*Inelastic Electron Scattering From Surfaces***TABLE OF CONTENTS**

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MASTER

I. PROGRESS REPORT:

(A) RESEARCH IN THE PREVIOUS GRANT PERIOD

In the study of new materials, it is often the case that the presence of an interface strongly influences the geometric and dynamical properties of a film. Our ability to properly characterize, modify and create novel interfacial properties by surface science techniques is central to new developments in a host of energy, communication and environmental research.

In the past two decades, we have witnessed a tremendous surge in the use of new or improved spectroscopic techniques for studying fundamental properties of surfaces and interfaces. Most of these probes study elastic processes.⁽¹⁾ However, from our experience with both molecular and solid state physics, we know that we often require knowledge not only of the static structure, but also of the dynamical response of a solid or epitaxial film to an external stimulus. It is also true that the dynamical response of a physical system is influenced strongly by its geometrical structure, so it is important to understand the relation between surface excitations and surface structure.

This proposal requests funds for the renewal of a theoretical program aimed at the quantitative study of two fundamental aspects of solids in the surface region: Surface dynamical processes such as vibrational and magnetic excitations in crystalline slabs, ultrathin-layered materials and chemisorbed systems on substrates and aspects of the geometric structure which are intimately connected to the dynamical excitations. The proposed research is one of very few funded programs that uses ab-initio and exact multiple scattering methods to determine quantitative information from state-of-the-art measurements.

To study excitations, one must either perform absorption spectroscopy, or study the inelastic scattering of a probe beam off the system of interest. In surface physics during recent years, there has been a major advancement in the spectroscopy of surface vibrations by the electron energy loss technique, and also by the inelastic scattering of slow, monoenergetic helium atoms from a surface. High-resolution electron-energy loss

spectroscopy (HREELS) is a powerful and versatile probe. It has provided finger-printing services to organic and molecular chemists, as well as to investigators in the field of heterogeneous catalysis. Because of the high surface sensitivity and wide spectra range of the technique, HREELS has emerged as a principal tool for studying vibrational properties of clean and adsorbate covered surfaces.

In past efforts supported by this grant, we have developed a multiple scattering theory of inelastic electron scattering by surface phonons.⁽²⁾ With this theory and a new generation of experiments, it is now possible to study surface phonons and the influence of bulk phonons on surface atom vibrations throughout the two dimensional Brillouin zone. The theory also allowed us to interpret experimental data quantitatively; indeed our early calculations outlined the conditions that must be realized in the laboratory for such experiments to be successful.

The use of inelastic electron scattering to study vibrations of crystal surfaces began around 1970. For many years, experiments were confined to the study of electrons which experienced very small angular deflections during the course of phonon excitation.⁽³⁾ The inelastic electrons thus emerged very close to the specular direction. In this angular regime, intense scattering from surface vibrations was produced by long-ranged Coulomb fields in the vacuum above the crystal, generated by atoms vibrating on the surface. This Coulomb scattering was strongest at low electron energies. Thus, the near specular energy loss experiments were performed with beam energies in the 1eV-10eV range. Under these conditions, where the electron was quite far above a surface ($\sim 100\text{\AA}$) when it encountered the long-ranged Coulomb field, the excitation cross-section contained little useful structural information. It was also the case that surface phonons excited in the experiment had wave vectors very near the center of the surface Brillouin zone ($\sim 10^6\text{cm}^{-1}$), so details of dispersion curves could not be explored.

Our theoretical analysis of off-specular electron scattering, where the wave vector of the modes excited may extend out to the boundary of the surface Brillouin zone, revealed the conditions required for such experiments to be realized in the laboratory. Most particularly, we found the off-specular excitation cross-sections *to be very much larger if electron energies are in the LEED range (50eV-300eV)* rather than the much lower

energies utilized in the near-specular experiments discussed in the previous paragraph. Furthermore, we found the energy and angle variations of the off-specular cross-sections to be quite sensitive to surface structure, and that modes forbidden in the near specular geometry by the dipole selection rule can be excited with substantial cross section in an off-specular measurement.⁽⁴⁾ This theory has proved to be very successful in interpreting the data in a quantitative manner and it has been used to guide the experimentalist in the choice of scattering geometry. It has also proved possible to study modes in which the vibrational motion of the surface atoms are parallel as well as perpendicular to the surface, and it has been demonstrated that the energy variation of the excitation is highly sensitive to surface structure.

Thus, while it has been clear for many years that electron energy loss spectroscopy can, in principle, be used to study dispersion curves of surface phonons with details comparable to that of neutron scattering of bulk phonons, it took more than a decade and quantitative theory to appreciate that high impact energies, in the range employed in low-energy electron diffraction, were the key to success. It is clear that such accurate microscopic theories will continue to play a central role in the future development of this spectroscopy, both in providing quantitative interpretation and in suggesting new measurements.

Recently, we have extended the analyses to study surfaces of ordered alloys. Here we have exploited the sensitivity of surface phonon cross-sections to geometry to extract structural information as well as information of the interatomic force constants from the data. For example, we have explored the relation between the structural results of Davis and Noonan for the (110) surface of the alloy NiAl with changes in the Ni and Al surface force constants, and studied the comparison between measured and calculated inelastic electron cross-sections.⁽⁵⁾ Results of the study indicated that the interatomic forces in the near-surface region were significantly different from the bulk values. The analysis also showed that along the $\bar{\Gamma} \bar{Y}$ (i.e., [100]) direction, the polarizations of the two lowest-frequency surface modes were interchanged as they approached the Brillouin-zone boundary. The surface-adjusted force constant model produced a Rayleigh mode whose first-layer Ni polarization switched to pure longitudinal at point $\bar{Y}$. This behavior was supported by the data, and such a switch was not present in the Rayleigh mode

calculated from bulk force constants. The force-constant changes indicated a surface rippling, where first-layer nickel atoms were displaced inwards and first-layer aluminum atoms were displaced outwards. This was consistent with a structural model based on low-energy electron diffraction (LEED) I-V spectra analysis by Noonan and David [Phys. Rev. Lett. **59**, 1714 (1987)] and a medium-energy ion-scattering (MEIS) study by Yalisove and Graham [Surf. Sci. **183**, 556 (1987)].

An important step to improve the accuracy of the theory was undertaken in the last grant period. We have incorporated results of first-principles phonon calculations into the multiple scattering inelastic electron cross-section theory. By combining ab-initio surface lattice dynamical results with phonon-loss cross-section calculations, we achieved a higher degree of accuracy in the microscopic description. There has been significant recent progress in the development of first-principles lattice dynamical calculations within the local-density-functional formalism. As was shown by Yin and Cohen in the bulk, it was possible to use ab-initio pseudopotentials and the Hellmann-Feynman theorem to calculate vibrational amplitudes and frequencies of metals and semiconductors. These methods have been applied to surfaces recently.

In collaboration with Dr. K. M. Ho of Iowa State University and Dr. K. P. Bohnen of KFA, Karlsruhe, Germany, we have used first-principles phonon eigenvectors and eigenfrequencies as inputs to the electron-energy-loss multiple scattering cross-section calculations.⁽⁶⁾ This improvement in the theory turned out to produce dramatic results. Calculations of Cu(001) and Ag(001), compared to data taken by Dr. M. Rocca of the University of Genova, Italy, and Dr. L. L. Kesmodel of Indiana University, showed that even on simple metallic surfaces, the earlier understanding based on parametrized models of surface force constants were in fact incomplete.^(7,8) The more accurate analysis revealed the existence of two new surface-localized modes: At $\bar{X}$ we found an S_2 mode with first-layer longitudinal displacement and second-layer shear vertical displacement, and at $\bar{M}$, we found an L_1 mode that had a longitudinal polarization which decayed into the bulk. With the discovery of these additional modes, previous discrepancies with data and mode misassignments were clarified and corrected. More on the research thrust for using ab-initio phonon calculations in the HREELS cross-section analysis will be discussed in Section III.

In a different area, we have studied the behavior of Auger and photoexcited electrons as they were forward-scattered by atoms in the surface region. The scattering produced a forward-focusing effect, which acted as a search-light seeking out crystallographic directions inside a solid.^(9,10) This technique thus provided a rare worm's eye-view of buried atoms in the interface region. In an article published in *Science*, we pointed out the difference between forward-focusing (the correct quantum mechanical interpretation of data) and forward-shadowing, which was suggested by another research group. This technique allowed layer-by-layer growth to be monitored. The presence of forward-focusing peaks in a system is evidence that an emitting atom is buried one, two or more atomic layers below the surface of a film. Another article explaining the differences in the forward-scattering phases between electrons and positrons is in print in *Surface Science Letters*. This phase difference causes electrons to exhibit forward-focusing while positrons to exhibit forward-shadowing. The concept of positron forward-shadowing is introduced for the first time by this article.

We have also completed a paper which introduced the concepts of low-energy electron holography and positron holography. This paper appeared recently in *Phys. Rev. Lett.*, Dec. 21, 1992. The new techniques demonstrate that vector positions of near-neighbor atoms within the out-going electron's mean-free path from an adatom can be determined. No prior knowledge of adsorption site, bond length, bond angle or type of atom is necessary. In achieving these high-fidelity 3D images with a 1 Å or less spatial resolution, it is demonstrated that holographic low-energy electron and positron holography have the potential of being accurate, direct structural tools in systems in which adsorbate-induced substrate distortions are small.

A patent of the multiple-energy phase-summing method for eliminating multiple-scattering artifacts in the holographic reconstruction process was granted to the P.I. in March, 1992.

A list of publications resulted from the research program supported by this grant appears in Section I(B).

(B) RESEARCH PAPERS COMPLETED DURING THE PAST GRANT PERIOD

Book:

- 1) *The Structure of Surfaces, III*, eds. S. Y. Tong, M. A. Van Hove, X. Xie and K. Takayanagi, Springer-Verlag, Berlin (1991).

Chapters in Books:

- 2) "Bonding and Structure on Semiconductor Surfaces," S. Y. Tong, H. Huang, C. M. Wei in *Chemistry and Physics of Solid Surfaces*, Vol. 8, R. Vanselow and R. Howe, eds., Springer-Verlag, Berlin (1990).
- 3) "The Study of Surface Phonons by Electron Energy Loss Spectroscopy: Theoretical and Experimental Considerations," D. L. Mills, S. Y. Tong, J. E. Black in *Surface Phonons*, ed. W. Kress, Springer, Heidelberg (1991).
- 4) "Forward Focusing Photoelectron Diffraction - A New Structural Tool for Surfaces and Interfaces," S. Y. Tong, Y. Chen, Hua Li and C. M. Wei, in *Surface Physics*, eds. X. Li et al., Gordon and Breach Science Publishers, Philadelphia (1992).

Journal Publications:

- 5) "Auger Electron Angular Distributions From Surfaces: Forward Focusing or Silhouettes?" X. D. Wang, Z. L. Han, B. P. Tonner, Y. Chen, S. Y. Tong, *Science*, 1129 (1990).
- 6) "Surface-Phonon Dispersion of NiAl(110)," M. Wuttig, W. Hoffmann, E. Preuss, R. Franchy, H. Ibach, Y. Chen, M. L. Xu, S. Y. Tong, *Phys. Rev. B* **42**, 5443 (1990).
- 7) "Electron-Energy-Loss Cross-Section and Surface Lattice-Dynamics Studies of NiAl (110)," Y. Chen, M. L. Xu, S. Y. Tong, M. Wuttig, W. Hoffmann, R. Franchy, H. Ibach, *Phys. Rev. B* **42**, 5451 (1990).
- 8) "Detection of Odd Symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory," J. L. Erskine, E.-J. Jeong, J. Yater, Y. Chen, S. Y. Tong, *J. Vac. Sci. Tech. A* **8**, 2649 (1990).
- 9) "Characterization of Surface Phonons on Cu(001) and Ag (001): First-Principles Phonon Calculations with Experimental and Theoretical Studies of High-Resolution Electron-Energy-Loss Spectra," Y. Chen, S. Y. Tong, Jae- Sung Kim, L. L. Kesmodel, T. Rodach, K. P. Bohnen and K. M. Ho, *Phys. Rev. B* **44**, 11, 394 (1991).

- 10) "High-Resolution Electron Energy-Loss Spectroscopy Analysis of Ag(001): Discovery of a New Surface Longitudinal Mode Using First-Principles Phonon Calculations," Y. Chen, S. Y. Tong, M. Rocca, P. Moretto, U. Valbusa, K. P. Bohnen and K. M. Ho, Surface Science Lett. **250**, L389 (1991).
- 11) "Surface Phonons and Structure of Epitaxial Nickel Layers on Cu(001)," Y. Chen, S. Y. Tong, Jae-Sung Kim, M. H. Mohamed, L. L. Kesmodel, Phys. Rev. B (Rapid Communications) **43**, 6788 (1991).
- 12) "Forward-Focusing and Shadowing Effects in Solids," Hua Li and S. Y. Tong, Surface Science Letters, in print.
- 13) "Low-Energy Electron and Low-Energy Positron Holography," S. Y. Tong, H. Huang and X. Q. Guo, Phys. Rev. Lett. **69**, 3654 (1992).
- 14) "First-Principles Phonon and Multiple-Scattering Electron-Energy-Loss Spectra Studies of Cu(111) and Ag(111)," Y. Chen, S. Y. Tong, K. P. Bohnen, T. Rodach, K. M. Ho, Phys. Rev. Lett., under review.

Patent Received:

U.S. Patent: "Method of Three-Dimensional Atomic Imaging," No. 5,095,207. Date: March 10, 1992.

Project History:

Project Performance Periods:	4/01/90-1/2/91;	2/01/91-1/31/92;	2/01/92-1/31/93
Project Fundings:	\$118,670	\$126,000	\$96,000

II. PAST GRADUATE STUDENTS AND POSTDOCTORAL ASSOCIATES

This program employs a postdoctoral research associate and a graduate student. Fifty percent of the graduate student's stipend is paid by the DOE grant. The other fifty percent is paid by the University as a matching fund to the grant. A list of past graduate students and postdoctoral associates who worked with the P.I. is given below, together with their current positions:

Table 1. Past Graduate Students and Postdoctoral Associates

<u>Name</u>	<u>Current Position</u>
• H.C. Poon – Ph.D. student (1985)	University of Singapore
• C.M. Wei – Ph.D. student (1990)	Nanking University, Taiwan
• B.M. Hall – Ph.D. student (1984)	Thinking Machines, Boston
• M.L. Xu – Ph.D. student (1988)	University of Toronto–Canada
• T.C. Zhao – Ph.D. student (1990)	NASA Space Epitaxy Center– Texas
• L. Maldonado – Ph.D. student (1981)	Lockheed International
• N. Stoner – Ph.D. student (1976)	University of Wisconsin–Whitewater
• M. Puga – Postdoctoral Associate (1984)	AT&T–Bell Laboratories
• A. Lubinsky – Postdoctoral Associate (1974)	Xerox Research Center
• C.H. Li – Postdoctoral Associate (1976)	Microsoft
• C.M. Wei – Postdoctoral Associate (1980)	University of Omaha, Nebraska
• M. Van Hove – Postdoctoral Associate (1975)	Lawrence Berkeley Laboratory
• W.M. Kang – Ph.D. student (1982)	AT&T–Bell Laboratories
• K.H. Lau – Postdoctoral Associate (1987)	AT&T–Bell Laboratories
• S. Nagano – Postdoctoral Associate (1986)	NEC–Tokyo

III. RESEARCH PROGRAM FOR THE NEXT PERIOD

Quantitative knowledge of surface excitations and their relation to structure is fundamental to a host of scientific questions critical to advances in energy and related research. In the next grant period, we shall focus the research in the following areas:

- (i) Interpretation of electron-phonon loss spectra using highly-precise first-principles models and inelastic multiple scattering theory for studying localized excitations at metal-semiconductor interfaces and ultrathin epitaxial metal layers.
- (ii) To explore the novel properties of electron and positron diffraction in solids for structural studies using a combination of elastic scattering and emission techniques, as well as imaging techniques based on the principle of holography. In some of these studies, the relation between structure and surface magnetism will also be explored.

In the following, we shall describe details of the research plan:

(i) For calculating the electron-energy loss cross-section of a given surface or resonance phonon, the displacement amplitudes of surface atoms at given $\vec{q}_{\parallel}$ are used as inputs. For this purpose, we use surface vibrational displacements generated by ab-initio calculations of surface phonons, rather than empirical force constant models. The reason for not using displacements from empirically determined force constants is that on many surfaces, interatomic force constants between five or more neighbors are needed to produce a good fit of experimental data. Even when a good fit is obtained, using at times as many as 15 parameters, such phonon dynamical models do not provide necessary insight to the microscopic mechanisms which control surface force constants. Also, phonon dynamical models based on parametrized force constants do not correlate between surface structural changes with variations in the surface force constants. An understanding of this correlation is particularly important on the (110) surface of metals, where large multilayer relaxation occurs, and on semiconductor surfaces, where the surface reconstructs.

As described in Section I, we have recently introduced an analysis of high-resolution electron energy loss spectroscopy (HREELS) of vibrational modes of Ag(001) using normal mode frequencies and displacements obtained from first-principles phonon calculations. The first-principles phonon calculations included the full microscopic electron screening at the surface and contained no adjustable parameters. The combined method of using eigensolutions from first-principles calculations and fully multiple scattering inelastic cross-section calculations represents the most sophisticated theoretical treatment to-date of this kind. The remaining assumptions in these new generation phonon calculations are the local density approximation and the adiabatic approximation. Such “parameter free” phonon calculations satisfy two self-consistency requirements: (i) That the calculations produce a surface equilibrium structure in agreement to the HREELS cross section intensity measurements; and (ii) that the calculated surface dispersion curves (dynamical forces) are in agreement with the energy-loss frequency measurements.

As discussed before, we have applied this combined microscopic approach to analyze EELS data of Cu(001) and Ag(001) at $\bar{X}$ and $\bar{M}$ points. The first-principles phonon calculations revealed an S_2 mode at $\bar{X}$ not present in simple force-constant models. This

new mode, together with the first-layer shear vertical displacements of bulk modes, were responsible for a previously unexplained feature observed in He-atom scattering experiments on Cu(001).

At $\bar{M}$, the strong energy dependence of the measured EELS loss peak was explained by the discovery of another new mode: The L_1 mode. Again, simple force-constant models could not explain the observed behavior because this new mode was absent in such models. The different cross-sectional behaviors for Cu(001) and Ag(001) were related to the different scattering potentials seen by the electron and the different structural constants. These results underlined the importance of using a microscopic (EELS) scattering theory, in conjunction with an accurate phonon model, for proper interpretation of measured electron-energy-loss data. Simply knowing the number of surface modes and their spectral densities were not sufficient for identifying which mode (or modes) were responsible for a particular loss peak measured at a given electron energy. With the discovery of two new localized phonons at $\bar{X}$ and $\bar{M}$ for Cu(001) and Ag(001), the phonon excitations of these surfaces are finally correctly characterized after 25 years of study.

In the next grant period, we plan to extend this research, carried out in collaboration with Dr. K. M. Ho (Ames Laboratory, Iowa State University) and Dr. K. P. Bohnen (KFK, Karlsruhe, Germany), to study the following systems: (i) A metal-semiconductor interface: Si(111) $\sqrt{3} \times \sqrt{3}$ R30°-Al, (ii) An ultrathin metal overlayer on substrate system: Cu(001) 1 $\times$ 1-Ni and (iii) A system with large surface relaxation: Pd(110). The theoretical results will be compared to new measurements taken in the laboratory of Professor Larry Kesmodel (Indiana University). The study of Pd(110) is important because it allows a test of the theoretical method on a system which undergoes large surface relaxations. The epitaxial growth of ultrathin films of Ni on Cu(001) allows a detailed study of the internal stress in epitaxial films as well as the relation between this stress and the appearance of film-induced localized phonons as a function of the film's thickness. Finally, the metal-semiconductor interfacial system is most interesting, because this system involves novel chemical bonding as well as geometric reconstruction at the interface of two unlike materials. The study will focus on the relation between surface geometry, chemical bonding and elementary vibrational excitations.

(ii) In tandem with studies of phonon excitations in the surface and interface regions, we shall investigate the structure of surfaces and interfaces. In addition to using diffraction and imaging methods of electrons in solids, we shall also explore the use of a different charged particle – the positron – as a structural tool. The reason for this interest is that positrons are close to being the ideal probe particles for surface structural studies because the positron-atom *elastic scattering is weak* while the positron-atom *inelastic damping is strong*. In other words, positron-solid scattering embodies the advantages of both photons (weak elastic scattering) and electrons (strong inelastic damping, hence a high surface sensitivity) in studying surface systems. Compared to electron diffraction, positron diffraction is rather new – the first observation of low-energy positron diffraction was made only a dozen years ago⁽¹¹⁾ (by contrast, LEED was first measured in 1927). Furthermore, the discovery of weak elastic scattering of positrons was made very recently (Tong et al., Phys. Rev. Lett. 69, 3654 (1992)), although earlier works contained ample hints that positron diffraction was considerably simpler to interpret than electron diffraction at the same energies. Because these findings are very recent, we elaborate in the following some of the novel properties of positron diffraction.

The most important difference between low-energy positron diffraction and electron diffraction is that positrons and the atomic nuclei repel because they have the same sign. This repulsive interaction has a significant consequence – i.e. the positron-atom elastic scattering is considerably weaker than that of the electron's. Classically, a repulsive Coulomb potential keeps a positron at distances larger than the turning point $R_t = \frac{Ze^2}{E_p}$, where E_p is the kinetic energy of the positron. By contrast, an attractive potential allows an electron to have considerable lifetime at distances $r \leq R_t$. The different pictures are shown schematically in Fig. 1. The weaker positron-atom scattering can also be seen by comparing the exact scattering factor given by:

$$f(\vec{k}_i, \vec{k}_f) = -\frac{m}{2\pi\hbar^2} \int e^{-i\vec{k}_f \cdot \vec{r}_1} \left\{ v(\vec{r}_1) \delta(\vec{r}_1, \vec{r}_2) + \right. \\ \left. + \frac{2m}{\hbar^2} v(\vec{r}_1) G(\vec{r}_1, \vec{r}_2) v(\vec{r}_2) + \dots \right\} e^{i\vec{k}_i \cdot \vec{r}_2} d\vec{r}_1 d\vec{r}_2 \quad (1)$$

Fig. 1

with the single-scattering (Born approximation) form:

$$f_B(\vec{k}_i, \vec{k}_f) = -\frac{m}{2\pi\hbar^2} \int e^{i(\vec{k}_i - \vec{k}_f) \cdot \vec{r}} v(\vec{r}) d\vec{r} \quad (2)$$

For example, we show in Fig. 1 the exact $|f_e(\theta)|$ and $|f_p(\theta)|$ for electrons and positrons respectively at 100 eV, plotted as a function of the scattering angle θ for a Cu atom. The positron's scattering factor, $|f_p(\theta)|$, falls off smoothly from $\theta = 0^\circ$ to 180° , similar to the behavior of the Born differential cross-section, while the electron's scattering factor, $|f_e(\theta)|$, has cusps at 80° and 145° and rises sharply at 110° and 180° . In typical LEED and LEPD experiments, the collected particles are back-scattered by angles near π . The scattered intensity scales as $|f(\theta_1) \cdot f(\theta_2) \cdot \dots|^2$ for a multiply scattered path. For electrons, because of the strong resonances in $f(\theta)$ (see Fig. 1), a doubly-scattered path such as $|f(20) \cdot f(160)|^2$ or $|f(30) \cdot f(110)|^2$, etc. has a large intensity and cannot be neglected. By comparison, the complete absence of strong resonances in a positron's $f(\theta)$ assures that multiple scattering terms such as $|f(\theta_1) \cdot f(\theta_2) \cdot \dots|^2$ are weaker than those of electrons.

Another important distinction between electron and positron diffraction is that the positron-atom potential is simpler to evaluate. We can understand this property by comparing the exact $|f_e(\pi)|$ (dotted line, inset of Fig. 1) and $|f_p(\pi)|$ (solid line, inset of Fig. 1) calculated from Eq. (1), as well as $|f_B(\pi)|$ (dashed line) calculated from Eq. (2). The Born approximation $|f_B(\pi)|$ for electrons and positrons are indistinguishable in the scale of Fig. 1. The positron's exact scattering factor at π is weaker in the energy range shown than its Born approximate value — they have a similarly smooth decay with energy — while the electron's exact scattering factor behaves drastically different as it rises through a strong resonance at $E \approx 190$ eV. An important consequence of the near-Born behavior of $|f_p(\pi)|$ is that at scattering angles near π , the momentum transfer, $q = |\vec{k}_i - \vec{k}_f| = 2k \sin \frac{\theta}{2}$, is large. This implies, from the integral of Eq. (2), that $f_p(q \approx 2k)$ is sensitive only to the small r region of $v(r)$, a region that is dominated by the electrostatic Coulomb potential. This explains why the back-scattered LEPD IV spectra are rather insensitive to the exact form of the exchange-correlation potential, a fact reported in the early work of Jona et al.⁽¹²⁾ For electrons, on the other hand, $|f_e(\pi)|$ is sensitive to all regions of $v(r)$ because of the higher-order terms in the expansion of Eq. (1). The physical consequence is that

positron diffraction spectra are less sensitive to the exact form of the exchange-correlation potential, thus making the construction of positron-atom scattering potentials simpler.

For positron diffraction, the exclusion principle is unimportant for its final state distribution in solids. This results in a larger inelastic damping for positrons than electrons at energies below 100 eV. At 100 eV or higher, a positron's inelastic damping is about the same as that of an electron's. The combination of weak elastic scattering and strong inelastic damping makes positron diffraction an attractive alternative for surface structural analysis. We plan to explore these unique properties of positron diffraction and determine how far this young technique can be developed as a structural and imaging tool. Because multiple scattering is less strong in positron diffraction, we plan to investigate approximation (i.e. perturbation) methods which have failed earlier for electron diffraction. We are hopeful that one or more such perturbation methods will work for positron diffraction. We shall also explore the potential for applying the holographic principle to invert positron diffraction spectra to produce 3D atomic images. The major difficulty of electron holography (as compared to optical holography) is that multiple scattering produces artifacts which distort the image and form "false atoms" at incorrect positions. To get rid of multiple-scattering artifacts, multiple-energy phase-summing methods were introduced. While such multiple-energy methods produced artifact-free atom images, they required the use of considerable data base in $(\theta, \phi \text{ and } k)$ space. Positron diffraction is well suited for holographic reconstruction because of positron's weak scattering in solids so that only a few energies are needed to produce high-fidelity images. An example of low-energy positron holography is shown in Fig. 2 for the Cu(001) $p(2 \times 2)$ -Se system. In the figure, we show the view through a plane $1.8 \text{ \AA}$ below the Se layer. This plane passes through the nuclei of the topmost Cu atoms. The images shown, from left to right, are reconstructed by using increasingly more energies. For electrons (top panels), strong artifacts appear at non-atomic positions with two energies. As more energies are added, the images at the atomic positions grow brighter while the intensities of the artifacts become dimmer. With five energies, the images, at least for the four nearest-neighbor atoms, are sharply formed, although one can still detect (weak) artifacts approximately midway between the farther atoms. By contrast, using the same energies with positrons, the atom images are already formed at approximately the

correct positions with only two energies. With increasing number of energies, the atomic positions marked by the images become more accurate while the intensities of the artifacts become weaker. Using five energies in the range $114 \text{ eV} \leq E \leq 166 \text{ eV}$, the images for the first twelve neighbors are sharply formed, and the view is essentially free from serious artifacts. These images provide a direct view of the surface structure. Each circle in Fig. 2 has a diameter of $1.1 \text{ \AA}$ and its center marks the correct atomic position. The images from positron holography are shifted by less than $0.1 \text{ \AA}$ for the nearest-neighbor atoms and by $\sim 0.3 \text{ \AA}$ for the next shell of atoms (for more details, see Tong et al., Phys. Rev. Lett. **69**, 3654, 1992)).

Currently, a limiting factor is the development of a positron source for diffraction experiments. However, tremendous progress has been made recently via the brightness enhancement concept. High brightness positron beams are available (e.g., the Brandeis positron facility) for measuring diffraction spectra. We shall collaborate with Prof. K. F. Canter at Brandeis University who has a leading experimental effort in positron diffraction and holography.

(iii) The richness of new epitaxially-stabilized phases is just beginning to be realized, since epitaxial strain offers structural possibilities that do not develop under hydrostatic strain. In recent work on Cu, a body-centered tetragonal phase was predicted by theory and the phase was found experimentally. Highly-precise self-consistent theory played an important role in predicting new stable structures (e.g., in predicting new lattice constants), as well as novel properties of the film. For example, Marcus and co-workers⁽¹³⁾ used the local-spin-density approximation (LSDA) and found that bcc Fe was necessarily ferromagnetic. In the fcc structure, however, the energy surface has a very different form: the global minimum corresponds to $M = 0$, indicating that this structure is normally non-magnetic. However, two local minima are found for high and low non-zero values of magnetization, indicating the existence of at least three different possible phases for fcc Fe. Such theoretical results indicate the possibility of designing new phases through epitaxially stabilized growth.

One of the primary motivations for studying ultrathin magnetic films (in the monolayer and bilayers range) is the expectation that the magnetic coupling would change between

bulk and thin films. Recent studies have shown that the direction of the magnetic moment as well as magnetic ordering are sensitively dependent on a film's thickness and the temperature at which the film is annealed. For example, Co films grown on Cu(111) do not exhibit a stable axis of magnetization, either in plane or along the surface normal. However, by gently heating (420°K) and cooling the films in the presence of a small (800 Oe) magnetic field, the perpendicular magnetization is stabilized. This stabilization is reversible: if the films are heated to 420°K in the absence of an applied magnetic field, the perpendicular magnetization exhibits no remanence. Dr. James Tobin of Lawrence Livermore National Laboratory has used circularly polarized x-rays from a synchrotron radiation source to study the exchange splitting and surface magnetic moment of Fe films grown on Cu(001) as well as Fe/Cr/Fe multilayer structures.⁽¹⁴⁾ They, and others have found a strong correlation between magnetic ordering with a film's thickness and temperature of growth. The evidence suggests that the microscopic structure of the film, i.e. geometric ordering strongly influences its magnetic coupling. We plan to explore the relation between the geometric structure of a film and its local magnetic properties. The systems to be studied include overlayer films of Gd/W(110), Co/Cu(001), Fe/Cu(001) and Fe/Cr/Fe multilayer lattices. Some most intriguing results have been reported recently by Thomassen et al. on the Fe/Cu(001) system. We plan to revisit this system in more detail. The experiments for the first two systems will be carried out by Prof. M. Onellion (University of Wisconsin-Madison) while the latter systems will be carried out in Dr. J. Tobin's laboratory at LLNL. We shall use a combination of diffraction methods: e.g. forward-scattering XPS (focusing peaks), photoemission (spin-independent and spin-dependent scan-energy photoelectron diffraction), LEED, as well as imaging techniques to study these systems.

References:

- 1) See, for example, the discussion presented by S. Y. Tong, *Physics Today* **37**, 50 (1984).
- 2) For a discussion of the primary general issues outlined by our theory, see C. H. Li, S. Y. Tong and D. L. Mills, *Phys. Rev. Letters* **44**, 407 (1980), and S. Y. Tong, C. H. Li and D. L. Mills, *Phys. Rev.* **B24**, 806 (1981).
- 3) H. Ibach and D. L. Mills, *Electron Energy Loss Spectroscopy and Surface Vibrations*, Academic Press, S.F., 1982.
- 4) For example, the off-specular electron loss cross sections show a very strong sensitivity to the spacing between the $c(2 \times 2)$ S overlayer on Ni(100), and the outermost layer of Ni atoms. See the detailed discussion presented by Z. Q. Wu, Y. Chen, M. L. Xu, S. Y. Tong, S. Lehwald, M. Rocca and H. Ibach, *Phys. Rev.* **B39**, 3116 (1989).
- 5) H. L. Davis and J. C. Noonan, *Phys. Rev. Letters* **54**, 566 (1988).
- 6) See, for example, K. M. Ho and K. P. Bohnen, *Phys. Rev.* **B38**, 12897 (1988); K. P. Bohnen and K. M. Ho, *Surf. Sci.* **207**, 105 (1988); A. M. Lakce, J. P. Toennies, C. H. Wöll, K. P. Bohnen and K. M. Ho, *Europhys. Lett.* **10**, 261 (1989); B. Voightlander, S. Lehwald, M. Ibach, K. P. Bohnen and K. M. Ho, *Phys. Rev.* **B40**, 8068 (1989).
- 7) Y. Chen, S. Y. Tong, M. Rocca, P. Moretto, U. Valbusa, K. P. Bohnen and K. M. Ho, *Surface Science Lett.* **250**, L389 (1991).
- 8) Y. Chen, S. Y. Tong, Jae-Sung Kim, L. L. Kesmodel, T. Rodach, K. P. Bohnen and K. M. Ho, *Phys. Rev.* **B44**, 11, 394 (1991).
- 9) W. F. Egelhoff, Jr. in *Critical Reviews in Solid State and Materials Sciences*, **16**, 213 (1990).
- 10) S. A. Chambers, in *Advances in Physics*, edited by S. Doniach (Taylor and Francis, London, 1991).
- 11) K. F. Canter, *Positron Scattering in Gases*, ed. J. W. Humberston, M.R.C. McDowell (Plenum, London, 1984).
- 12) F. Jona, D. W. Jepsen, P. M. Marcus, I. J. Rosenberg, A. H. Weiss, K. F. Canter, *Solid State Commun.* **36**, 947 (1980).
- 13) V. L. Moruzzi, P. M. Marcus, K. Schwarz, and P. Mohn, *Phys. Rev.* **B34**, 1784 (1986).
- 14) J. G. Tobin, G. D. Waddill, and D. P. Pappas, *Phys. Rev. Lett.* **68**, 3642 (1992); G. D. Waddill, J. G. Tobin, and D. P. Pappas, *Phys. Rev.* **B46**, 552 (1992).

IV. COLLABORATION WITH EXPERIMENTALISTS AND OTHER THEORISTS

An important aspect of this program is the close collaboration with experimental work. We have planned joint projects with a number of research laboratories in the U.S. We have had an excellent record of working with experimentalists (over 100 of my papers contained results obtained from such collaborations). We have also very successful collaborations with other theorists. Table 2 contains a list of the planned collaborations.

Table 2. Planned Projects

<u>Technique</u>	<u>Materials</u>	<u>Collaborators</u>
High-resolution EELS	Pd(110) Si(111) $\sqrt{3} \times \sqrt{3}$ R30°-Al Cu(001) 1×1 -Ni	L.L. Kesmodel (Indiana U.)
Positron Diffraction Holography	GaAs(110) Si(111) 2×1 Cu(001) $p(2 \times 2)$ -Se	K.F. Canter (Brandeis U.) F. Jona (SUNY-Stony Brook)
Forward-scattering XPS, Photoelectron Diffraction, Electron Holography	Gd/W(110) Co/Cu(001) Fe/Cu(001) Fe/Cr/Fe	M. Onellion (U. of Wisconsin) M. Onellion (U. of Wisconsin) J.G. Tobin (Lawrence Livermore Nat. Lab.) J.G. Tobin (Lawrence Livermore Nat. Lab.)
Ab-initio Phonon Calculations	Pd(110) Si(111) $\sqrt{3} \times \sqrt{3}$ R30°-Al Cu(001) 1×1 -Ni	K.M. Ho (Iowa State U.) and K.P. Bohnen (KFK Karlsruhe, Germany)
Spin-wave Excitations, Spin LEED	Gd/W(110) Fe/Cu(001)	H. Hopster (U. California-Irvine) D.L. Mills (U. California-Irvine)

V. Curriculum Vita

David S. Y. Tong

Distinguished Professor of Physics and
Director, Laboratory for Surface Studies
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Employment History: The University of Wisconsin-Milwaukee
Distinguished Professor, Department of Physics, 1988-present.
Professor, Department of Physics, 1979-1988
Director, Laboratory for Surface Studies, 1980-present
Associate Professor, 1977-79; Assistant Professor, 1973-77
National Science Foundation - Washington, D.C.
Program Director, Condensed Matter Theory Section, Division of
Materials Research, Washington, D.C., 1988-89 (on loan to Federal
Government Agency from Univ. of Wisconsin-Milwaukee)
The University of Wisconsin-Madison
NSF Senior Visiting Investigator, Synchrotron Radiation Center,
UW-Madison, 1982-84 (concurrent appointment with Univ. of
Wisconsin-Milwaukee)
University of California-Irvine
Visiting Professor, 1978
University of California-Berkeley
Visiting Professor, 1978
Arhus University-Denmark
Visiting Professor, 1980
North Dakota State University
Assistant Professor, 1972-73
Cornell University
Postdoctoral Fellow, 1969-72

Education: Degree of Doctor of Philosophy in Physics, 1969, University of
California-Irvine
Degree of Master of Science, 1967, University of California-Irvine
Degree of Bachelor of Science, 1964, University of Hong Kong

Panels, Official Appointments and Awards:

- Consultant to Lawrence Livermore Laboratory, 1990-92.
- Consultant to the IBM Thomas J. Watson Research Center, Yorktown Heights, NY. 1974, 1975, 1981, 1983.
- Consultant to the Semiconductor and Surface Physics Division, Naval Research Laboratory, Washington, DC, 1973, 1975, 1977, 1980.
- Consultant to the Lawrence Radiation Laboratory, Berkeley, CA, 1978, 1980.
- Consultant to the Solid State Division, Oak Ridge National Laboratory, Oak Ridge, TN, 1981.

- Panelist of The Structure of Small Molecules Adsorbed on Surfaces, sponsored by CECAM, Europe, Gargnano del Garda, Italy, June 1979.
- Panelist of Symposium Sobre Finica de Superficies. A Workshop sponsored by UNAM, Mexico City, July 1979.
- Panelist of 50th Anniversary of the Discovery of Electron Diffraction. A Workshop sponsored by the British Institute of Physics, Imperial College, London, September 1977.
- Co-authored a 192 page report for the Resource Council for Materials Science, U.S. Department of Energy, Washington, DC, 1979.
- Consultant to NASA Space Epitaxy Program, University of Houston, 1990-92.
- Member of the Ad Hoc Advisory group for the Solid State Sciences Committee (SSSC), the U.S. National Research Council, 1980.
- Co-organizer of 3rd International Summer Institute in Surface Science (ISISS), August 15-19, 1975. Conference was sponsored by ONR and NSF.
- Co-organizer of 1st Conference on Physical and Chemical Properties of Solid Surfaces (PCPSS), October 28-30, 1979. Conference was sponsored by AVS.
- Member of the Program Committee of Conference on Low-Energy Electron Diffraction for Surface Structure Determination, June 10-13, 1980. Conference was sponsored by NSF and IBM.
- Member of the Program Committee of International School on Condensed Matter Physics, August 15-25, 1980. School was sponsored by the Bulgarian Academy of Sciences.
- Panel Member and Consultant to the Taiwan Synchrotron Radiation Center Project, 1984.
- Organizer of 1st International Conference on the Structure of Surfaces, August, 1984, at Berkeley, CA.
- Local Chairman, Physical Electronics Conference, Milwaukee, WI, June 1985.
- Member of the Organizing Committee, 2nd International Conference on the Structure of Surfaces, June 1987, at Amsterdam, The Netherlands.
- Local Chairman, 3rd International Conference on the Structure of Surfaces, July 1990, Milwaukee, WI.
- General Chairman, 4th International Conference on the Structure of Surfaces, 1993, Shanghai, China.
- Presidential Young Investigators Program, National Science Foundation Panel, Washington, D.C., 1990.
- Atomic Resolution Microscopy Panel, National Science Foundation, Washington, D.C., 1992.
- Symposium Organizer, Materials Research Society, Nov. 30-Dec. 4, 1992, Boston, MA.
- SRI International Panel on Assessment of Research Activity in the People's Republic of China, NSF and Science and Technology Policy Program, Washington, DC, Sept. 17, 1992.

Editorial Work, Officers and Awards:

- Editor, CRC Press, Critical Reviews in Solid State and Materials Sciences, 1976 and 1978.
- President of the American Vacuum Society, Wisconsin Chapter, 1979 (also Vice-President in 1978 and Treasurer in 1977).
- Executive Committee Member of the Surface Science Division, The American Vacuum Society, 1982-1986.
- Program Chairman, Surface Science Division of The American Vacuum Society, 1985.
- Chairman, Surface Science Division of The American Vacuum Society, 1985-1986.
- Recipient of the Fullbright East-West Center Award, 1965.
- Recipient of the University of Wisconsin-Milwaukee Foundation Distinguished Research Award, 1979.

- Distinguished Visiting Scientist, High-Resolution Electron Microscopy Facility, Arizona State University, Tempe, AZ, 1988.
- Distinguished Lecturer, Advanced Topics Lecture Series, Ministry of Education, Taiwan, 1987.
- Distinguished Lecturer, China Center of Advanced Science and Technology (CCAST), Beijing, 1991.

Honors and Invited Articles and Talks in 1993:

- Royal Society Kan Tong Po Visiting Professorship at the University of Hong Kong, July-August, 1993.
- Invited Lecturer, International School of Advanced Studies (ISAS), Trieste, Italy, June 1993.
- Invited Lecturer, "Workshop on Automation Algorithms in Surface Diffraction," University of Cambridge, England, March 1993.
- Invited Lecturer, "U.S.-Japan Symposium on Surface Characterization," Kona, Hawaii, March 1993.
- Invited to write a chapter for *Handbook of Surface Science*, Elsevier, North-Holland, The Netherlands.
- Invited by *Surface Science* to write an overview article describing the historic development of surface structure by electron diffraction to be included in a commemorative volume marking the first 30 years of research and development in this area.
- *Physics World*, England, is preparing an article to feature publication #156 "Low-Energy Electron and Low-Energy Positron Holography."
- Invited to write an advanced text on "Atomic Scale Imaging of Surfaces and Interfaces" by Cambridge University Press, United Kingdom.

Publications:

The P.I. has over 150 publications which, besides papers in refereed journals, include 4 books, 9 review papers and 24 chapters in books. Five of his papers were cited in "Physics News" by the American Institute of Physics in 1986.

VI. Publications During Past Five Years:

Books:

- 108) *The Structure of Surfaces III*, eds. S. Y. Tong, M. A. Van Hove, X. Xie and K. Takayanagi, Springer-Verlag, Berlin (1991).

Chapters in Books:

- 109) "Accurate Dynamical Theory for RHEED Rocking-Curve Intensity Spectra," S. Y. Tong, T. C. Zhao and H. C. Poon, in "RHEED and Reflection Electron Imaging of Surfaces," eds. P. K. Larsen and P. J. Dobson, Plenum Press, N.Y. (1988).
- 110) "Bonding and Structure on Semiconductor Surfaces," S. Y. Tong, H. Huang, C. M. Wei, in *Chemistry & Physics of Solid Surfaces*, Vol. 8, R. Vanselow and R. Howd, eds., Springer-Verlag, Berlin (1990).

- 111) Chapter in Book: "Angular Diffraction Patterns of Photoelectrons and Auger Electrons From Single-Crystal Cu(111)," X. D. Wang, Y. Chen, Z. L. Han, S. Y. Tong, B. P. Tonner, in *The Structure of Surfaces III*, eds. S. Y. Tong et al., Springer, Heidelberg, (1991).
- 112) Chapter in Book: "The Study of Surface Phonons by Electron Energy Loss Spectroscopy: Theoretical and Experimental Considerations," D. L. Mills, S. Y. Tong, J. E. Black, in *Surface Phonons*, ed. W. Kress, Springer, Heidelberg (1991).
- 113) Chapter in Book: "New Method for a Lensless Electron Microscopy: Achieving High Resolution and Overcoming Effects of Multiple Scattering," S. Y. Tong, H. Huang and Hua Li., eds. T. C. Haug, P. I. Cohen, and D. J. Eaglesham, MRS Symp. Series 208, 13 (1991).
- 114) Chapter in Book: "Photoelectron Diffraction of Magnetic Ultrathin Films: Fe/Cu(001)," J. G. Tobin, M. K. Wagner, X. Q. Guo and S. Y. Tong, Mat. Res. Soc. Symp. Series 208, 283 (1991).
- 115) "Forward Focusing Photoelectron Diffraction: A New Structural Tool for Surfaces and Interfaces," S. Y. Tong, Y. Chen, Hua Li and C. M. Wei, in *Surface Physics*, eds. X. Li et al., Gordon and Breach Science Publishers, Philadelphia (1992).

Journal Publications:

- 116) "Two-Dimensional Boundary Conditions and Finite Size Effects in Angle-Resolved Photoelectron Emission Spectroscopy, LEED and HREELS," S. Y. Tong and H. C. Poon, *Phys. Rev. B* 37, 2884 (1988).
- 117) "Surface Structure Analysis Using Reflection High Energy Electron Diffraction," K. D. Jamison, D. N. Zhou, P. I. Cohen, T. C. Zhao and S. Y. Tong, *J. Vac. Sci. Technol. A* 6(3), 611 (1988).
- 118) "Low-Energy Electron-Diffraction Analysis of the Si(111) 7x7 Structure," S. Y. Tong, H. Huang, C. M. Wei, W. E. Packard, F. K. Men, G. Glander and M. B. Webb, *J. Vac. Sci. Technol. A* 6(3), 615 (1988).
- 119) "Atomic Geometry of Si(111) 7x7 by Dynamical Low-Energy Electron Diffraction," H. Huang, S. Y. Tong, W. E. Packard and M. B. Webb, *Phys. Letters A* 130(3), 166 (1988).
- 120) "Multiple Scattering Analysis of Reflection High-Energy Electron Diffraction Intensities from GaAs(110)," S. Y. Tong, T. C. Zhao, H. C. Poon, K. D. Jamison, D. N. Zhou and P. I. Cohen, *Phys. Letters A* 128(8), 447 (1988).
- 121) "Characterization of Surface and Resonance Phonons for the Ni(100) - c(2x2)S System," Y. Chen, Z. Q. Wu, M. L. Xu, S. Y. Tong, K.-M. Ho and X.-W. Wang, *Phys. Review B* 37, 9978 (1988).
- 122) "Role of Adsorption Site on Electron-Energy-Loss Cross Sections of Single-Layer Substrate Modes," S. Y. Tong, Y. Chen, and Z. Q. Wu, *Phys. Review* 38(3), 2192 (1988).
- 123) "Dynamical Calculation of RHEED Rocking Curves for Ag(001) and Pt(111)," T. C. Zhao and S. Y. Tong, *Ultramicroscopy* 26, 151 (1988).

- 124) "Invariant-Embedding R-Matrix Scheme for Reflection High-Energy Electron Diffraction, T. C. Zhao, H. C. Poon and S. Y. Tong, Physical Review B38(2), 1172 (1988).
- 125) "Adsorption Distance of S on Ni(001): An Electron-Energy-Loss-Spectroscopy Cross-Section Analysis of the Ni(001-c(2x2)S system," Z. Q. Wu, Y. Chen, M.L. Xu and S. Y. Tong, Phys. Rev. B39(5), 3116 (1989).
- 126) "Vibrational Properties of Epitaxial Films on Metals. I. Fcc Ni on the Ni(001) Surface," S. Y. Tong, Y. Chen, J. M. Yao, and Z. Q. Wu, Phys. Rev. B 39(9), 5611 (1989).
- 127) "Vibrational Properties of Epitaxial Films on Metals. II. Fcc Ni on the Cu(001) Surface," Y. Chen, Z. Q. Wu, J. M. Yao, and S. Y. Tong, Phys. Rev. B 39(9), 5617 (1989).
- 128) "A Comparison of Green's Function and Slab Methods of Calculating Surface Vibration Spectral Densities: p(2x2)O on Ni(100) as an Example," Y. Chen, Z. Q. Wu, and S. Y. Tong, Sur. Sci. 210, 271-281 (1989).
- 129) "Observation and Structural Determination of $(\sqrt{3} \times \sqrt{3})R30^\circ$ Reconstruction of the Si(111) Surface," W. C. Fan, A. Ignatiev, H. Huang, and S. Y. Tong, Phys. Rev. Letters 62(13), 1516 (1989).
- 130) "The First Interlayer Spacing of Ta(100) Determined by Photoelectron Diffraction," R. A. Bartynski, D. Heskett, K. Garrison, G. Watson, D. M. Zehner, W. N. Mei, S. Y. Tong, and X. Pan, J. Vac. Sci. Technol. A 7(3), 1931 (1989).
- 131) "Quantative Structural Determination of Metallic Film Growth on a Semiconductor Crystal: $(\sqrt{3} \times \sqrt{3})R30^\circ T(1 \times 1)$ Pb on Ge(111)," H. Huang, C. M. Wei, H. Li, B. P. Tonner, and S. Y. Tong, Phys. Rev. Letters 62(5), 559 (1989).
- 132) "The First Interlayer Spacing of Ta(100) Determined by Photoelectron Diffraction," R. A. Bartynski, D. Heskett, K. Garrison, G. Watson, D. M. Zehner, W. N. Mei, S. Y. Tong and X. Pan, Phys. Rev. B40, 5340 (1989).
- 133) "Atomic Structure of Si(111)- $(\sqrt{3} \times \sqrt{3})R30^\circ$ -Al Studied by Dynamical Low-Energy Electron Diffraction," H. Huang, S. Y. Tong, W. S. Yang, H. D. Shih, F. Jona, Phys. Rev. B42, 7483 (1990).
- 134) "Atomic Structure of Si(111) $(\sqrt{3} \times \sqrt{3})R30^\circ$ -B by Dynamical Low-Energy Electron Diffraction," H. Huang, S. Y. Tong, J. Quinn, F. Jona, Phys. Rev. B41, 3276 (1990).
- 135) "Surface-Phonon Dispersion of NiAl(110)," M. Wuttig, W. Hoffmann, E. Preuss, R. Franchy, H. Ibach, Y. Chen, M. L. Xu, S. Y. Tong, Phys. Rev. B42, 5443 (1990).
- 136) "Electron-Energy-Loss Cross-Section and Surface Lattice-Dynamics Studies of NiAl(110)," Y. Chen, M. L. Xu, S. Y. Tong, M. Wuttig, W. Hoffman, R. Franchy, H. Ibach, Phys. Rev. B42, 5451 (1990).
- 137) "Detection of Odd Symmetry Shear Modes at Metal Surfaces by Inelastic Electron Scattering: Experiment and Theory," J. L. Erskine, E.-J. Jeong, J. Yater, Y. Chen, S. Y. Tong, J. Vac. Sci. Tech. A8, 3649 (1990).

- 138) "The Structure of Si(111) $\sqrt{3} \times \sqrt{3}$ R30°-Ag, Reply Comment," Phys. Rev. Lett. 64, 492 (1990).
- 139) "Quantitative Structural Determination of Metallic Film Growth on a Semiconductor Crystal, Reply Comment," H. Haung, C. M. Wei, B. P. Tonner, S. Y. Tong, Phys. Rev. Lett. 64, 1183 (1990).
- 140) "Growth of Co Layers on Cu(111) Studied by Forward-Focusing Angle-Resolved X-Ray Photoemission Spectroscopy and Real-Space Imaging," C. M. Wei, T. C. Zhao, S. Y. Tong, Phys. Rev. Lett. 65, 2278 (1990).
- 141) "Adsorption Geometry of (2x1) Na on Si(001)," C. M. Wei, H. Huang, S. Y. Tong, G. Glander, M. B. Webb, Phys. Rev. B42, 11284 (1990).
- 142) "Auger Electron Angular Distributions from Surfaces: Forward Focusing of Silhouettes?" X. D. Wang, Z. L. Han, B. P. Tonner, Y. Chen, S. Y. Tong, Science 248, 1129 (1990).
- 143) "Angle-Resolved X-Ray Photoemission Spectroscopy from HCP Co(0001): Forward-Focusing and Atomic Imaging," C. M. Wei, T. C. Zhao, S. Y. Tong, Phys. Rev. B43, 6354 (1991).
- 144) "Characterization of Surface Phonons on Cu(001) and Ag(001): First-Principles Phonon Calculations With Experimental and Theoretical Studies of High-Resolution Electron-Energy-Loss Spectra," Y. Chen, S. Y. Tong, Jae-Sun Kim, L. L. Kesmodel, T. Rodach, K. P. Bohnen and K. M. Ho, Phys. Rev. B44, 11 394 (1991).
- 145) "Energy-Extension in 3-Dimensional Atomic Imaging by Electron Emission Holography," S. Y. Tong, Hua Li and H. Huang, Phys. Rev. Lett. 67, 3102 (1991).
- 146) "High-Resolution Electron Energy-Loss Spectroscopy Analysis of Ag(001): Discovery of a New Surface Longitudinal Mode Using First-Principles Phonon Calculations," Y. Chen, S. Y. Tong, M. Rocca, P. Moretto, U. Valbusa, K. P. Bohnen and K. M. Ho, Surface Science Lett. 250, L389 (1991).
- 147) "Phase Shift Correction in 3-Dimensional Imaging Using Forward-Scattering Photoemission and Auger Spectroscopies," S. Y. Tong, C. M. Wei, T. C. Zhao, H. Huang, Hua Li, Phys. Rev. Lett. 66, 60 (1991).
- 148) "The Registry of Honeycombs in the Structure of Si(111) ($\sqrt{3} \times \sqrt{3}$) R30°-Ag," S. Y. Tong, H. Huang, Surface Science Lett. 243, L46 (1991).
- 149) "Surface Phonons and Structure and Epitaxial Nickel Layers on Cu(001)," Y. Chen, S. Y. Tong, Jae-Sung Kim, M. H. Mohamed, L. L. Kesmodel, Phys. Rev. B (Rapid Communications) 43, 6788 (1991).
- 150) "Three-Dimensional Imaging of Atoms Using Source Waves From Deeply Buried Atoms and Overcoming Multiple-Scattering Effects," H. Huang, Hua Li and S. Y. Tong, Phys. Rev. B44, 3240 (1991).
- 151) "Principles of Energy Extension in Electron-Emission Holography," Phys. Rev. B46, 4155 (1992).

- 152) "Momentum-Space Images of Surface Dimers on GaAs(001)-(2x4) by High-Energy Auger and X-ray Photoelectron Diffraction," J. Vac. Sci. and Technol. B10, 2092 (1992).
- 153) "Method for Spatially Resolved Imaging of Energy-Dependent Photoelectron Diffraction," S. Y. Tong, H. Huang and C. M. Wei, Phys. Rev. B46, 2452 (1992).
- 154) "Direct Atomic Structure by Holographic Diffuse LEED," C. M. Wei and S. Y. Tong, Surface Sci. Lett. 2174, L577 (1992).
- 155) "Forward-Focusing and Shadowing Effects in Solids," Hua Li and S. Y. Tong, Surface Science Letters, in print.
- 156) "Low-Energy Electron and Low-Energy Positron Holography," S. Y. Tong, H. Huang and X. Q. Guo, Phys. Rev. Lett. 69, 3654 (1992).
- 157) "R-matrix Method for Calculating Wavefunctions in Reflection High-Energy Electron Diffraction," T. C. Zhao and S. Y. Tong, Phys. Rev. B, in print.
- 158) "Imaging Atoms in Surface Dimers of GaAs(001) c(2x8)/(2x4) by Electron-Emission Holography," Surface Sci., in print.

VII. APPENDICES

Facilities

The Department of Physics and the Laboratory for Surface Studies at UW-Milwaukee have made major commitments to basic and applied research in surface science. The latter is an interdepartmental research center with 16 full time faculty members (in the Departments of Physics, Chemistry and Materials Science) and over 50 research staff and graduate students working on a span of surface related research. The Principal Investigator is the Director of the Laboratory for Surface Studies. Experimental work on LEED, synchrotron radiation and laboratory based photoemission, Auger electron spectroscopy, STM, infrared and Raman spectroscopies, electron desorption, thin film growth and characterization, heterogeneous catalysis, oxidation reactions and interface studies of metal-semiconductor compounds are among the research projects being carried out here.

The Laboratory for Surface Studies also sponsors the following programs as part of its activities:

- LSS-Undergraduate Research Participation Program (LSS-URP) — Qualified undergraduate students from colleges and universities in Wisconsin and neighboring states are granted LSS-URP-Fellowships during each summer period. The students work for about 8 weeks with a professor in the Laboratory for Surface Studies. During their stay they attend special seminars which familiarize them with the LSS research programs and the research equipment available.
- Surface Studies Seminar — At the weekly Surface Studies Seminars (held on Tuesdays, 3:30–4:30 p.m.), we invite industrial, academic and foreign visitors to lecture on their areas of specialization.
- E.W. Müller Lectureship — In the Spring of 1978, UWM received permission from the personal representative of the late Professor E.W. Müller to use his name for a special lectureship award. The E.W. Müller lectureship award is given annually to a scientist with outstanding achievements in surface science. Under the conditions of the award,

the recipient presents a series of lectures in surface studies during the UWM summer session and also cooperates in research projects with faculty members of LSS.

- The International Summer Institute in Surface Science (ISISS) — The Summer Institutes are held biennially during the month of August on the UWM campus. Twenty-one internationally recognized surface scientists present tutorial review talks on their area of specialization. The first ISISS was held in 1973. In 1992, the Laboratory hosted its 10th Summer Institute. The papers from the Summer Institutes were published collectively in "Critical Reviews of Solid State and Materials Sciences." Also since ISISS 1975, a book entitled *Chemistry and Physics of Solid Surfaces* has been published by Springer-Verlag. In 1993, the Summer Institute papers will be published in *Surface Science Reports*.

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