

# An Angle-Resolved Photoemission Extended Fine Structure Study of Clean Ni(111) Surface Structure

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## INTRODUCTION

Angle-Resolved Photoemission Extended Fine Structure<sup>1,2</sup> (ARPEFS) has been successfully applied to various adsorbate systems since its inception twenty years ago. It generally yields very precise bond length and inter-layer distance information in the neighborhood of 0.02Å to 0.05Å. When applying Fourier Transform to ARPEFS data, strong peaks emerge at photoelectron Path Length Differences (PLD) which can be derived from geometrical settings of experimental apparatus. Most of these peaks can be understood in light of single backscattering and the cluster model.

However, when we measure photoemission from adatoms, which are usually sparsely placed on surface, the scattering between the emitter atoms themselves is weak, and there is no forward focusing/defocusing phenomenon involved. When we turn to a clean metal surface, like Ni(111), we have a unique opportunity to look at the photoelectron diffraction process inside the top layer itself, as well as the complication of many layers of emitter atoms in one experiment<sup>3</sup>. We report here the complete ARPEFS of Ni3p and Ni3s photoelectrons and their respective fittings through a new version of a multiple-scattering calculation program based on Rehr-Albers separable propagator.

## EXPERIMENT

The experiment was performed in an Ultra-high vacuum chamber (base pressure of  $4 \times 10^{-11}$  torr), equipped with a PHI hemispherical electron energy analyzer and a liquid-Nitrogen-cooled 5-degrees-of-freedom sample manipulator, on beamline 9.3.2 at the Advanced Light Source of Lawrence Berkeley National Laboratory. The Ni(111) crystal was cleaned by the standard procedure of ion sputtering and annealing cycles. The surface order and cleanliness were periodically monitored with synchrotron XPS and LEED. The sample surface temperature was kept at 120K throughout the data collection. The photon polarization vector was oriented 30° from electron analyzer lens axis. Every ARPEFS curve is reduced from a series of photoemission spectra, with each spectrum looking at the constant initial state with particular photon energy to provide equal 0.05Å<sup>-1</sup> steps in terms of photoelectron wavevector. The data reduction process is described in detail elsewhere<sup>4</sup>.

## RESULTS AND DISCUSSION

A comparison between experiment and calculation (Fig.1) reaffirms the validity of the cluster model in describing photoelectron diffraction process in a system much more complicated than the prototypical S/Ni(100) case. The R-factor of the fit in this case is as good as that of the benchmark S/Ni(100). The determined surface structure is a bulk-terminated surface with little or no relaxation.

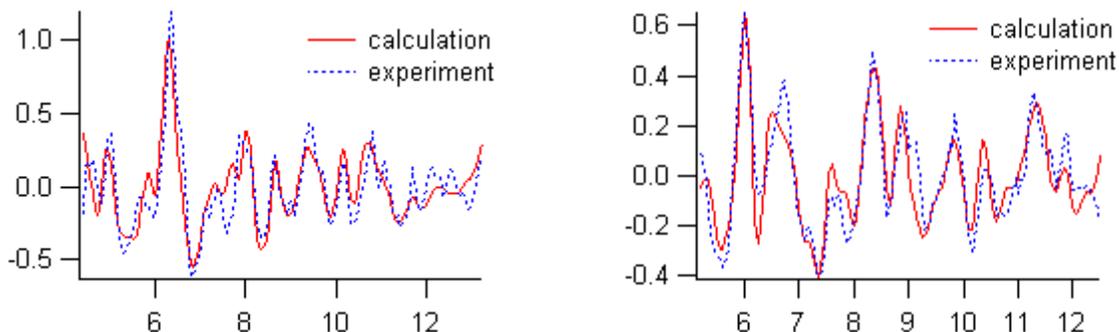


Figure 1. Normal emission ARPEFS. Left panel is Ni3s, right panel is Ni3p. The x-axis is the photoelectron wavevector in  $\text{\AA}^{-1}$ .

More analysis is underway for off-normal emission data and the 6eV and 12eV satellites of the Ni3p core-level.

## ACKNOWLEDGMENTS

We thank G.Andronaco, N.Hartman, M.Z. Hasan, S.A.Kellar, K.Kellogg, J.K.Lee, X.-J. Zhou, G.-R.Zhuang, for their help in the experiment.

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This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Science Division, of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098.

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