obtained from the ARPES of Pd(110). Black portion indicates the strongest spectral intensity. By the fits of a momentum distribution curve (MDC), an intensity distribution curve as a function of momentum for a

given binding energy, with a Lorentzian on a linear background, the peak positions at rectangle region of Fig. 1 (a) were evaluated as Fig. 1(b) shows. One can clearly recognize a kink structure, or a sudden change of the gradient of the energy-band dispersion, at $E \sim 30$ meV, which coincides well with the energy scale of the Debye temperature, $\Theta_D = 350$ K ($k_B \Theta_D \sim 30$ meV)[4].

The real part of the self-energy $\text{Re}\Sigma(k, \omega)$ can be evaluated by the energy shift from the non-interacting band ε_k [5]. Here we assumed that ε_k is a parabolic function as shown by a solid line in Fig. 1(b). Fig. 2 shows thus obtained $\text{Re}\Sigma(k, \omega)$ (white circles) being compared with a theoretical $\text{Re}\Sigma$ due to the EPI [2]. The experimental $\text{Re}\Sigma(k, \omega)$ is well reproduced by the theoretical curve, indicating that the kink structure originates from the EPI. One can evaluate the electron-phonon coupling constant by the gradient of $\text{Re}\Sigma$ at E_F (dashed line in Fig. 2), namely, $\lambda = \partial \text{Re}\Sigma / \partial \omega|_{E_F}$ [5]. We obtained $\lambda = 0.41 \pm 0.03$, which agrees well with the theoretical values, $\lambda = 0.377$ [4] ~ 0.405 [6].

The coupling constants for the $\Sigma_{1\uparrow}$ and $\Sigma_{1\downarrow}$ bands of Ni are $\lambda = 0$ and 0.33 , respectively [2], and that for the Σ_1 band of Cu is $\lambda = 0.15$ [7]. The coupling constant for the s-like FS in Pd is larger than those in Ni and Cu, which qualitatively agree with the theoretical estimation [8].

In conclusion, high-resolution ARPES of Pd(110) has been done. A kink structure has been observed at $E \sim 30$ meV, which is derived from the EPI. We have obtained the coupling constant $\lambda = 0.41$, which agrees well with the theoretical calculation.

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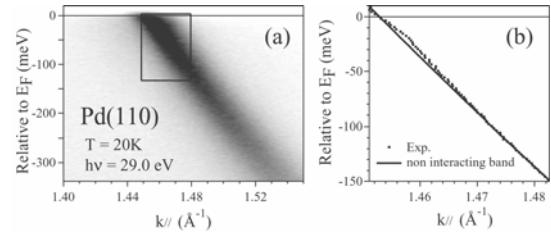


Fig.1. ARPES of Pd(110) at 20 K. (a) Intensity plot. (b) Evaluated peak positions (dots) for the region in the rectangle in (a). Solid line in (b) is assumed to be non-interacting band ε_k .

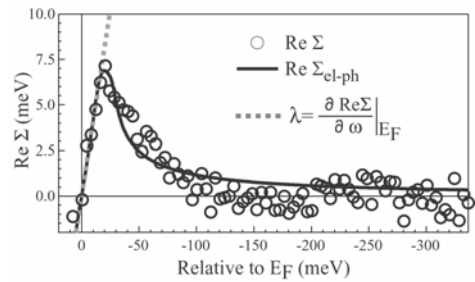


Fig. 2. Evaluated $\text{Re}\Sigma$ (white circles). Solid and dashed lines indicate theoretical $\text{Re}\Sigma$ and the gradient of the experimental $\text{Re}\Sigma$ at E_F , respectively.