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Dynamics of Gas-Surface Interactions

AFOSR-88-0194

Final Technical Report for November 1, 1988 - October 31, 1992

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Abstract: This research initiative deals with the interaction of neutral particle, electron, and optical beams with well-characterized single crystal surfaces. These studies are motivated by a desire to understand and control surface reactions, such as surface oxidation, the technological need to characterize the physical properties of thin films and surfaces, and the desire to understand how energy and momentum are exchanged at the surface of a material when it is subjected to gas-surface collisions, electron-surface collisions, optical illumination, or chemical reaction. Experiments aimed at determining the surface phonon dispersion relations for a variety of clean and adsorbate covered systems play a central role in this program. Such measurements are crucial for elucidating how the force constants at the surface differ from those characteristic of the bulk for a given material, and how adsorption of atomic and molecular species modify the force constants, and hence electron density distributions, at and in the vicinity of the surface. The experimental program utilizes two, now fully operational, scattering laboratories that were constructed with significant DoD funding. One of these is a high resolution (energy and momentum) neutral particle scattering apparatus which routinely carries out single phonon inelastic as well as diffractive scattering measurements. The other laboratory houses an inelastic electron scattering instrument which also produces momentum-resolved inelastic scattering data. The capabilities of these two facilities complement each other in many important and useful ways. To our knowledge, we are the only research group in the world which currently has both inelastic neutral particle and electron scattering capabilities at its disposal. Especial attention is also being given to elucidating which surface vibrational modes actively participate in collision induced energy exchange, and determining under which energy regimes single phonon, multi-phonon, and electron-hole pair processes are significant energy absorption mechanisms. Structural studies employing helium atom scattering also form a key part of this program. During the past grant period our efforts have concentrated on (i) structural and inelastic helium scattering studies of the model superalloy $\text{Cu}_3\text{Au}(001)$, (ii) the initial stages of oxidation for a stepped metallic surface, $\text{Ni}(977)$, where we have examined a fascinating step doubling phenomenon with diffractive helium scattering, (iii) helium scattering and molecular dynamics simulations of stepped surfaces; (iv) inelastic electron scattering studies of $\text{Ni}(111)$ and $\text{O}/\text{Ni}(111)$, (v) the use of inelastic electron scattering to probe previously unobserved frustrated vibrations for $\text{CO}/\text{Ni}(111)$, (vi) the use of resonantly enhanced inelastic electron scattering to probe the femtosecond dynamics of transiently formed CO^- on $\text{Ni}(111)$, (vii) implementation of an intense neutral particle beamline for use with our electron scattering apparatus, and (viii) development of lattice dynamics, scattering, and, most recently, molecular dynamics calculations for analyzing our helium and electron scattering results.

I. Introduction

The scattering of atomic, molecular, and electron beams from well-characterized single crystal surfaces is proving to be an incisive method for studying the dynamics of gas-surface and electron-surface interactions. Perhaps even more importantly, scattering measurements can be used to probe the structure, surface vibrational properties, and reactivity of clean and adsorbate covered surfaces. This final technical report gives an overview of the research accomplished under the auspices of the AFOSR during the past grant period. This experimental program utilizes two, now fully operational, scattering laboratories that were constructed with significant DoD funding. One of these is a high resolution (energy and momentum) neutral particle scattering apparatus which routinely carries out single phonon inelastic as well as diffractive scattering measurements. The other laboratory houses an inelastic electron scattering instrument which also produces momentum-resolved inelastic scattering data. As will be seen in this document, the capabilities of these two facilities complement each other in many important and useful ways. These measurements are supported by appropriate in-house theoretical efforts, such as lattice dynamics calculations, quantum scattering calculations, and most recently, molecular dynamics (MD) simulations. The MD simulations are an important addition as they allow surface vibrational dynamics to be calculated at elevated temperatures.

Areas being explored cover elastic, inelastic, and reactive scattering. During the past grant period our efforts have concentrated on (i) structural and inelastic helium scattering studies of the model superalloy $\text{Cu}_3\text{Au}(001)$, (ii) the initial stages of oxidation for a stepped metallic surface, $\text{Ni}(977)$, where we have examined a fascinating step doubling phenomenon with diffractive helium scattering, (iii) helium scattering and molecular dynamics simulations of stepped surfaces; (iv) inelastic electron scattering studies of $\text{Ni}(111)$ and $\text{O}/\text{Ni}(111)$, (v) the use of inelastic electron scattering to probe previously unobserved frustrated vibrations for $\text{CO}/\text{Ni}(111)$, (vi) the use of resonantly enhanced inelastic electron scattering to probe the femtosecond dynamics of transiently formed CO^- on $\text{Ni}(111)$, (vii) implementation of an intense neutral particle beamline for use with our electron scattering apparatus, and (viii) development of lattice dynamics, scattering, and molecular dynamics calculations for analyzing our helium and electron scattering results. The scientific projects being studied in this program are motivated by a desire to understand and control heterogeneous surface chemistry, including surface oxidation, the technological need to characterize the physical properties of thin films and surfaces, and the desire to understand how energy and momentum are exchanged at the surface of a material when it is subjected to gas-surface collisions, electron-surface collisions, optical illumination, or chemical reaction. The energy transfer questions being addressed here are central to a microscopic understanding of thermal accommodation, momentum accommodation (aircraft drag), and chemical adsorption.

II. Personnel

Our research program has been quite successful in attracting and educating some of the best young scientific talent in the country, including undergraduates, graduate students, and postdoctoral fellows. For example, during the 1988-92 time period four students received their doctorates based upon AFOSR sponsored research, and two more are expected during the next few months. Our research group currently consists of seven graduate students, two postdoctoral fellows, and two outstanding undergraduates. Listed in order of seniority, these include: Dr. Kevin Gibson, Dr. Wei Li, Suzanne King, Glenn Tisdale, Kevin Peterlinz, Licheng Niu, Jennifer Colonell, Michael Stimiman, Errol Sanchez, Jason Fleischer, and Sarah O'Conner. There are also two graduate students studying with Prof. John Light who are working on problems related to our AFOSR sponsored experiments. Our program has continued to attract students of unusual ability, including Dr. Thomas Curtiss, the James Franck Fellow in Experimental Physical Chemistry (one such fellowship is given every two years in our institute), Jennifer Colonell (an AT&T Fellow and a McCormick Fellow), and Mike Stimiman (a Dept. of Education GANN Fellow).

Recent alumni (*primary effort on AFOSR sponsored projects)

Graduate Students:

- *Daniel Koleske (Ph.D. - Chemistry, Dec. 1991, now at IBM Yorktown Heights)
- David Padowitz (now at Berkeley)
- *Warren J.C. Menezes (Ph.D. - Chemistry, March 1990, now at LK Technologies after postdoc at Argonne Natl. Lab)
- *Barbara Gans (Ph.D - Chemistry, June 1990, now at Naval Res. Lab)
- Kevin Gibson (now at Chicago after postdoc at AT&T Bell Labs)
- Chien-fan Yu (now at IBM Fishkill after postdoc at Columbia Univ.)
- *Yaw-Wen Yang (Ph.D - Chemistry, June 1988, now at Brookhaven Natl. Lab after postdoc at U. of Washington, Seattle)

Other Graduate Students (doctoral work done on theoretical problems generated by our DoD funded activities):

- *Peter Knipp (now at Christopher Newport U.(faculty) after postdoc at NRL, PhD-Physics, 6/90 with U. Fano)
- Birgitta Whaley (now at Berkeley (faculty) after postdoc in Israel, PhD with J. Light)

Postdoctoral Fellows:

- *Thomas Curtiss (now at Univ. of Utah - faculty)
- Wesley Natzle (now at IBM Fishkill - perm. staff)
- Larry Brown (now at Texas A&M - faculty)
- *Jeong Sook Ha (now at Electronics and Telecomm. Res. Institute, Korea)

Undergraduate Research Students (all benefited from AFOSR supported facilities)

- *Jeanette Sperhac (graduate student-Univ. of Colorado, Boulder)
- *Sei Lee (teaching science in high school-Mississippi)
- *Joe Zwanziger (Berkeley PhD - now at Indiana Univ., Bloomington - faculty)
- *Jesus Melendez (working in Phoenix, Az)
- *Scott Silence (MIT PhD - current postdoc at IBM, Almaden)
- *Mark Kramer (MD, U. of Chicago)
- *Eriko Yagi (working in SF, CA)

To conclude this section, we wish to emphasize that we have been quite successful in attracting qualified women and minorities to our program (see above) and hope to continue this important trend in the future. At the present time three of our group members are women who are citizens of the US. The PI fully recognizes that the future vitality of the American science enterprise will depend on the successful involvement of women and under-represented minorities at all levels of training.

III. Research Accomplishments

Our AFOSR funded activities have been in several areas during the past grant period. For the purposes of this Final Technical Report, we summarize this activity in 8 sections as listed below:

- (1) **Facilities Overview**
- (2) **Elastic and Inelastic He Scattering Studies of Cu₃Au(001)**
- (3) **Initial Stages of Oxidation for a Stepped Metallic Surface, Ni(977): Observation of Step and Terrace Doubling Via He Scattering**
- (4) **He Scattering and Molecular Dynamics Simulations of Stepped Surfaces**
- (5) **Inelastic Electron Scattering Studies of Ni(111) and O/Ni(111)**
- (6) **Low Energy Frustrated Vibrations of c(4x2)-CO-Ni(111)**
- (7) **Resonantly Enhanced Inelastic Electron Scattering: A Femtosecond Probe of Adsorbate Dynamics**
- (8) **Instrumentation Development**

(1) Facilities Overview

This experimental program utilized two, now fully operational, scattering instruments that were constructed with significant DoD funding. We are currently the only research group in the world which has both inelastic neutral particle and electron scattering capabilities at our disposal.

One of these is a high resolution (energy and momentum) neutral particle scattering apparatus, Figure 1, which routinely carries out single phonon inelastic as well as diffractive scattering measurements. This novel neutral particle scattering instrument has been optimized for a variety of high energy resolution single-phonon scattering measurements. It has successfully met its design criteria of simultaneously achieving an extremely low background in its detector (10 counts per second), high angular (momentum) resolution, and, most importantly, excellent time-of-flight energy resolution (300 μ eV is routinely being obtained at this time). Inelastic atom scattering is, in principle, a nearly ideal probe of *low energy* microscopic surface vibrations. This can be

attributed to several factors including excellent surface sensitivity, high energy resolution (sub-meV), and, most importantly, the fact that both the energy *and momentum* of thermal energy helium beams are well matched to those of surface phonons. We note in particular that excellent surface sensitivity is realized in the neutral particle scattering experiments since the classical turning points of the incident trajectories occur at the surface—penetration depth problems similar to those associated with electron diffraction do not occur.

The other laboratory houses an inelastic electron scattering instrument, Figure 2, which also produces momentum-resolved inelastic scattering data. It operates at high sensitivity with high energy resolution (5 meV), and with incident beam energies of up to 240 eV. The inelastic electron scattering measurements provide complementary information (at lower resolution) to the helium measurements in that other higher lying vibrational modes can also be interrogated; electron scattering can also provide access to sub-surface features under appropriately chosen scattering conditions. Together, these techniques can provide a very extensive mapping of the acoustic and optical modes that are present at surfaces—crucial information for developing a clear understanding of the forces which govern the dynamical behavior of interfaces.

The aforementioned experimental programs are supported by appropriate in-house theoretical efforts, such as lattice dynamics calculations, quantum scattering calculations, and most recently, molecular dynamics (MD) simulations. The MD simulations are an especially important addition as they allow surface vibrational dynamics to be calculated at elevated temperatures.

Financial support came in four forms: this AFOSR grant and three separate DoD-University Research Instrumentation Program grants. (Early "seed" funding for this project also came from the University of Chicago, the Research Corporation, the Camille and Henry Dreyfus Foundation, and the NSF-Materials Research Laboratory at the University of Chicago.)

(2) Elastic and Inelastic He Scattering Studies of Cu₃Au(001)

Understanding the chemical and physical properties of alloy surfaces is important for the further development of heterogeneous catalysts and for the custom design of material interfaces able to withstand corrosive and high temperature environments. To date, there have been only a few surface studies of intermetallic compounds which comprise ordering binary alloys [1-3]. A₃B intermetallic compounds often form fcc lattices of which a simple cubic sublattice consists solely of minority atoms. These are interesting because they exhibit high strength even at elevated temperatures. Samples consisting of both ordered and disordered regions are of further interest, as their physical properties, such as resistance to dislocation propagation and brittleness, can be optimized for a specific application given our present understanding of the relationship between

microstructure and micromechanics. For this reason 'superalloys' are currently used in high performance applications of the aerospace industry. These alloys exhibit increased hardness in their ordered phase as compared to their disordered phase or their single metal constituents. In our group we have initially focussed on the model system $\text{Cu}_3\text{Au}(001)$, with two of the primary goals being to investigate how interatomic forces differ between the surface and bulk regions of an intermetallic compound, and how the surface structure changes in the vicinity of the disordering temperature of the alloy -- ideally revealing how the ordered and substitutionally disordered surface domains evolve as a function of temperature.

$\text{Cu}_3\text{Au}(001)$ exhibits a high degree of long range order, with the surface existing as a $c(2 \times 2)$ structure. Planes perpendicular to the (001) direction consist of alternating layers of either 50% Cu-50% Au or 100% Cu composition. The low energy ion scattering study (LEIS) of Buck and Wheatly [4] has shown that the (001) surface of the ordered phase terminates exclusively with a layer consisting of 50% Cu-50% Au composition, ordered in a $c(2 \times 2)$ arrangement.

Cu_3Au is particularly interesting because the bulk undergoes a *first order* phase transition ($T_c=663$ K) to form a substitutionally disordered phase at a temperature well below its melting temperature ($T_m=1226$ K). Recent theory [5] and experimental work [6,7] on the order-disorder transition at the (001) surface indicates that the transition may occur *continuously*. Although the symmetry is reduced when going from the ordered state to the disordered state, the material maintains an fcc lattice--in contrast to a surface melting transition. Because of this the structural and vibrational properties both above and below the transition temperature can be investigated in the same way.

We have employed both elastic (for diffraction) and inelastic (for surface vibrational studies) helium atom scattering to characterize the structure and vibrational properties of $\text{Cu}_3\text{Au}(001)$. Neutral helium atom scattering is especially well suited for this study since it has extreme sensitivity to the outermost layer of the alloy; i.e., it offers a high degree of "contrast" between the surface and the selvedge region. Figure 3 shows a series of He diffraction scans for this surface as a function of surface temperature. The superior energy resolution (0.25-1.0 meV) available with inelastic helium scattering allows clear identification of low frequency modes, that may only be separated in energy by a few meV. Such measurements can be viewed as a two-dimensional, surface sensitive, analog to inelastic neutron scattering.

During the past year we have completed the analysis of the dynamical properties of the ordered (001) surface. Inelastic helium atom scattering has been used to measure the surface phonon dispersion curves for the (001) face of the ordered phase of Cu_3Au along the $\langle 100 \rangle$ (i.e., $\bar{\Gamma}-\bar{M}$) direction. Figure 4 shows a series of time-of-flight spectra for this surface. We have

spectroscopically observed two surface phonon modes on this fcc alloy. The lower energy surface phonon mode, the Rayleigh wave, has an energy of $7.1 (\pm 0.5)$ meV at $\bar{M}'$. The higher lying feature is an optical mode with an energy of $12.5 (\pm 1.0)$ meV, which shows little dispersion across the surface Brillouin zone. This phonon mode might be interpreted as a folded Rayleigh mode. The experimentally measured dispersion curves do not agree with those generated by a lattice dynamical slab calculation which uses a pair potential force-field that successfully models the bulk vibrations of the ordered alloy, Figure 5A. The best fit to our experimental data indicates that the force constant between the first and second layer Cu atoms needs to be stiffened by approximately 20% with respect to the corresponding bulk value, Figure 5B. This is approximately the same amount of stiffening needed to match the HREELS data for the Rayleigh wave on Cu(001) [8].

Further efforts have been concerned with the surface structure and phonon spectra at temperatures near the surface phase transition and above it, when both the surface and the bulk of the alloy become disordered. The spectra shown in Figure 6 demonstrate that single phonon scattering events can be followed up to and through the surface disordering transition. We hope to elucidate whether, and if so to what extent, the surface force constants differ between the ordered and substitutionally disordered phases of the alloy. We also are making a major effort to study how the surface structure changes in the vicinity of the bulk disordering temperature. We have recently seen that the surface begins to disorder at temperatures well below T_c for the bulk, i.e. 664 K, exhibiting similar behavior as been seen in LEED studies. Figure 3 shows temperature dependent diffraction measurements of the alloy surface which demonstrate the gradual onset of surface disorder as a function of temperature, beginning well below the bulk critical temperature. A continuous phase transition is suggested by examination of the temperature dependence of the long-range order parameter for this system. We wish to emphasize again that neutral helium atom scattering is especially well suited for this study since it has extreme sensitivity to the outermost layer of the alloy; i.e., it offers a high degree of structural "contrast" between the surface and the selvedge region.

We have also conducted *kinetic measurements* in an attempt to observe in real time how the surface orders following quenching from above T_c to temperatures below T_c . Our preliminary results have already revealed that the surface orders much more rapidly than the bulk (!!!) [9]. Figure 7 demonstrates that even for a relatively shallow quench (to $T_c - 5$ deg.) only two minutes is required for surface order to develop, in sharp contrast to related bulk measurements which take hours to occur [10-13]. Our work forms a nice complement to depth dependent evanescent wave x-ray scattering experiments [3]. Such dynamical measurements should reveal new details about the approach to equilibrium. Higher resolution studies on this or other interfacial systems may be

used to reveal how quenched systems evolve through the various stages of nucleation, ordering, and coarsening [10,14].

Finally, yet another surprising result appears to be emerging from our studies of surface disordering as a function of sample temperature. Examination of superlattice peak linewidths and integrated areas has shown that, for certain regions of our target crystal, that the peaks actually narrow before reaching the bulk critical temperature, and that the peak intensity vs. surface temperature curve has a related small bump, as shown in Figure 8. This suggests that in some instances the surface domain structure may actually improve as T_c is approached from below, implying that domain boundaries may be relaxing.

(3) Investigation of the Initial Stages of Oxidation for a Stepped Metallic Surface, Ni(977): Observation of Step and Terrace Doubling Via He Scattering

Stepped surfaces have a long history of acting as model systems for interfaces which contain known densities and types of structural defects [15]. In our group we have conducted a series of helium diffraction experiments, including time-resolved diffraction (kinetics) measurements, to examine the initial stages of oxidation on a stepped metallic surface, Ni(977) [also labelled as Ni(S)-{8(111) x 1(100)}], Figure 9. This regularly stepped surface has a (111) terrace that is 8 atoms wide with step edges composed of (100) faces.

We see very strong helium diffraction from the clean Ni(977) surface, as can be seen in the upper panel of Figure 10. The positions and intensities of these peaks are well understood by us, having been modelled with a simple scattering calculation. We were greatly surprised to find that exposure of this surface to only ca. 0.05 Langmuirs of oxygen at temperatures in the vicinity of 500 K led to a massive structural change of the surface— helium diffraction, as well as LEED, showed that the steps and terraces double in size under these conditions, i.e. a Ni(S)-{15(111) x 2(100)}-O surface is formed. The lower panel of Figure 10 shows an additional diffraction spot at 34 deg. which is the signature for this restructuring. We have since undertaken extensive energy dependent helium diffraction data to confirm our findings. So-called drift spectra, in which the DeBroglie wavelength of the helium is allowed to monotonically decrease while collecting diffraction data, convincingly confirm that this structural change occurs. Figure 11 shows a comparison of experimental and calculated drift spectra which span the beam temperature range from 70-300 K. The left panels (experiment and theory for the clean surface) in this figure exhibit four "waves" while the right panels (experiment and theory for the slightly oxidized surface) each show six such features. Diffraction data at different incident angles further confirm the observation of step doubling. The observed step "coalescence" requires as little as 4-6% oxygen coverage,

suggesting that the reconstruction must involve oxygen-step interactions. Similar structural evolution has been seen previously with LEED for Pt(755) [16].

This oxidation study of the Ni(977) surface agrees with the initial oxidation results conducted by MacRae on Ni(111) [17], who concluded that NiO growth was initiated at steps with a (100) step face. Once these initial NiO nucleation sites are established which are 2-3 layers in depth, the NiO grows parallel to the surface [18]. Because the Ni(977) surface has regularly spaced (100) step faces, it is an ideal candidate for a more thorough understanding of how Ni surfaces oxidize. Furthermore, the diffraction intensities from surfaces which consist of both Ni(977) and Ni(S)-{15(111) x 2(100)}-O regions surface can be related to the number of single and double steps that appear on the surface, giving us a superb system for studying domain growth and domain boundary aggregation. Monte Carlo simulations of this system may be carried out.

Finally, we are just beginning to examine the kinetics, i.e. oxygen coverage and temperature dependence, of this remarkable structural transformation. Our plans for the next grant period include *time-resolved He diffraction* measurements which will monitor the structural evolution of the surface following either oxygen exposure or temperature jumps (we already know that the process is thermally activated; temperatures above ca. 425 K seem to be needed for the doubling to occur.) We have especially high hopes for the new information that will come from these measurements, such as Ni diffusion coefficients on partially oxidized surfaces. Additional surface phonon studies are also planned which will tell us about the surface forces which are present on clean and oxidized metallic interfaces (see next section).

(4) He Scattering and Molecular Dynamics Simulations of Stepped Surfaces

We have embarked on the study of stepped surfaces with the intent of studying their structural and dynamical properties with low energy helium scattering. Complementing the experimental work are lattice dynamics and molecular dynamics calculations from our group [19-21]. The MD simulations are an important addition as they allow surface vibrational dynamics to be calculated at elevated temperatures. The computational codes have been completed and are now being used in advance of the experimental measurements. The scientific goal is to understand how surface vibrations behave in the vicinity of a surface defect, with stepped crystals providing us with a "controllable two-dimensional defect". Since stepped surfaces contain step atoms with lower coordination than the relevant basal plane, the step atoms should be especially sensitive to the anharmonic part of the potential. Furthermore, recent calculations from our group [19-21] and Gottingen [22] have shown that new vibrational modes ω exist at extended defects, such as stepped surfaces. Figure 12 shows such a calculation for a LJ(755) surface which clearly shows

two new features, labelled E1 and E2, which are "edge" phonons which are localized along the step.

Anharmonic effects are another key focus of these studies. Temperature dependent studies of the surface phonon dispersion relations for FCC (100), (110), and (111) faces using molecular dynamics (MD) simulations and Lennard-Jones potentials have been carried out [19-21]. Here we examined the temperature dependence of the $\bar{Q}$ -resolved phonon spectral density function. At higher temperatures some of the phonon linewidths changed from having a linear to a quadratic dependence on T . The temperature at which this T to T^2 change occurs is surface dependent and occurs at the lowest temperature on the (110) surface. The T^2 dependence arises from the increasing importance of higher order phonon-phonon scattering terms. This is especially true for the linewidth of the S_1 mode at $\bar{X}$ on the (110) surface, Figure 13, where, at $T \sim 15-23\%$ of the melting temperature, the RMSD perpendicular to the atomic rows become larger than the RMSD normal to the surface. Our results indicate that the dynamics on the (110) surface may be significantly influenced by anharmonic potential terms at temperatures as low as 15% of the melting temperature. We propose to experimentally examine such effects. Calculations are also in progress using more realistic Finnis-Sinclair potentials to model the temperature dependent dynamics of various Ni surfaces.

After theoretically examining the frequencies and polarizations for the "step modes" which should exist on a wide variety of surfaces, we decided to make Ni(977) our first stepped crystal for experimental examination. High resolution diffraction and phonon measurements on this surface are well underway.

(5) Inelastic Electron Scattering Studies of Ni(111) and O/Ni(111)

One of the central concerns in surface science today is to ascertain how the properties (static and dynamic) of surfaces differ from those of bulk matter. A very direct way to explore the dynamical aspects of this problem is to study the interatomic force constants in the vicinity of a surface. Under AFOSR auspices we have been studying the surface dynamical properties of clean Ni(111) as examined by high resolution electron energy loss spectroscopy (HREELS) operating at high incident energies, in the off-specular impact scattering regime. The experimental results are analyzed using lattice dynamical and quantum multiple-scattering calculations. Ni(111) presents an excellent opportunity for studying the dynamical properties of a closest-packed surface which has nearly ideal termination with respect to its bulk geometry. Bulk nickel dispersion curves are fit extremely well by a simple force-constant model which assumes that the interatomic potential $\phi(r)$

is only nonzero between nearest neighbors. The first and second derivatives ϕ' and ϕ'' dictate the harmonic vibrations. Deviations of dynamical surface properties from "ideal termination" can be expressed in terms of $\phi_{ij}(r) \neq \phi(r)$, where $\phi_{ij}(r)$ is the (nearest-neighbor) potential between atoms in layers i and j . Previous studies indicate that the geometrical spacing between this unreconstructed surface and the second layer is within 1% of the bulk value. Hence, $\phi_{ij}(r) - \phi(r)$ is expected to be small.

Our results [23-25] demonstrate that the surface force field for Ni(111) differs from expectations based upon simple extrapolation from bulk behavior. The intraplanar surface force constant is approximately 11% softer than in bulk nickel. In addition, tensile surface stress is present at the (relatively low) level of +1.6 N/m, indicating that the surface atoms have a desire to be more closely spaced than in the bulk. This level of stress has been predicted theoretically for a number of metal surfaces. These surface force field assignments were derived from lattice dynamical fits to the spectroscopic results, Figure 14, and were independently confirmed by quantum multiple scattering calculations, Figure 15. Work that is currently being prepared for publication shows that energy dependent scattering measurements are quite sensitive to the lattice dynamical model used. By varying the experimental parameters, we can now selectively resolve different phonon features under favorable circumstances. Our precision surface phonon measurements have recently stimulated accurate electronic structure calculations of Ni(111) [25,26] (effective medium calculations by P. Ditlevsen from Copenhagen). Surface phonons derived from this electronic structure calculation have just been shown to be in excellent agreement with our measurements, Figure 16.

Note that our results on intraplanar softening results were largely based on the successful spectroscopic detection of a longitudinally polarized surface mode, the so-called S2 gap mode. This 11% is quite similar to recent values for Cu(111) that were determined with inelastic electron scattering [27], but is much smaller than those reported for the (111) surfaces of Cu [28], Ag [28,29], and Pt [30] as examined by inelastic helium scattering.

Our experimental focus has now shifted to O/Ni(111). Experimental measurements and related lattice dynamics calculations are nearly completed. The obvious goal here will be to see how the initial stages of oxidation modify the surface force constants of the Ni surface. Predictions have been made which suggest that the tensile stress present at the surface should be relieved upon formation of an ordered adsorbate overlayer. Our measurements should be able to quantitatively test this prediction.

(6) Low Energy Frustrated Vibrations of c(4x2)-CO-Ni(111)

Precise information about the vibrational modes of molecules adsorbed at well characterized surfaces is essential for improving our understanding of molecular bonding at interfaces. Two primary techniques, infrared spectroscopy (IRS) and high resolution electron energy loss spectroscopy (HREELS), have been used with much success to study the *high*-frequency vibrational modes of adsorbates for many systems. In contrast, very little is known about the *low*-frequency frustrated, i.e. hindered, translation and rotation modes for adsorbed molecules. This is unfortunate since these modes play a very important role in determining the dynamical behavior of adsorbed systems. These low-frequency modes are the first to become excited upon thermal excitation. Information on the energy and amplitude of these low energy modes is important for understanding such fundamental processes as surface diffusion, thermal desorption, and the vibrational dephasing of higher lying excitations.

In our laboratory we have been using inelastic electron scattering at high incident energies (impact scattering) to spectroscopically observe such frustrated vibrations for CO/Ni(111) [31]. Bridge-bonded CO molecules have six nondegenerate normal modes: C-O internal stretch (ω_1), metal-CO stretch (ω_2), two "frustrated rotations" (ω_3 , ω_4), and two "frustrated translations" (ω_5 , ω_6). We have seen two previously undetected low energy vibrational modes for bridge-bonded CO arranged in a c(4x2) structure on Ni(111). These are the frustrated translation, ω_6 , located at 11.8 meV at $T_s=120$ K, Figure 17, and the frustrated rotation, ω_4 , located at 37.5 meV at $T_s=170$ K. In addition to these measurements we also studied the dispersion curve for the frustrated translation mode along the $\langle 11\bar{2} \rangle$ symmetry direction of Ni(111) and found it to be dispersionless, indicating that there is no significant lateral interaction between adjacent CO molecules in this structure. These measurements will be useful for improving our understanding of chemical bonding, vibrational dephasing, surface diffusion, and desorption processes for this well defined adsorption system. This work will be extended to other adsorption systems. Initial measurements on NO/Ni(111) are currently getting underway.

(7) Resonantly Enhanced Inelastic Electron Scattering: A Femtosecond Probe of Adsorbate Dynamics

We have recently begun to use resonantly enhanced inelastic electron scattering to study the dynamical properties of chemisorbed molecules. The classic review articles of George Schulz [32,33] provide a rather remarkable tutorial on the origin and characteristics of such "temporary negative ions" in the gas phase. These articles, and the work referenced therein, provide a solid framework for initiating studies of adsorbed species. One of the great hopes here is that such

studies will enable us to probe the short-time dynamics of transiently bound negative-ions on surfaces which were formed by the injection of an incident electron into a shape resonance of the molecule. Another hope is that electrons scattering by such resonant processes will be able to couple with normally forbidden spectroscopic transitions, yielding new information on the normal modes for adsorbed species.

Our initial measurements are focussing on the $c(4\times 2)$ -CO-Ni(111) system since all of the adsorbed molecules reside in a bridge-bonded configuration. CO is known to have a shape resonance around 19.5 eV in the gas phase [34], which has also been studied in physisorbed films [35,36] and for CO chemisorbed on Ni(110) [37]. We have already seen that resonant scattering couples rather strongly with two modes in particular: one of the frustrated rotations (which had not been seen before), Figure 18, and the intramolecular CO stretch [31,38]. We have studied the cross sections for these events as a function of incident electron energy and final scattering angle, Figures 19 and 20. The electron energy loss intensities of both modes were found to peak broadly around $E_i=18$ eV, presumably due to scattering into a Σ shape resonance at this energy. The intensities of these modes also increased as the final scattering angle was moved towards the surface normal, providing further confirmation of the postulated scattering mechanism. To our knowledge, these measurements are the first to demonstrate that a *molecule-surface* mode can be excited for a chemisorbed system due to resonant scattering.

Such measurements hold the promise, in favorable cases, of becoming useful for examining the femtosecond dynamics of chemisorbed systems. Wavepacket arguments suggest that by observing which *molecule-surface* vibrational modes become excited following transient negative ion formation we can obtain useful information about the femtosecond dynamics for chemisorbed systems [39]. The scheme, shown schematically in Figure 21, is as follows:

- (1) Inject incident electron under resonant conditions to form the transiently bound negative ion. Probability of injection depends upon electron energy and incident angle.
- (2) Nuclear coordinates evolve on the negative ion potential energy surface for femtosecond timescales for transiently bound shape resonances.
- (3) Ejected electron is energy analyzed, as a function of final scattering angle, to examine excitation in both the intramolecular and molecule-surface vibrational degrees of freedom on the ground state potential energy surface. The presence (or absence) of vibrational excitation is a

given coordinate gives a snapshot of short timescale nuclear coordinate evolution for the system in the excited state.

Our observation of a frustrated rotation seems to imply that the molecule starts to bend over in the negative ion state, possibly due to attraction of its image. One should note that our observations are the complement to electron induced desorption experiments which proceed via stimulated adsorbate rotation [40]. They also add new supporting information for surface photochemistry experiments which, in many instances, actually proceed via electron attachment

During the coming year we hope to complete our analysis of CO/Ni and move on to other systems which exhibit resonant scattering. One of the main goals will be to find systems which live long enough to reveal truncated overtone progressions with respect to gas phase behavior. Such overtone progressions will be able to serve as clocks for the excited state lifetimes when combined with wavepacket calculations [39], Figure 22. Preliminary searches in our laboratory have found just the first overtone for the CO stretch, implying an exceedingly short existence for the negative ion in this instance. Recent theoretical work suggests that longer lived excited states should indeed exist and be experimentally accessible [41].

(8) Instrumentation Development

During the past year we completed the construction of our new neutral particle beamline and have recently connected it to our electron scattering apparatus for conducting so-called beam-EELS experiments. The intensity of the room temperature supersonic beams that have been generated to date have exceeded our design goal of 10^{18} molecules/sr/sec. This new combined instrument gives us the capability to monitor the nascent reaction intermediates that form upon molecular adsorption (via in situ vibrational spectroscopy). Film growth experiments with, for example, organometallic reagents are also anticipated. Parameters under our control will include both the kinetic and internal energy of the incident molecules. This beam-EELS combination will allow us to expand our studies of surface oxidation to include highly energetic oxidants. We would especially like to construct an atomic oxygen beam source [42] for studies involving excited oxidants, such as O^3F , O^1D , and $O_2(^1\Delta)$.

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V. Figure Captions and Figures

Figure 1. Schematic diagram of the high resolution neutral particle scattering apparatus.

Figure 2. Schematic diagrams of the combined molecular beam/electron scattering instrument. Upper Panel: Top view of the HREELS scattering plane. Lower Panel: Side view of the new differentially pumped molecular beam line attached to the electron scattering spectrometer.

Figure 3. Top: Diffraction scan for $\text{Cu}_3\text{Au}(001)$ along the $\langle 100 \rangle$ ($\bar{\Gamma}-\bar{M}$) direction. The open circles are the diffraction data and the solid line is a simulation of the diffraction scan taking into consideration the instrument function. Bottom: Angular profiles of the superlattice peak versus crystal temperature. The superlattice peak disappears with increasing temperature.

Figure 4. Inelastic HAS data taken on the $\text{Cu}_3\text{Au}(001)$ surface. a). A series of time-of-flight (TOF) spectra taken with fixed incident kinematics. The (+)'s are the experimental data and the solid lines are fits to the data. b). Energy transformed TOF data from (a). c). The solid lines are scan curves for the initial and final scattering conditions: $\theta_i=31.8^\circ$, $E_i=30.8$ meV, and $\theta_f=39.0^\circ$, 40.0° , 41.0° , 42.0° , and 43.0° . The elastic flight time occurs at 902 μsec for these spectra. The dashed line is representative of the Rayleigh wave dispersion, and is a sinusoid scaled in energy to 7.1 meV.

Figure 5: Slab Calculations as outlined in the text. a). Model using $\phi_{j,s}'$ and the unmodified $\phi_{j,b}''$. b). Same as (a) except $\phi_{2,s}''$ has been stiffened by 20%. The open circles are the data folded onto the first surface Brillouin zone. The dashed lines represent the continuum of the bulk modes.

Figure 6. Temperature dependent inelastic helium scattering data for $\text{Cu}_3\text{Au}(001)$ taken below, near, and above T_c . These spectra show that single phonon scattering peaks can be seen for metallic superalloys even at temperatures above their critical temperatures.

Figure 7. Helium diffraction lineshapes for the $\text{Cu}_3\text{Au}(001)$ superlattice peak which show that the surface has essentially ordered after only two minutes (!) following a temperature quench from above T_c , much more rapidly than has been reported for the bulk, which may take on the order of an hour or more to order.

Figure 8. Top: Superlattice peak linewidths which show that the surface quality (domain size) actually improves as the temperature is raised near T_c for some parts of the target crystal. Lower Panel: Plateaus (or even small bumps) in the surface order vs. T_s plots near 650 K, such as shown here, suggest that grain boundaries, or other surface defects, may relax prior to reaching the bulk critical temperature, $T_c = 664$ K.

Figure 9. Schematic view of Ni(977).

Figure 10. Upper Panel: He diffraction from clean Ni(977). Lower Panel: He diffraction from partially oxidized Ni(977). Note the extra peak in the lower panel, a clear signature for step and terrace doubling.

Figure 11. Comparison of experimental and calculated helium diffraction runs, as a function of incident beam energy (so-called drift spectra) which definitively show that the presence of oxygen

on Ni(977) at elevated temperatures leads to step and terrace doubling. The agreement between theory and experiment is excellent.

Figure 12. Molecular dynamics calculation for a stepped LJ(775) surface which shows the existence of two new surface phonon modes which are localized near the step edge. Scattering experiments are underway to study these new E_1 and E_2 phonon modes. Such studies will improve our understanding of how surface forces are modified in the vicinity of a step.

Figure 13. Temperature dependent phonon lineshapes calculated from molecular dynamics simulations of various Lennard-Jones surfaces. Note the quadratic rise in phonon linewidth for the (110) surface at the X-point, which is indicative of anharmonicity in the surface forcefield.

Figure 14. Surface phonon dispersion for Ni(111) along the $\bar{\Gamma}$ $\bar{M}$ direction. The uncertainty of the data is typically $\Delta E = \pm 0.3$ meV and $\Delta \zeta = \pm 0.01$. Long-dashed lines are the lattice dynamics results for S_1 and S_2 using as input the bulk force constant whereas the short-dashed lines are for 11% intraplanar softening and 1.6 N/m tensile surface stress. Solid lines with cross-hatching indicate the boundaries of the bulk phonon bands. At $\bar{M}$, the values of S_1 , S_2 , and R_1 are 17.2 meV, 32.2 meV, and 23.1 (± 0.6) meV, respectively.

Figure 15. Experimental spectra and quantum scattering calculations for kinematic conditions which optimized sensitivity to (a) S_1 (Rayleigh wave), (b) S_2 (gap mode), and (c) R_1 (resonance due to second layer transverse displacements). The dashed line in each panel represents the estimated multiphonon contribution. Surface force constant model: 11% intraplanar softening and 1.6 N/m tensile surface stress.

Figure 16. Effective medium electronic structure calculations of P. Ditlevsen for Ni(111) which are in excellent agreement with our scattering experiments (solid points). First layer transverse signal is due to the Rayleigh wave, first layer longitudinal signal is due to the gap mode, while the signal appearing near the zone edge (embedded in the bulk density of states) is a "surface resonance" which has its origin in second layer transverse displacements.

Figure 17. Typical electron energy loss spectrum of c(4x2)-CO-Ni(111) with impact energy $E_i=190$ eV. Inset figure shows the geometric displacements for the frustrated translation of bridge-bonded CO where molecular motion is perpendicular to the Ni-Ni bonding axis. The spectrum was collected along the $\langle 11\bar{2} \rangle$ direction of Ni(111) with $\Theta_i=60^\circ$ and $\Theta_f=33^\circ$, and an accumulation time of 30 sec/chan. The weak feature near 50 meV may be due to impact scattering

excitation of the C-Ni stretch. The solid line is a nonlinear least squares fit to the data which used Gaussian fitting functions.

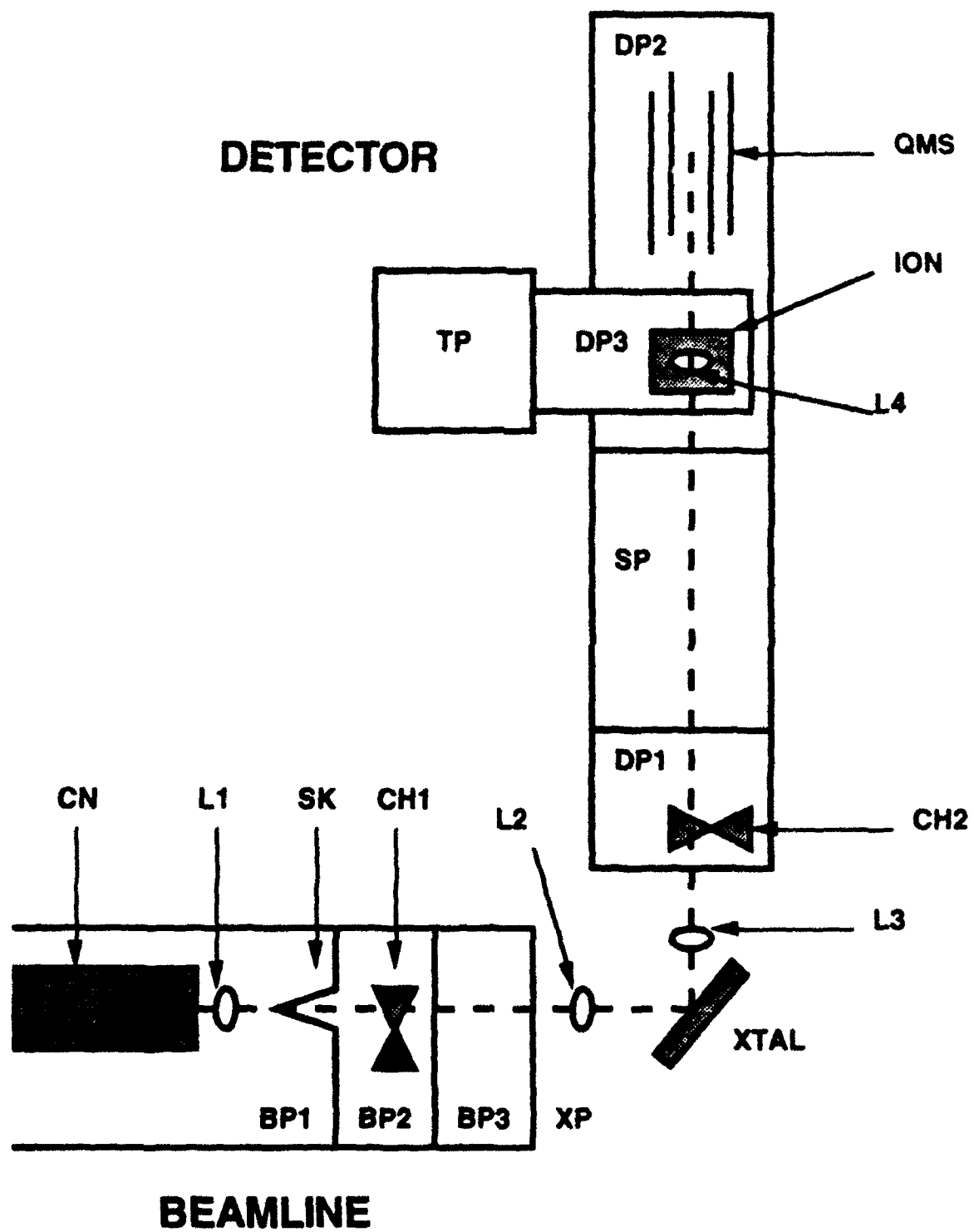
Figure 18. Resonance enhancement of the inelastic electron scattering cross-section for bridge-bonded CO/Ni(111). Note that there is a Σ -shape resonance for chemisorbed CO at approximately 18 eV, corresponding to the maximum frustrated rotation peak intensity in this figure. The observation of this frustrated rotation implies that the geometry of the CO/Ni(111) system must change during the femtosecond scale lifetime of the excited state in such a way as to lead to slight rotation of the molecule on the surface.

Figure 19. Energy dependence of shape resonance scattering leading to excitation of CO stretch and CO frustrated rotation modes.

Figure 20. Angle dependence of the emitted electron following injection into the CO Σ -shape resonance at $E_i = 18$ eV. The angular distributions for electrons coupling to either the CO stretch or CO frustrated rotation peak along the CO axis, i.e., normal to the surface.

Figure 21. Schematic view of the resonantly enhanced scattering process.

Figure 22. Schematic wavepacket diagram for transient negative ion scattering which illustrates femtosecond timescale propagation on the excited potential energy surface. The resulting overtone progression on the ground state contains information on the negative ion lifetime. For simplicity, not all Franck-Condon allowed transitions are shown.



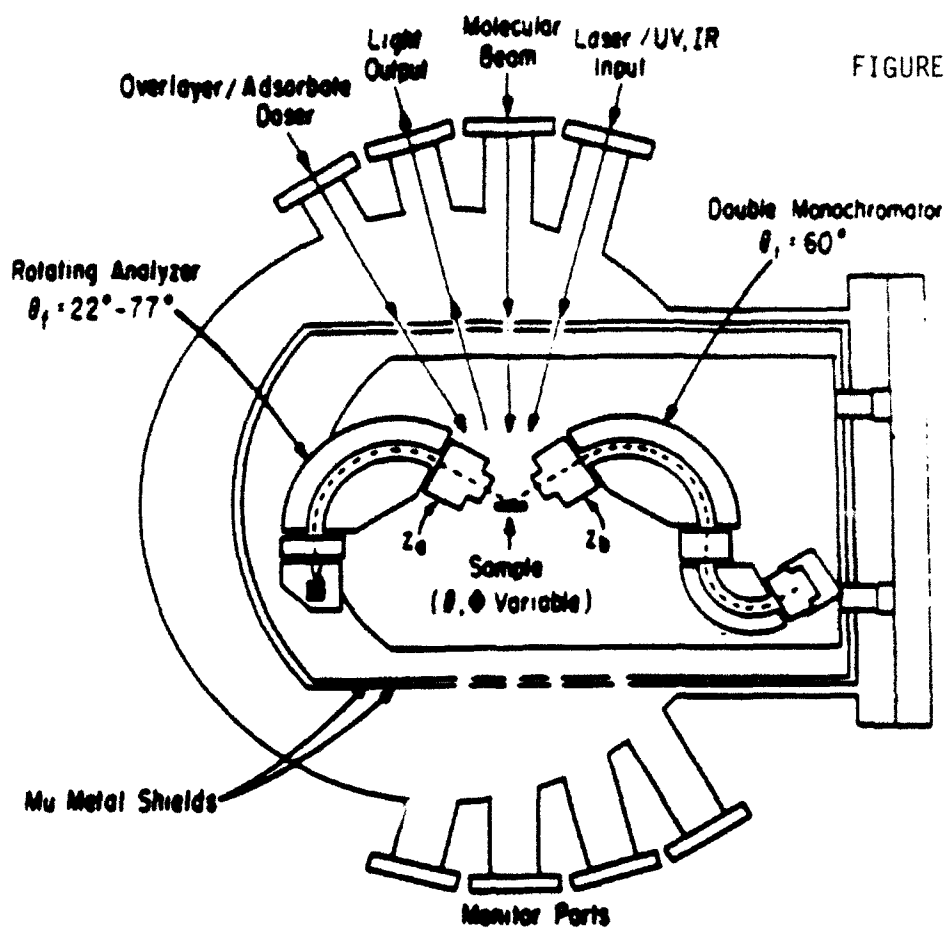
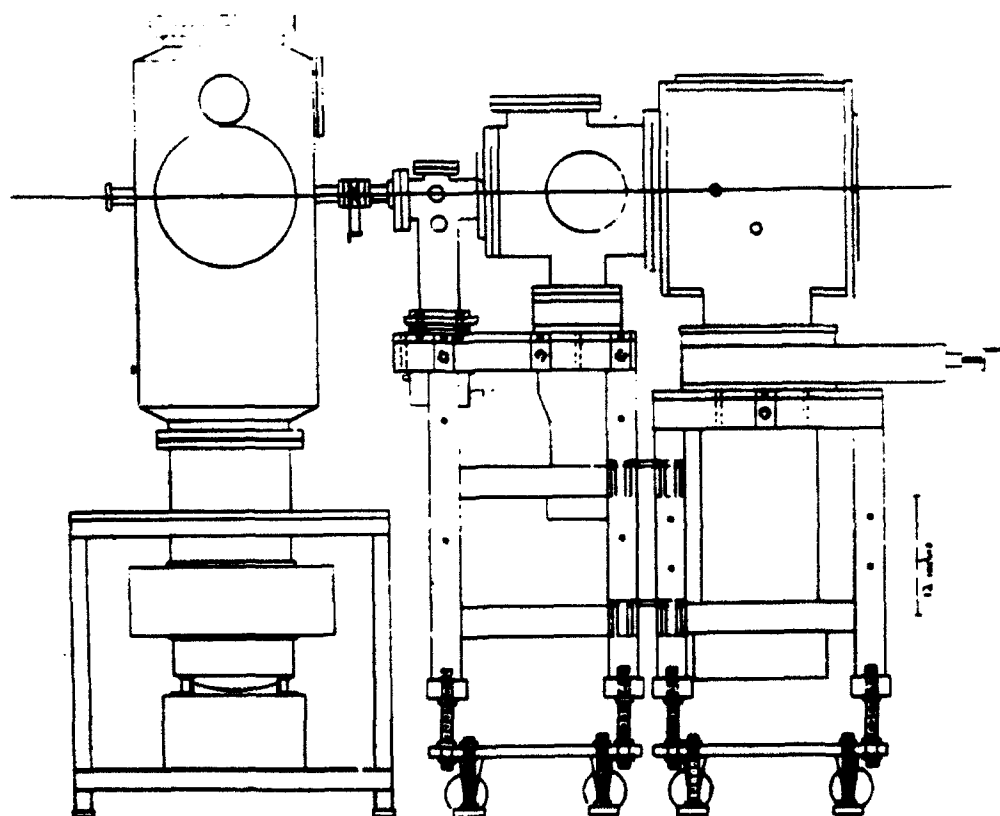
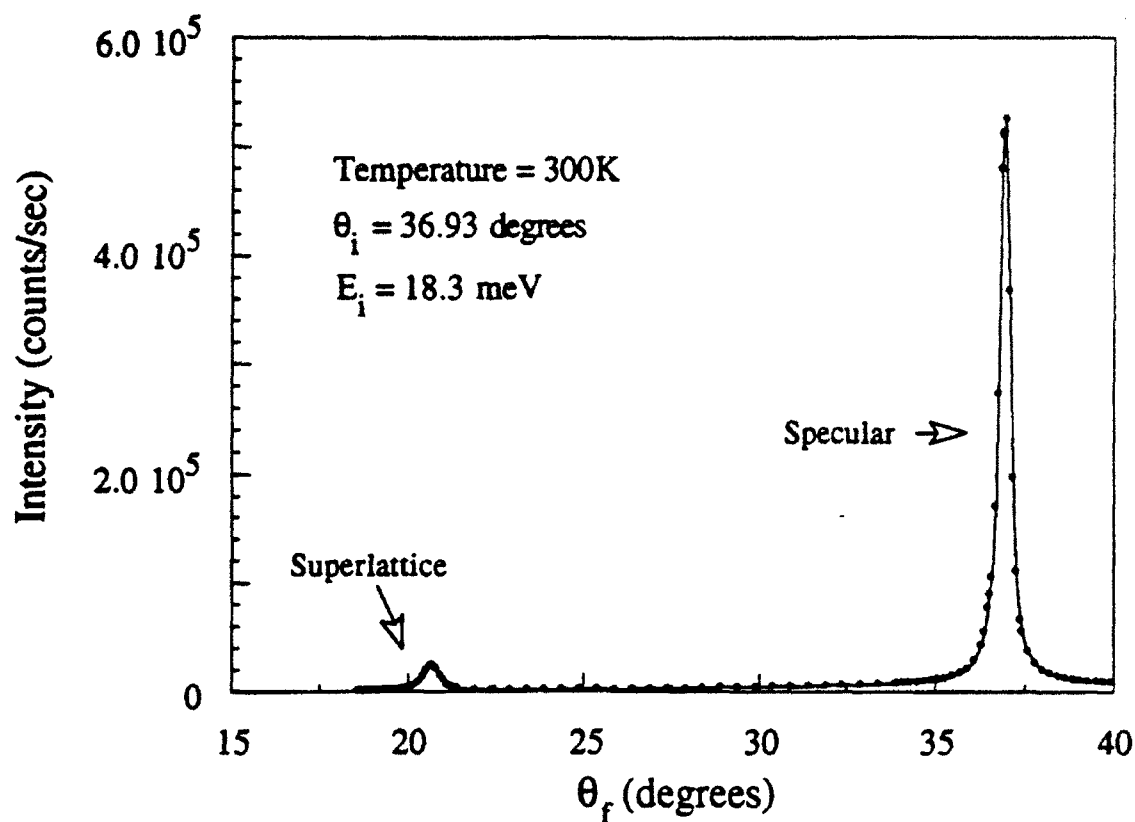
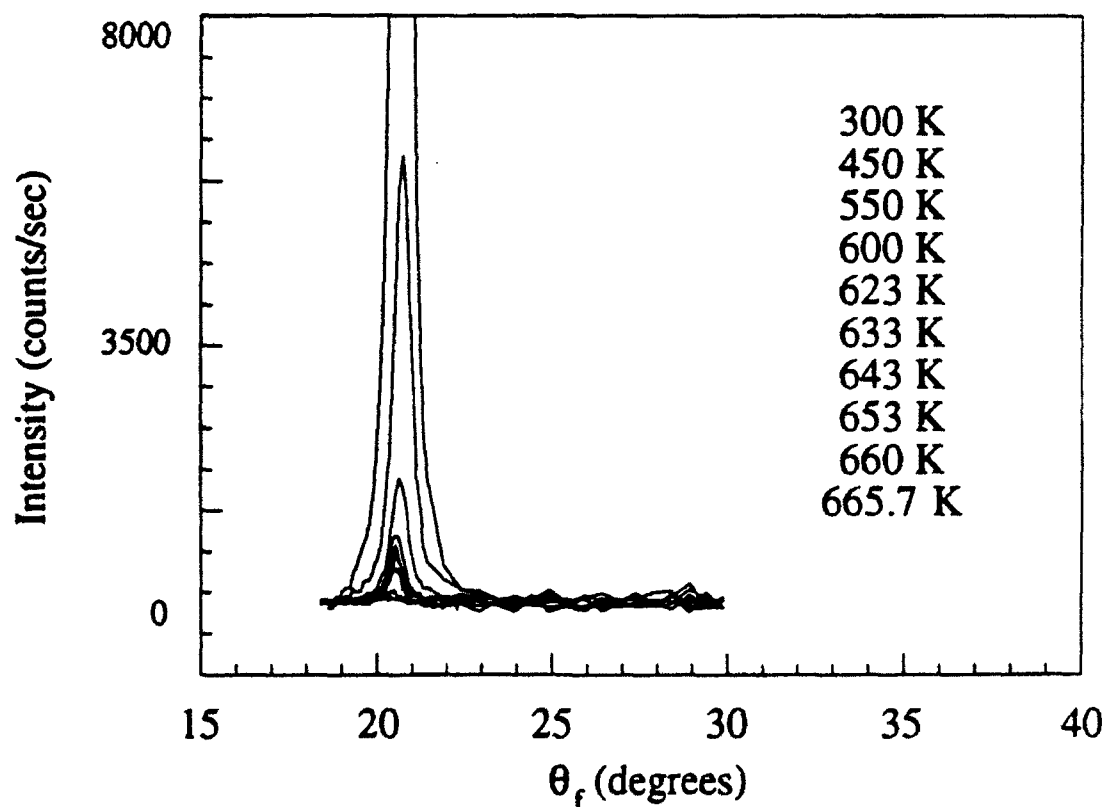
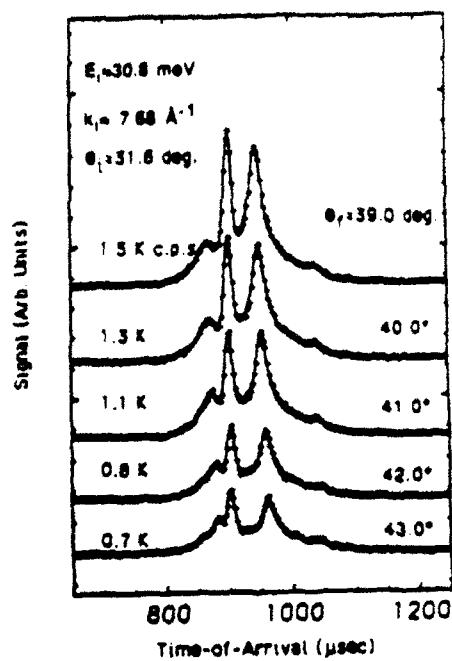


FIGURE 2

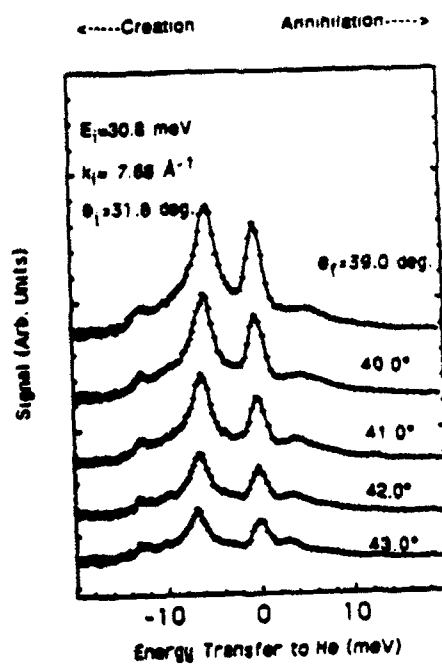


 Cu_3Au (001) Attenuation of Superlattice Peak with Temperature

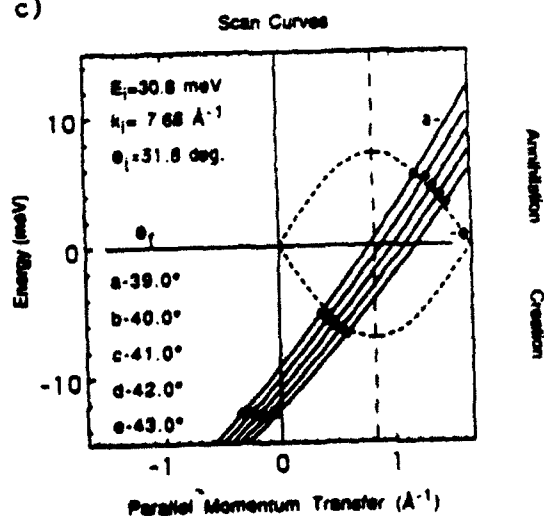
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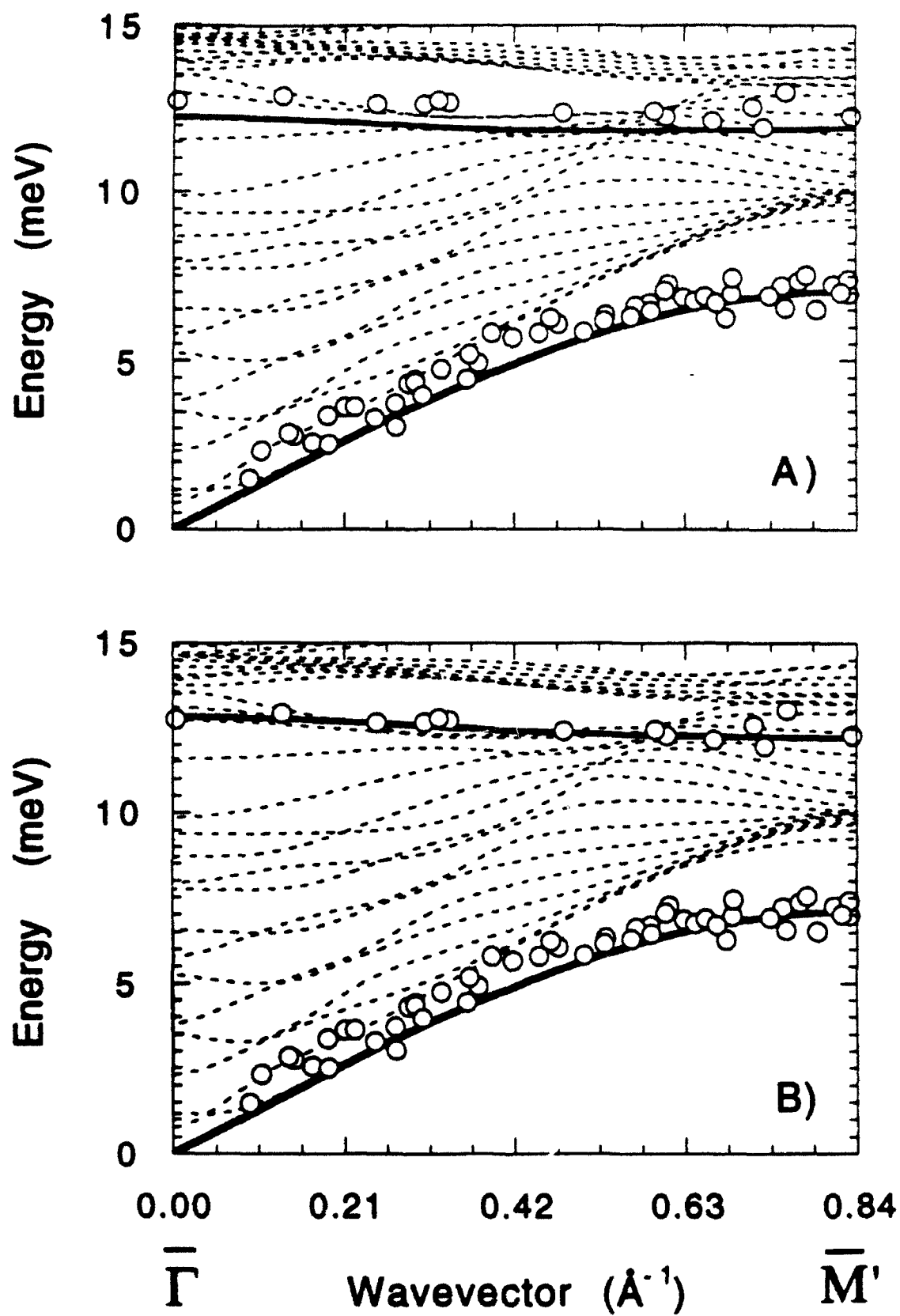


b)



c)





Temperature Dependence of Cu_3Au Surface Phonons Through Tc

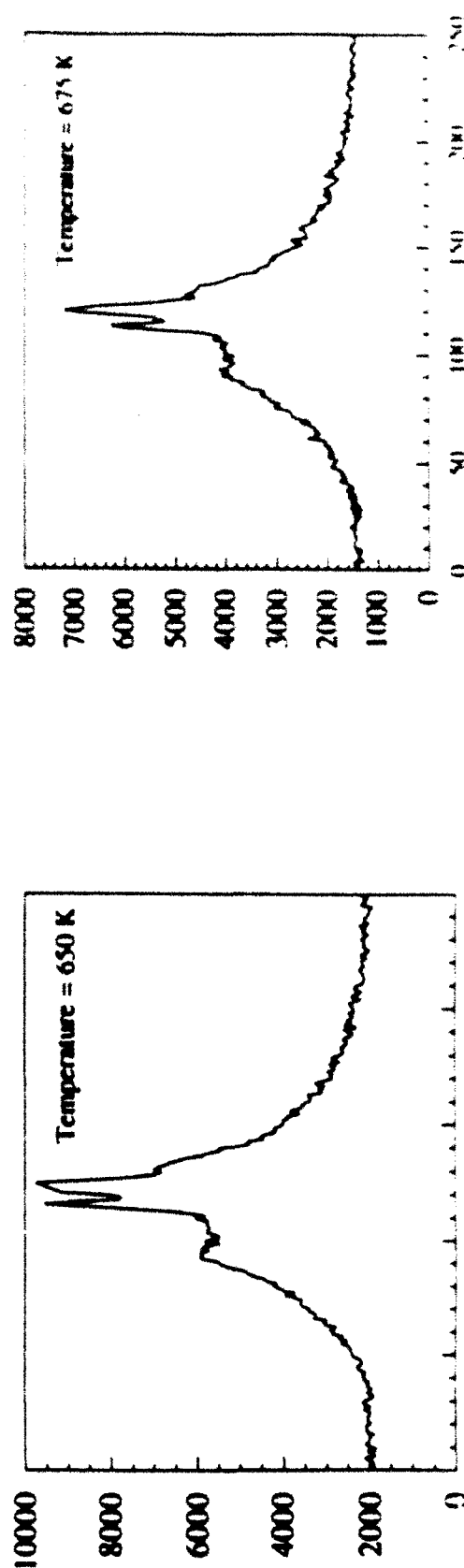
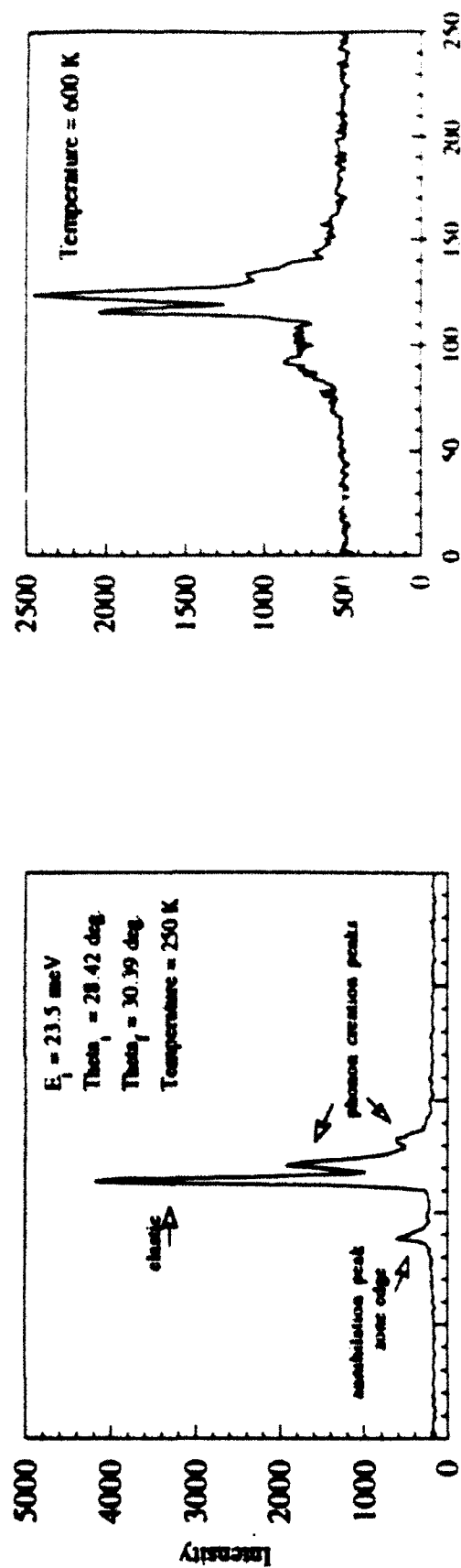
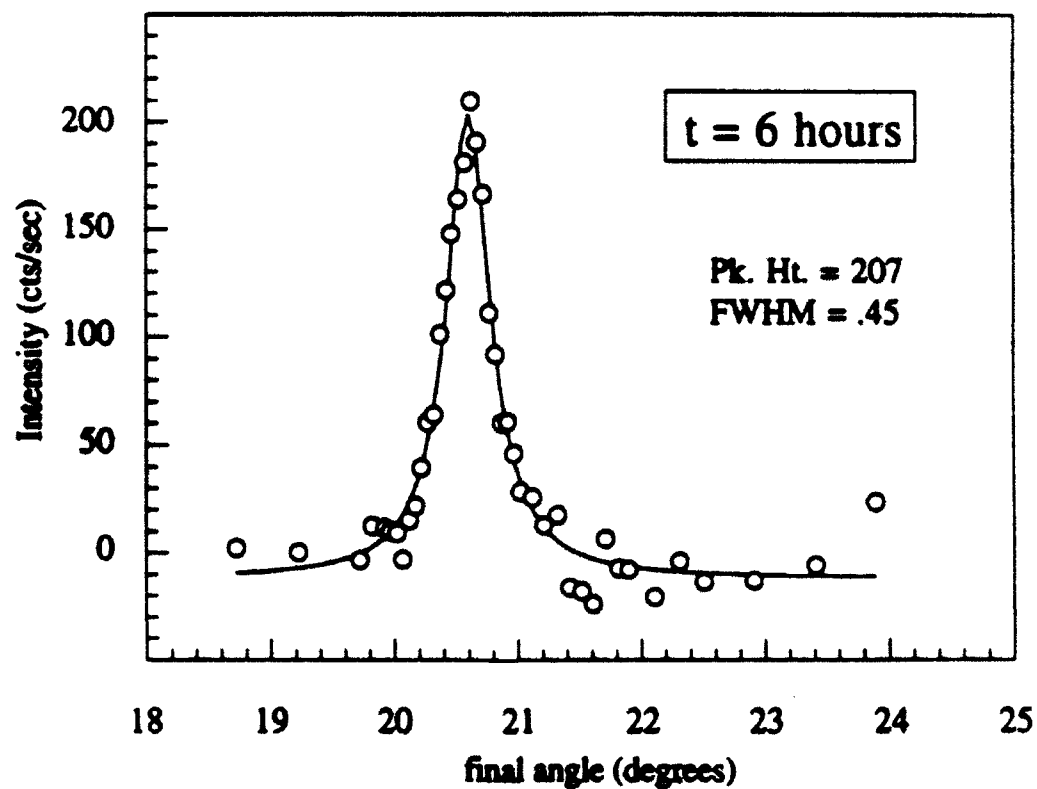
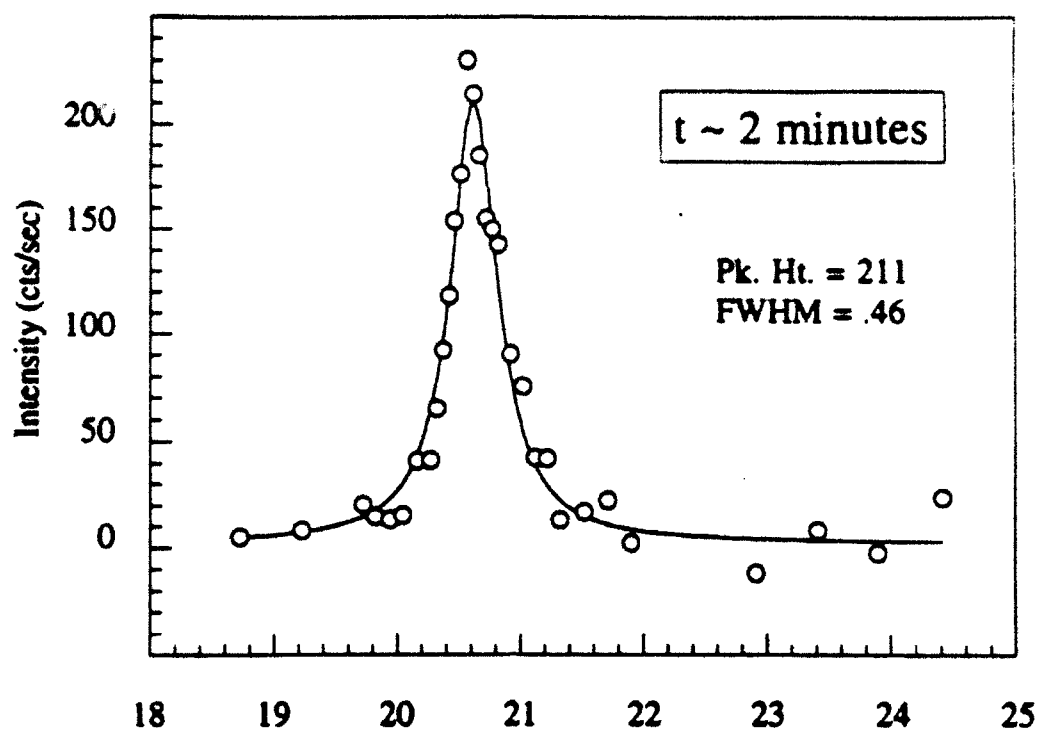


FIGURE 6

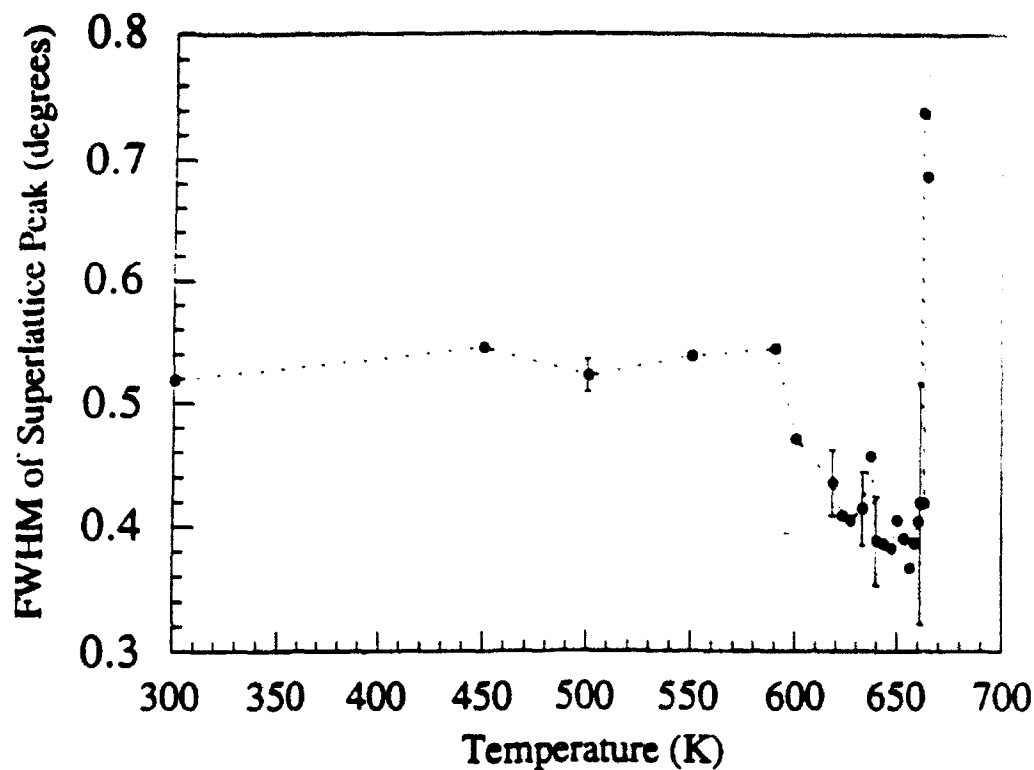
Cu₃Au(001) Superlattice Peak
Quench from 720K to 660K (T_c-5K)



Width of Cu_3Au Superlattice Peak vs Temperature

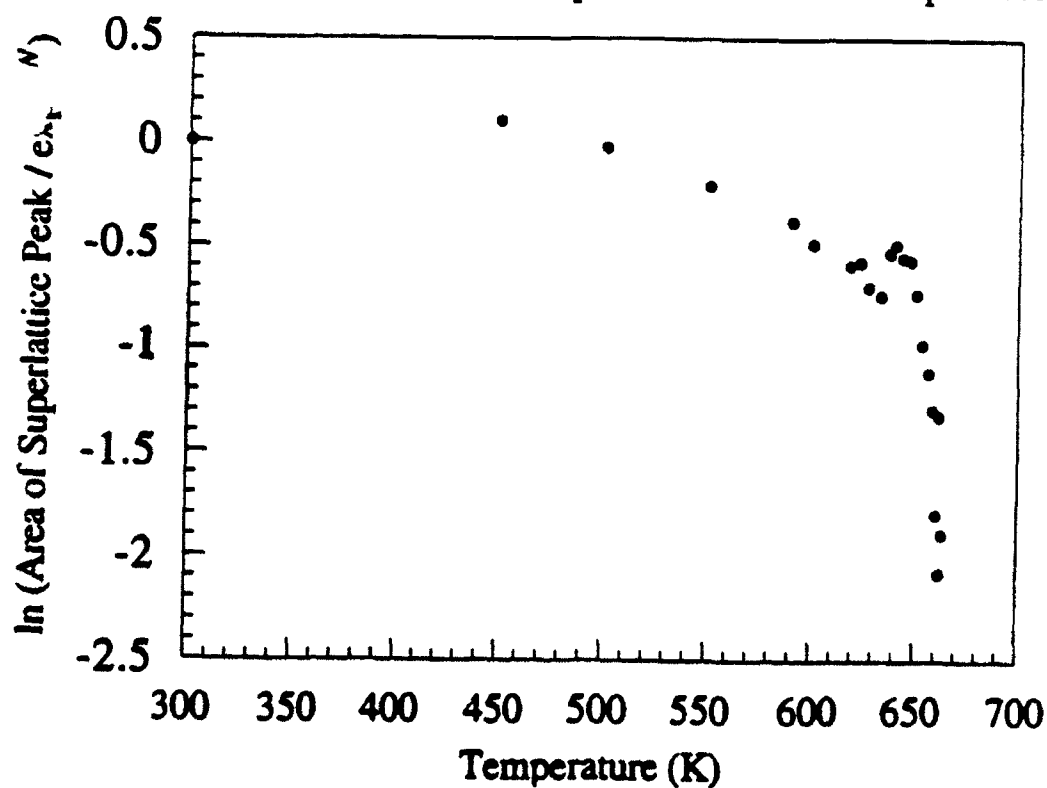
FIGURE 8

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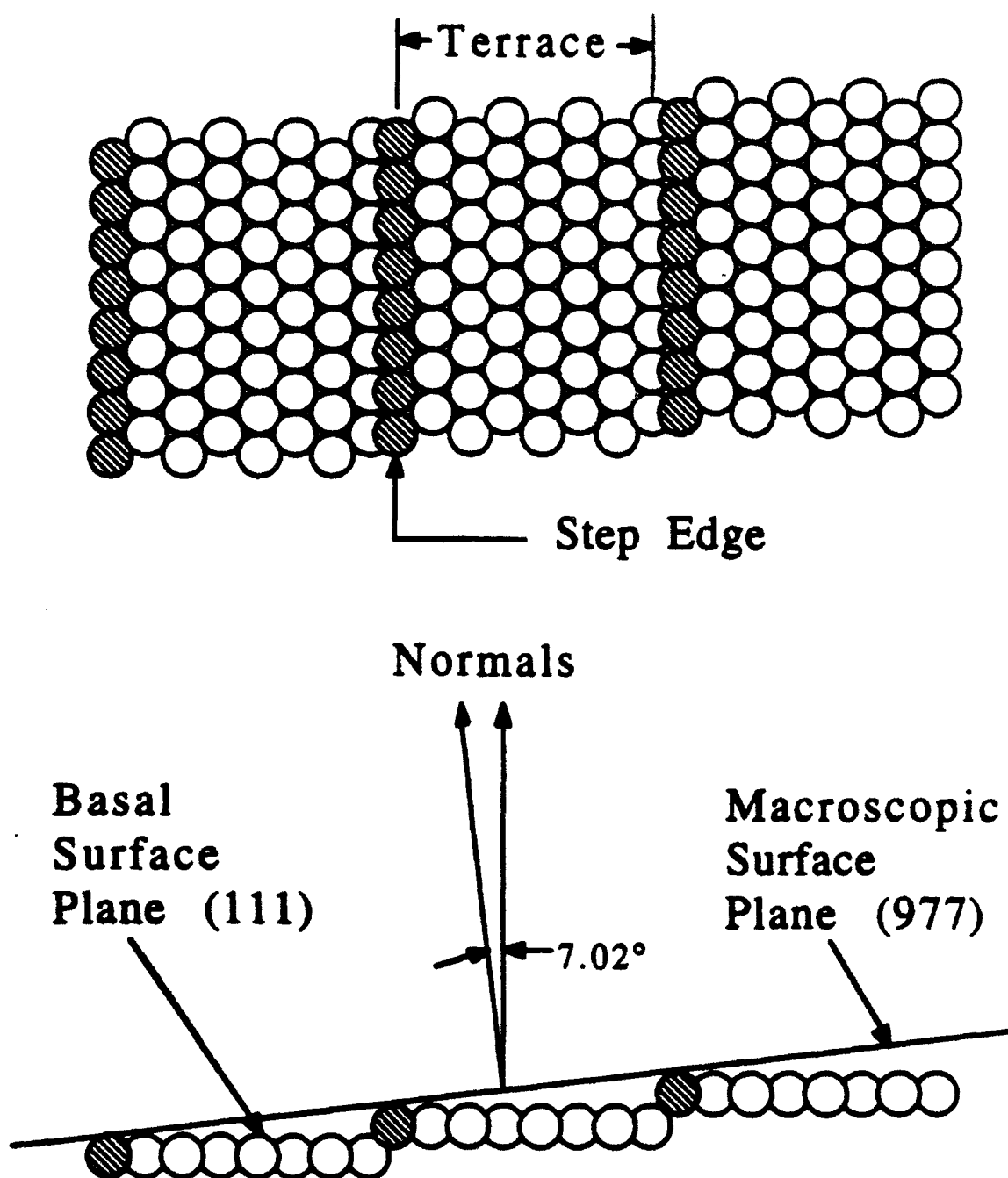


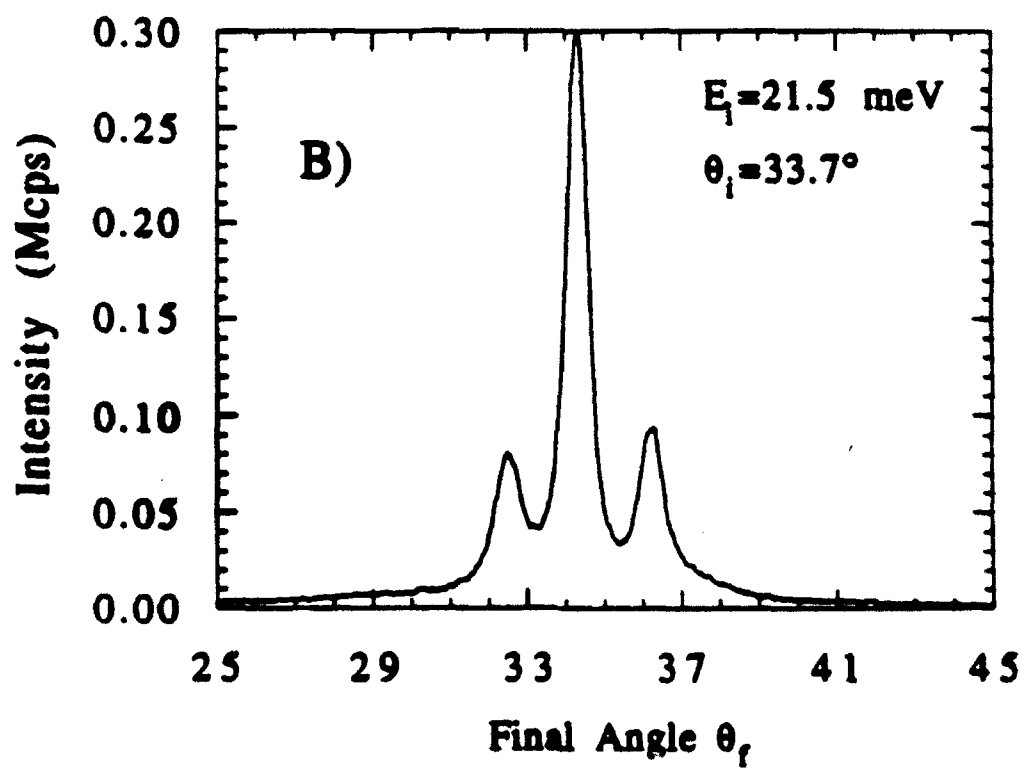
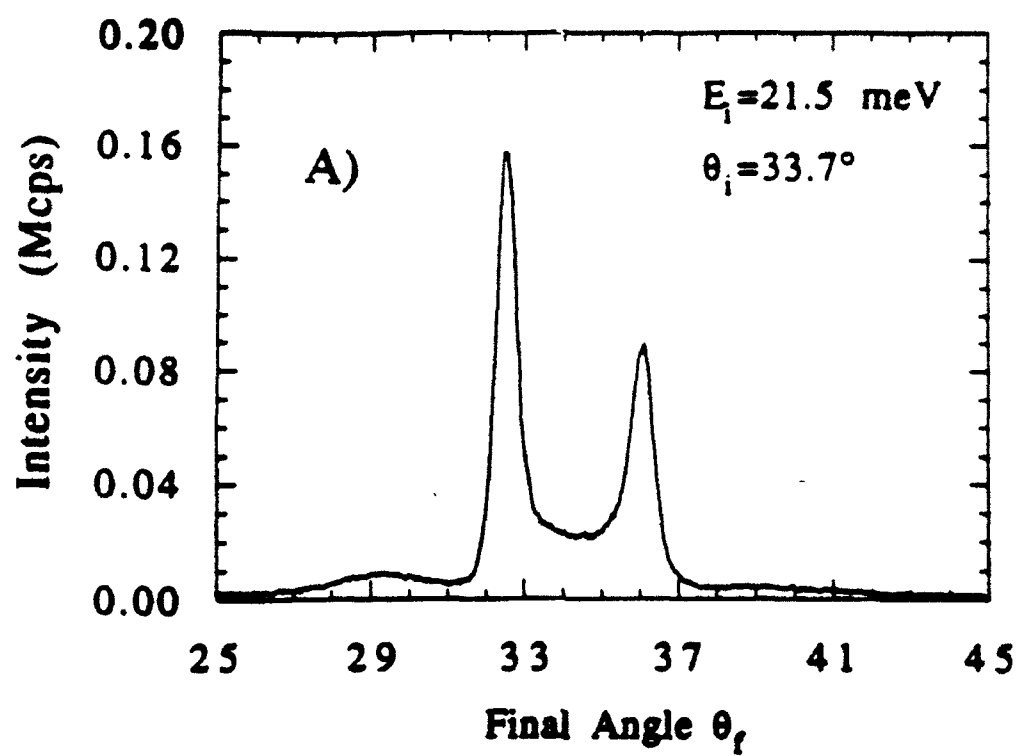
Cu_3Au (001)

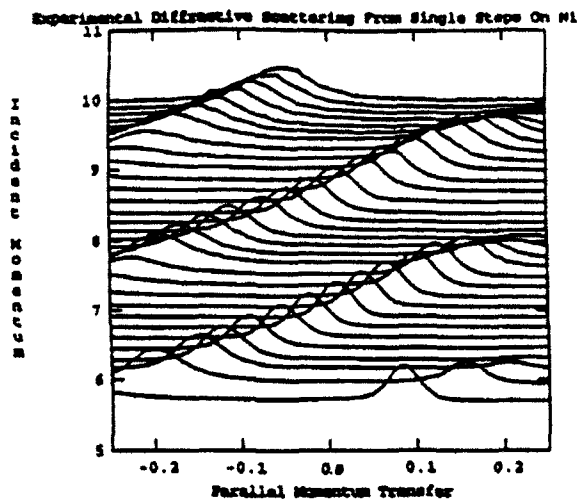
Debye-Waller Corrected Superlattice Peak vs Temperature



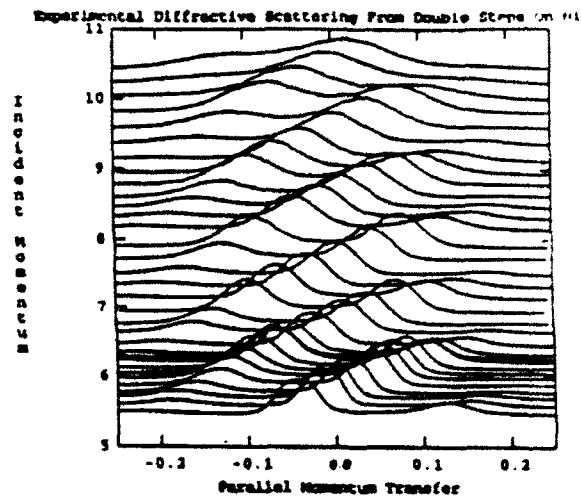
Ni(977)



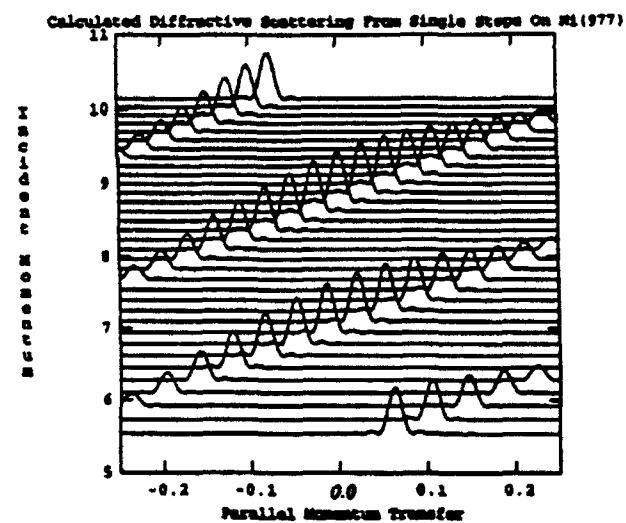




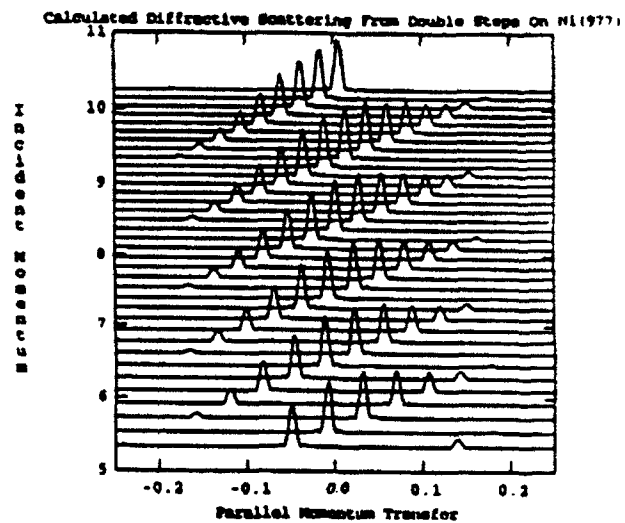
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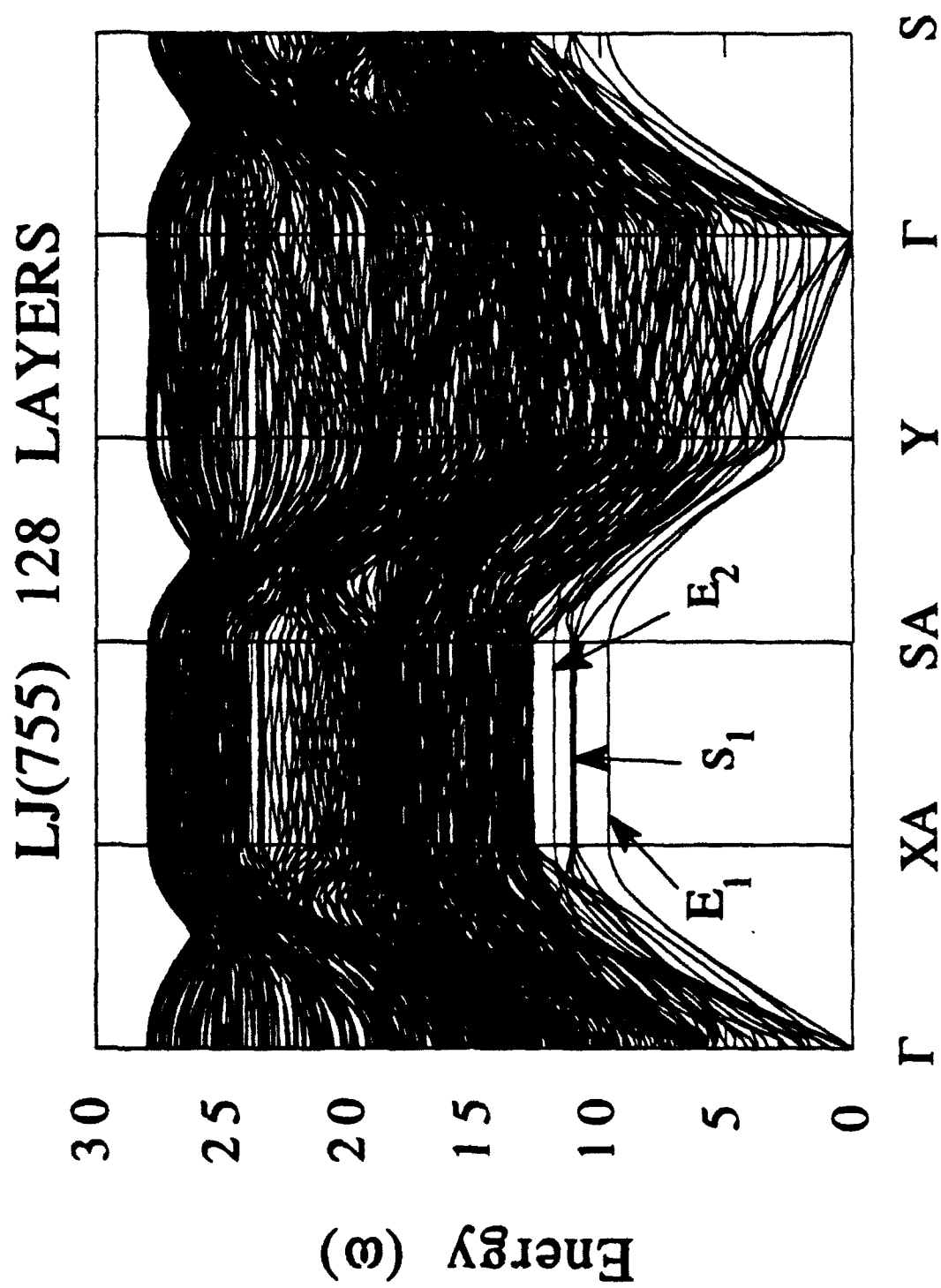
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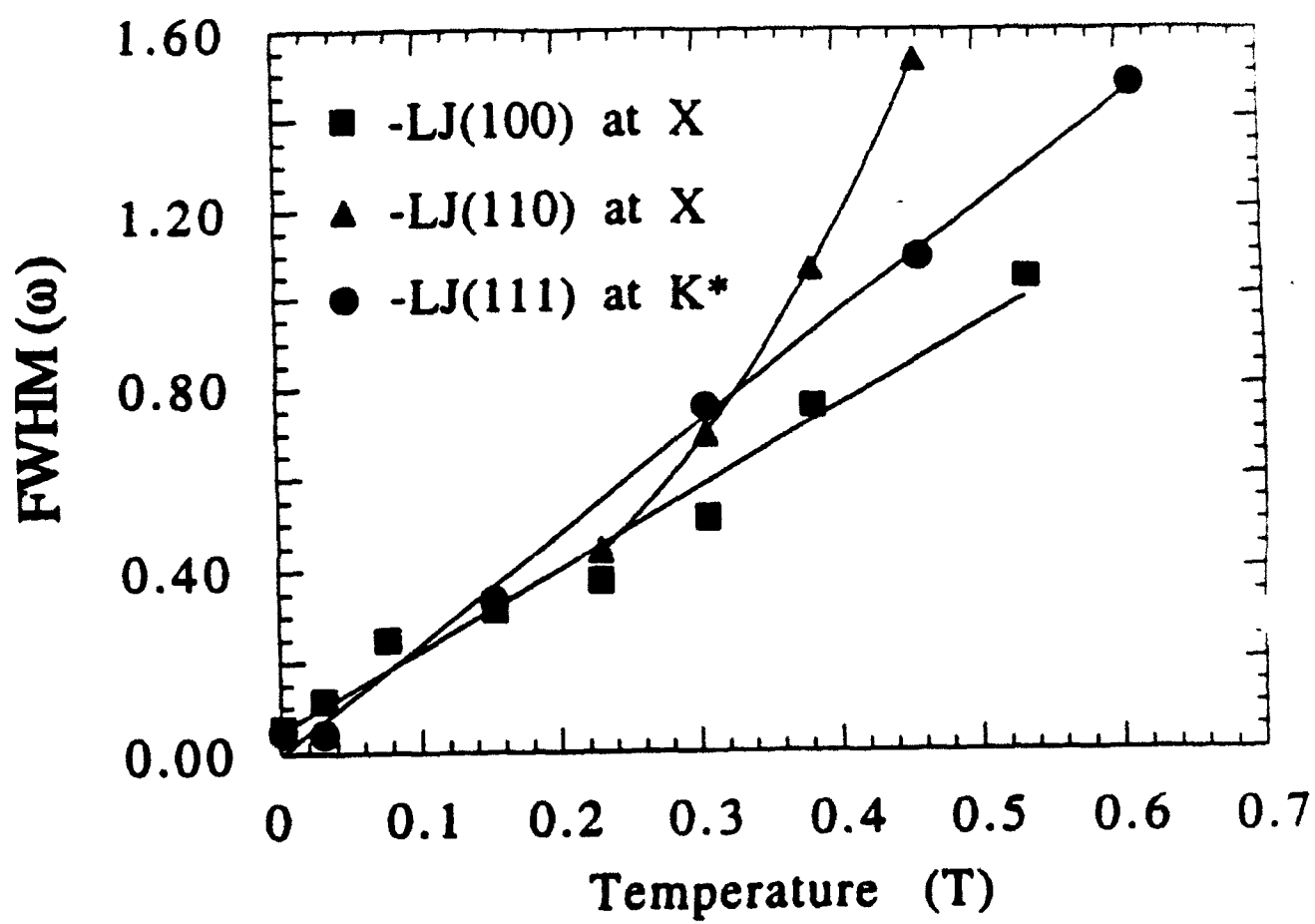


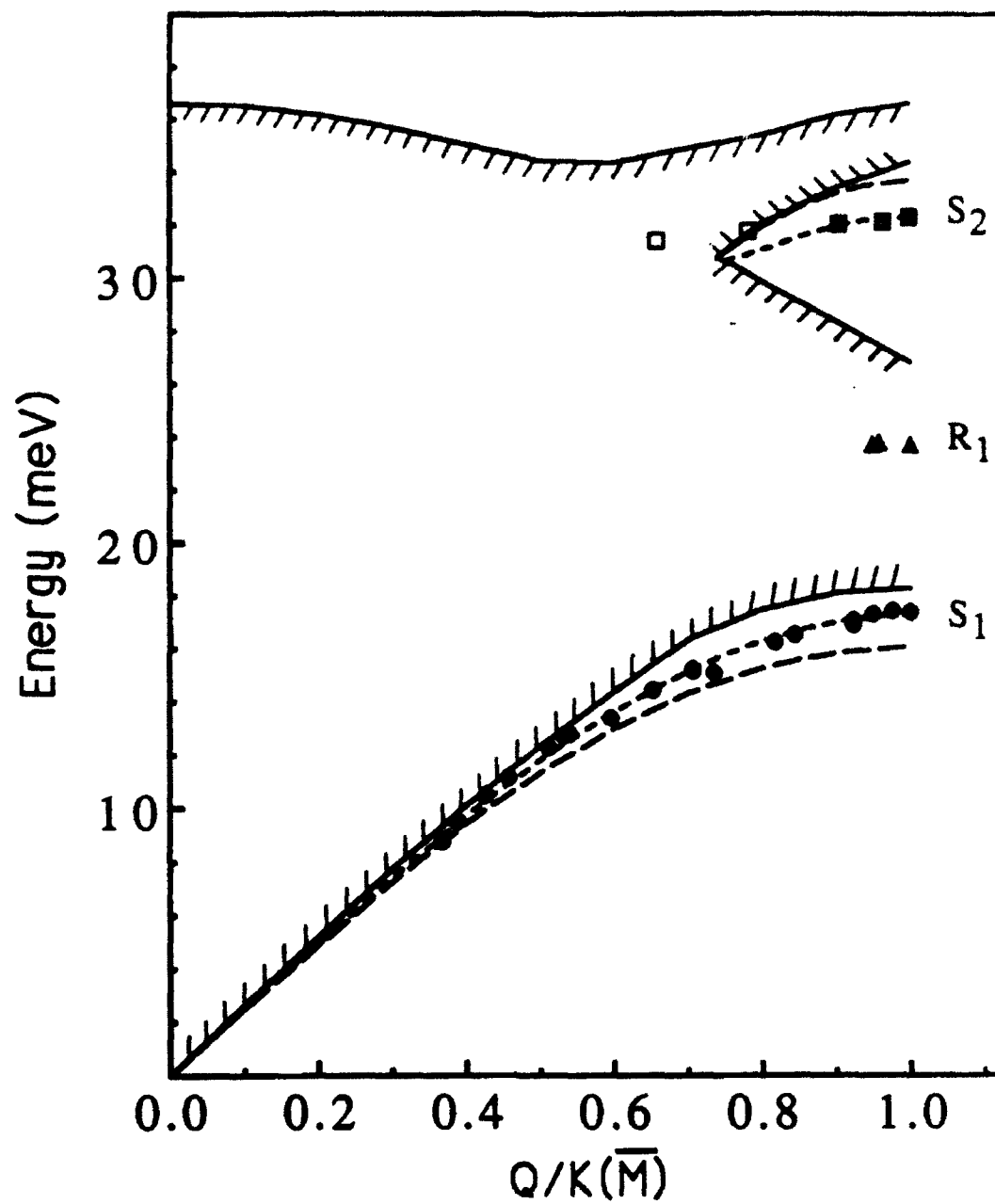
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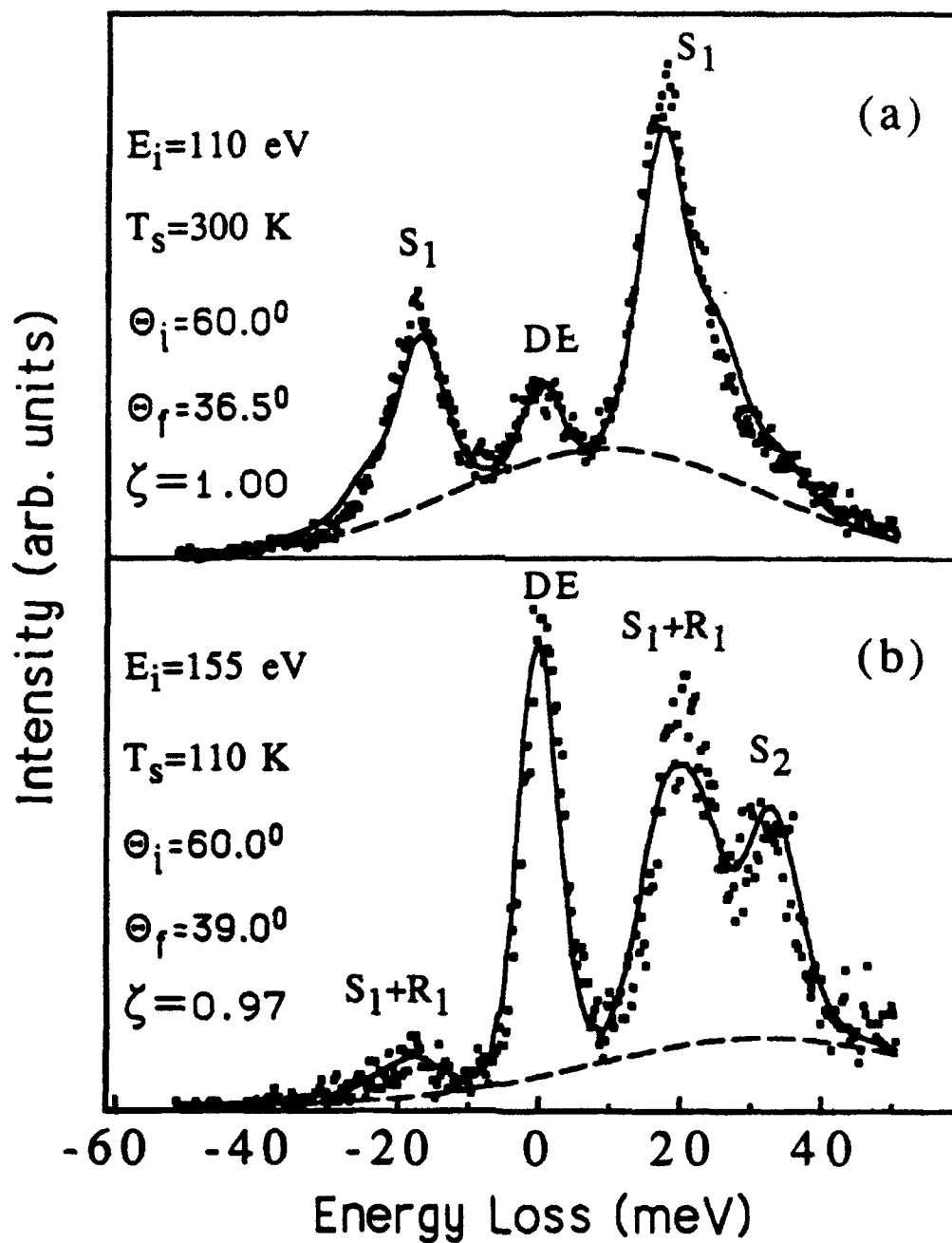


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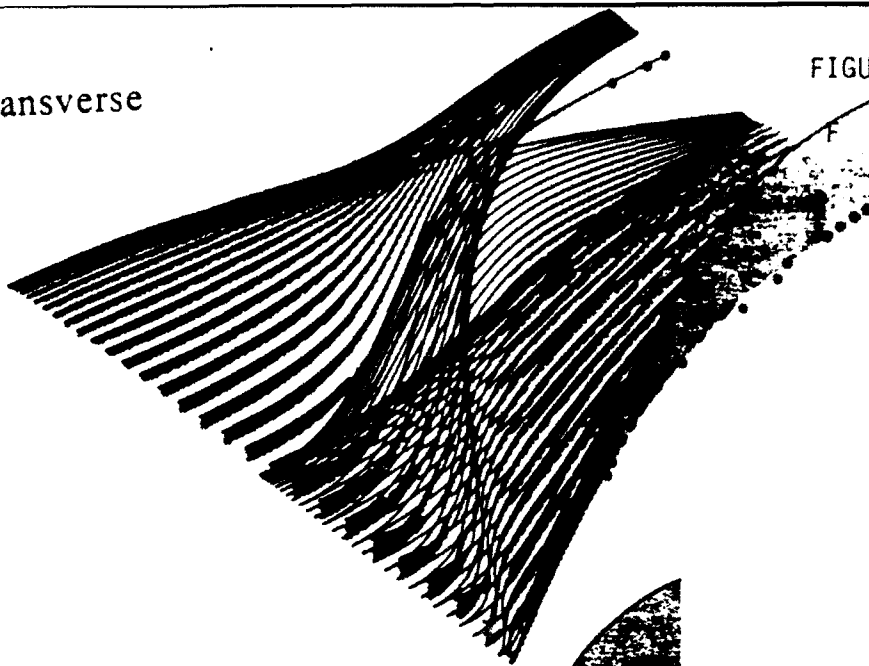




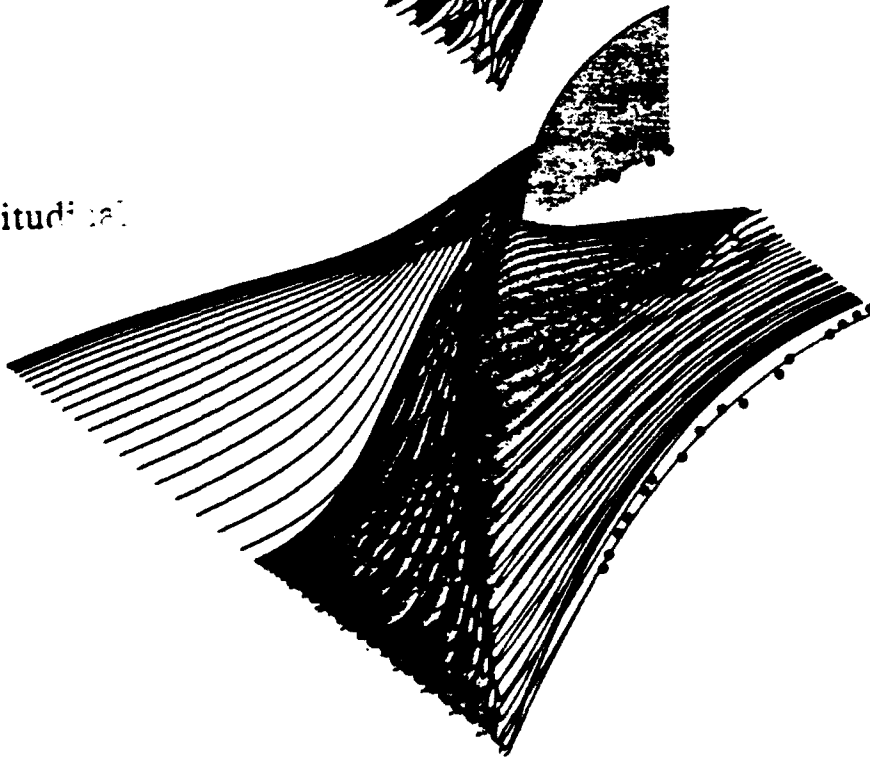




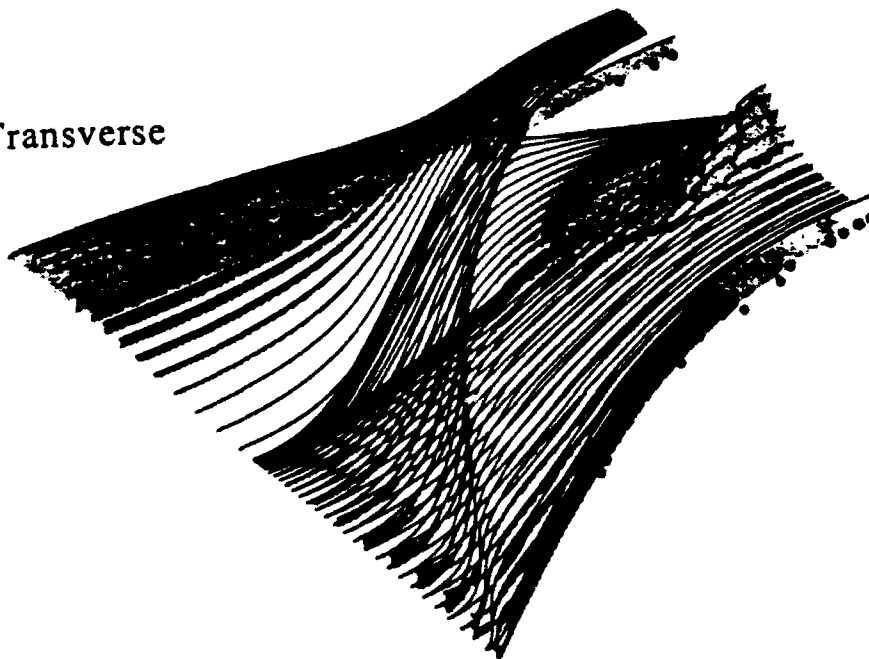
1st Layer Transverse

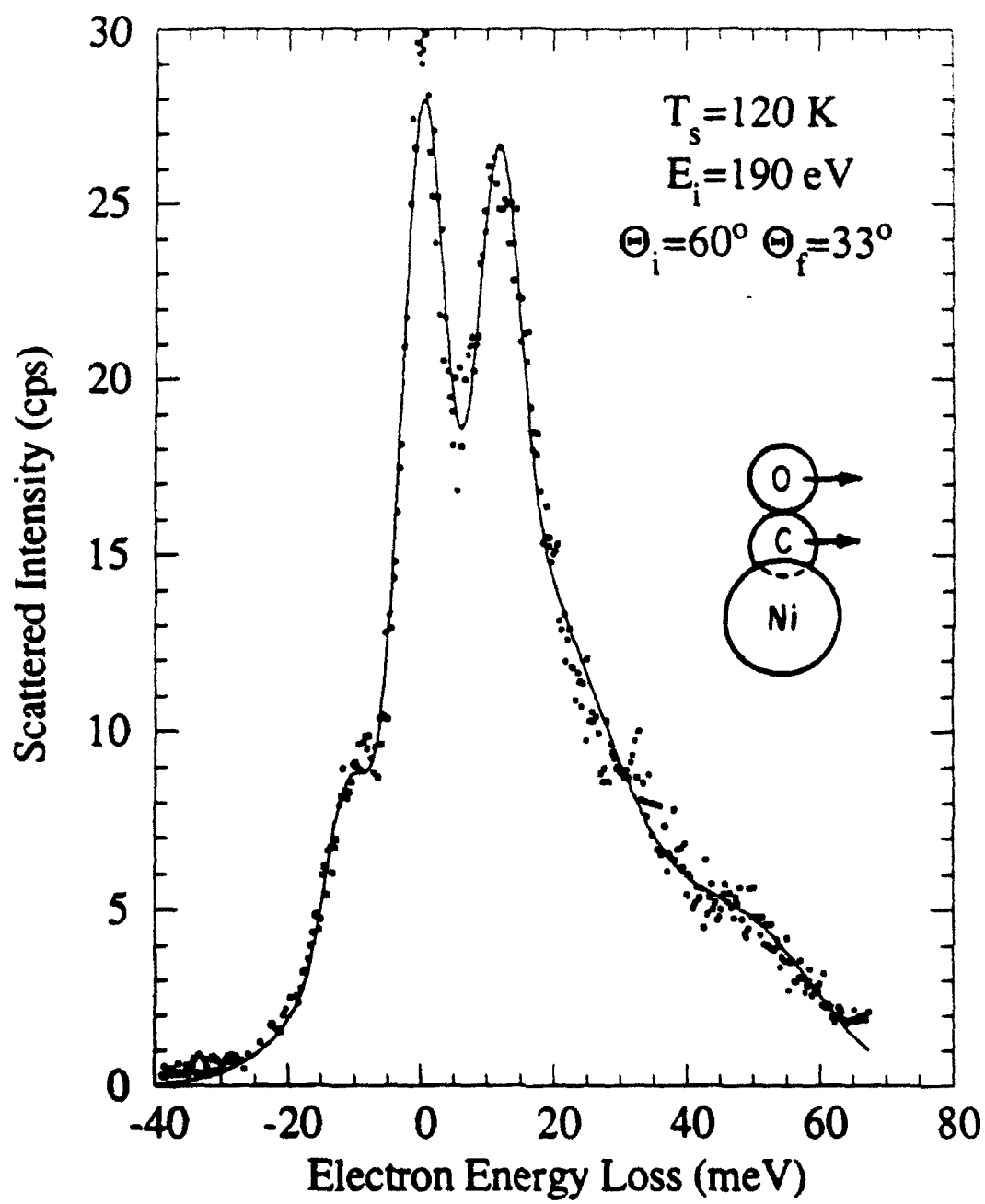


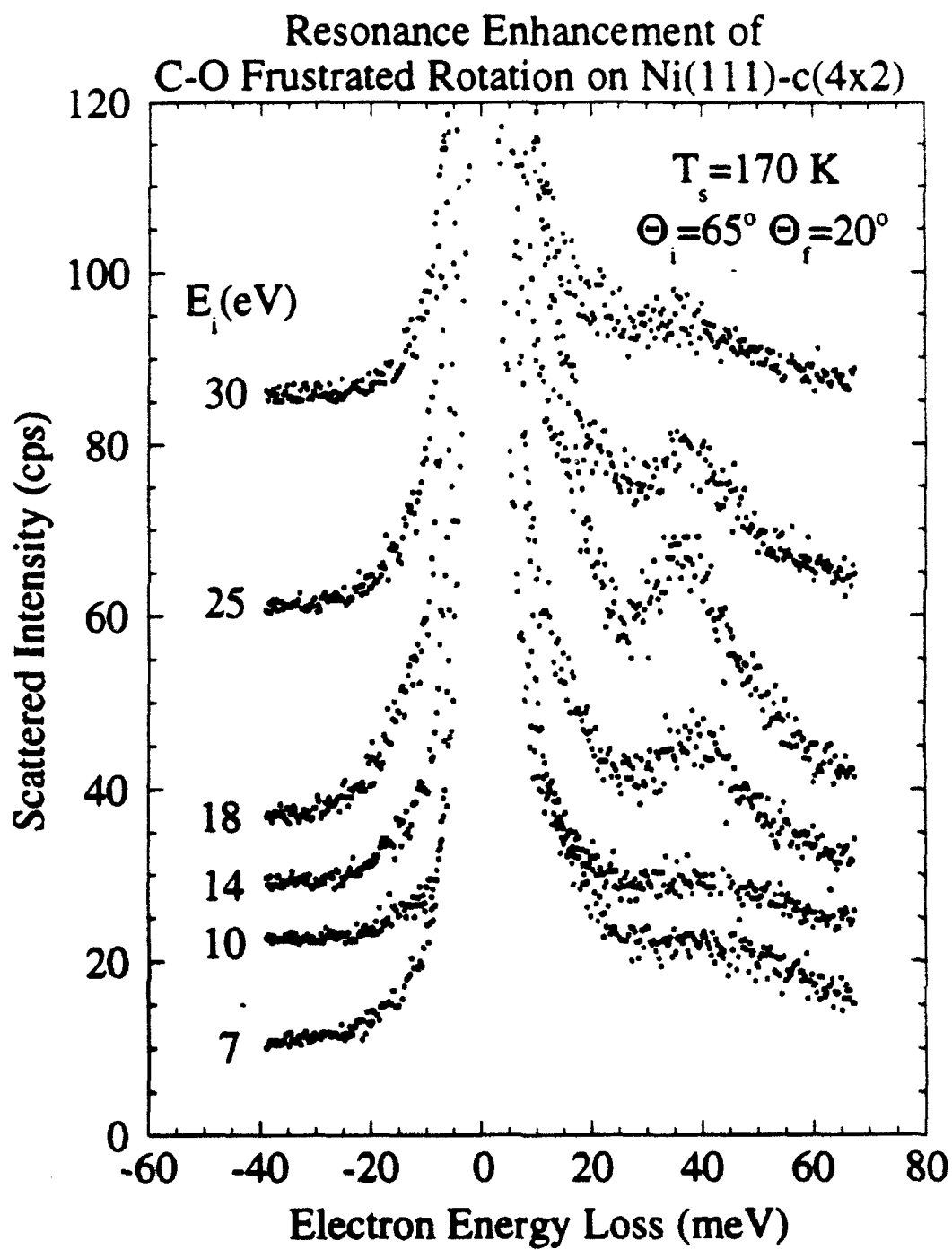
1st Layer Longitudinal

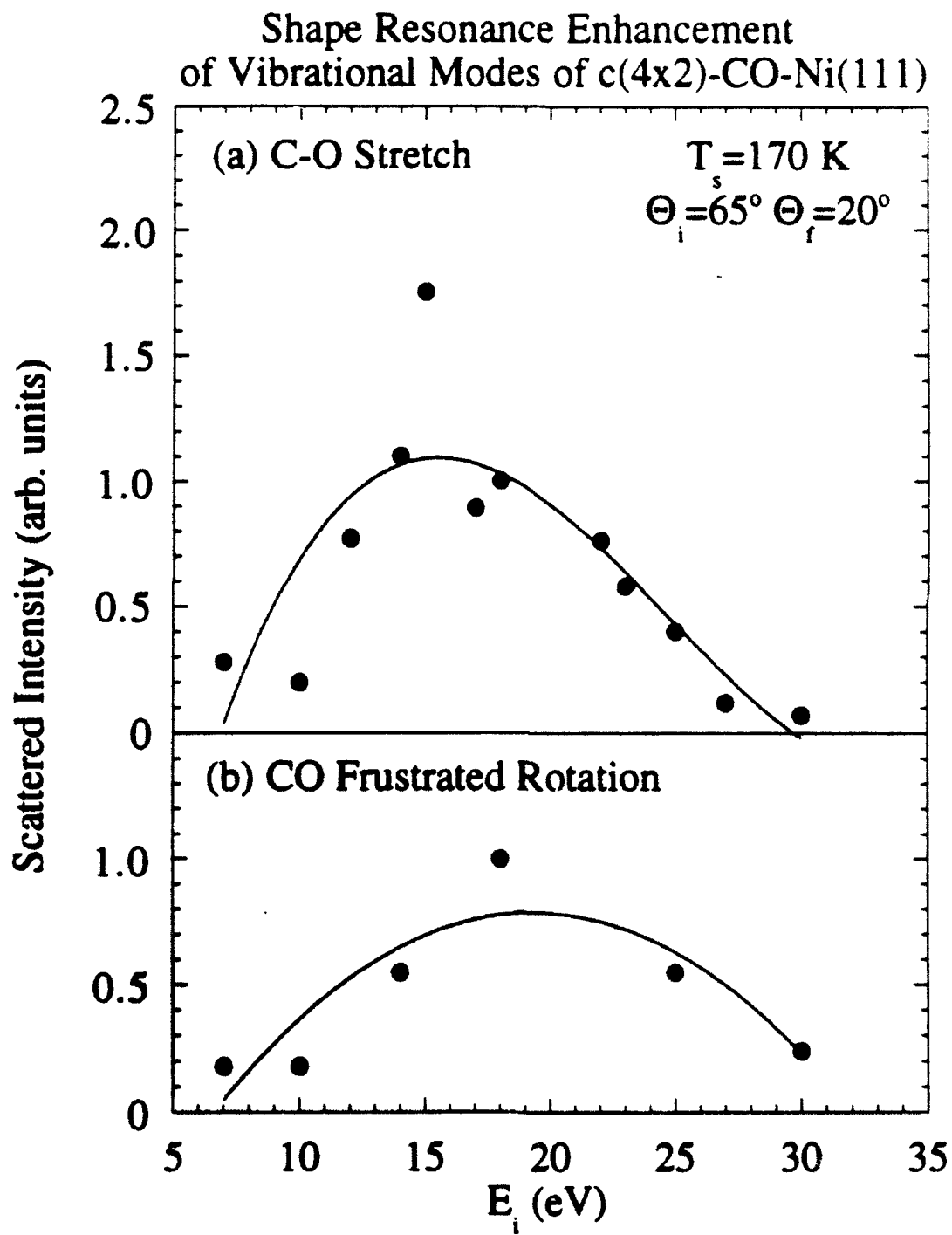


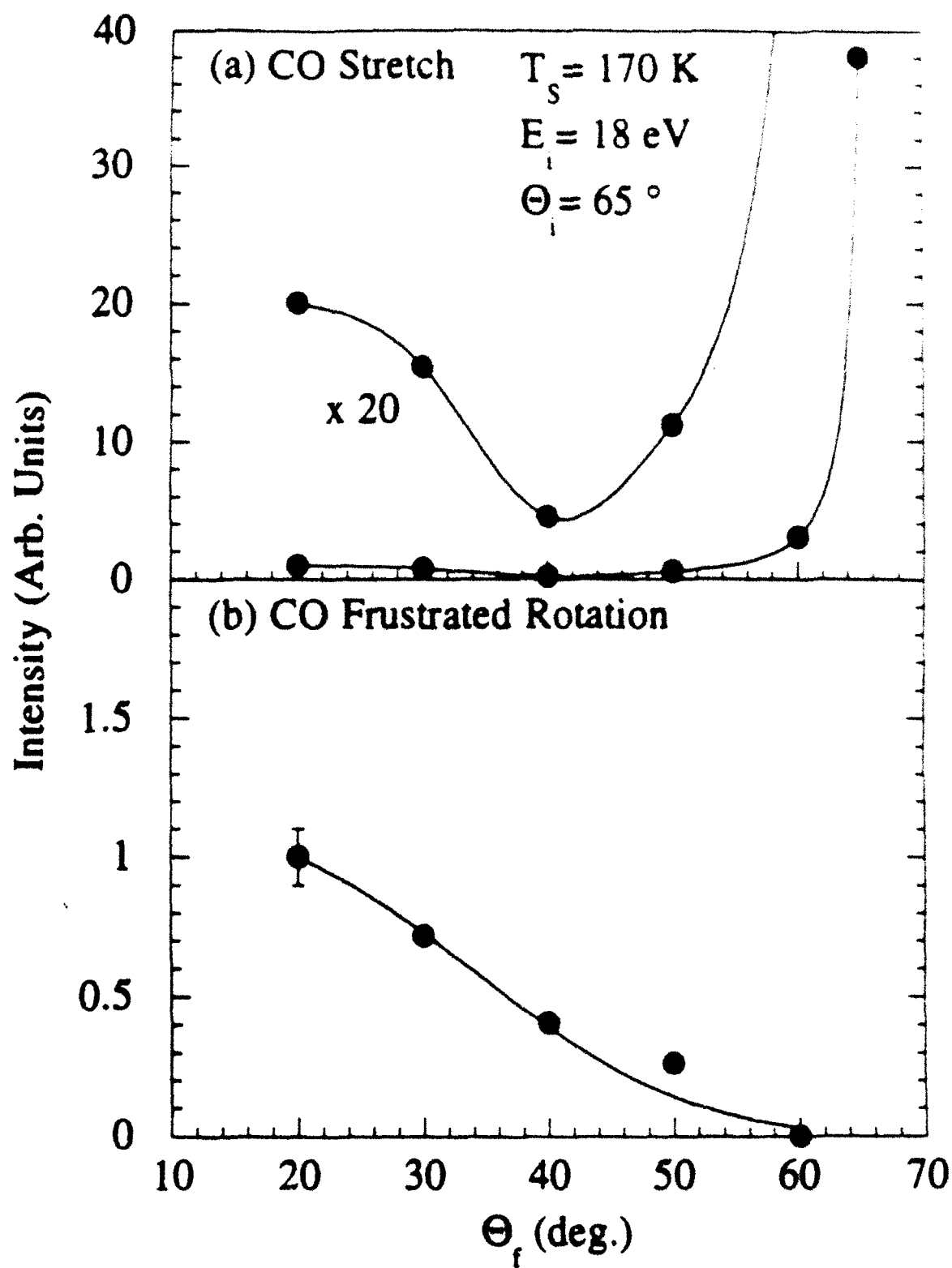
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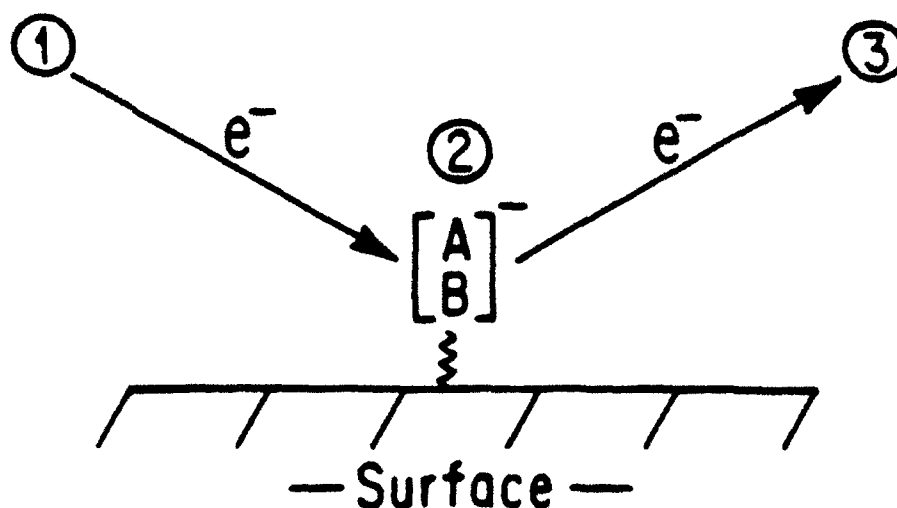








Experimental Arrangement

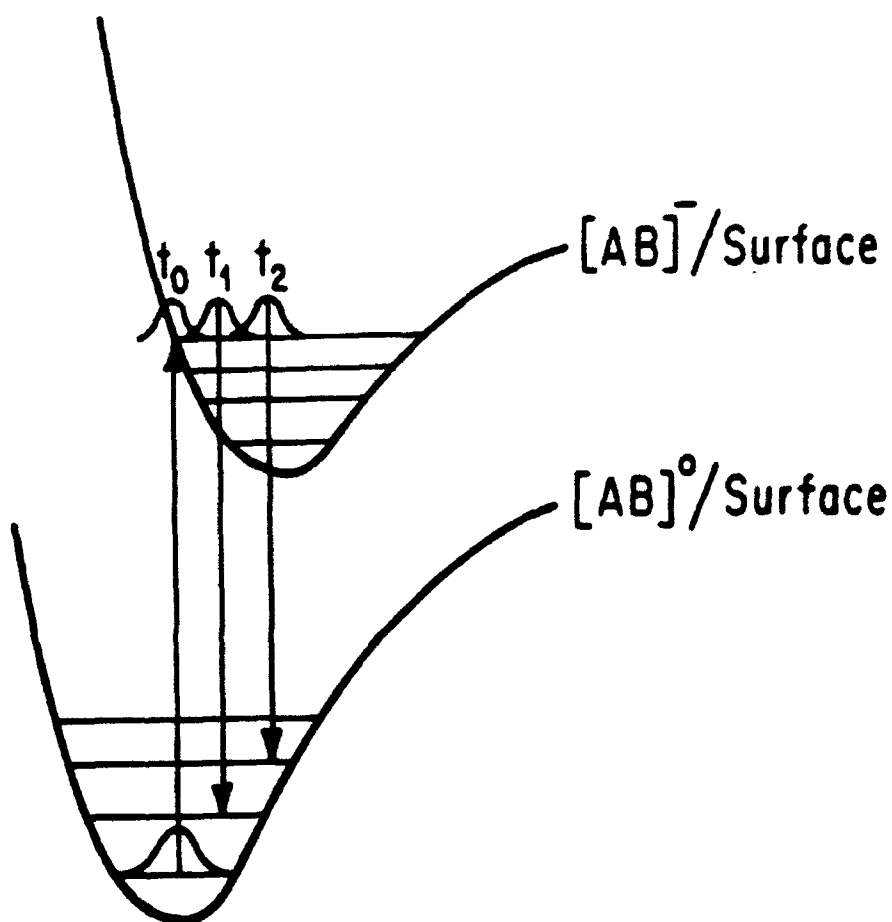


(1) Inject incident electron under resonant conditions to form the transiently bound negative ion. Probability of injection depends upon electron energy and incident angle.

(2) Nuclear coordinates evolve on the negative ion potential energy surface for femtosecond timescales for transiently bound shape resonances.

(3) Ejected electron is energy analyzed, as a function of final scattering angle, to examine excitation in both the intramolecular and molecule-surface vibrational degrees of freedom on the ground state potential energy surface. The presence (or absence) of vibrational excitation in a given coordinate gives a snapshot of short timescale evolution for the system in the excited state.

**Simplified Wavepacket Schematic
For A-B Stretch Excitation due
to Transient Negative Ion Formation**



**Note: Transient Negative Ion States
Can Lead to Both Fundamental and
Overtone Vibrational Excitations
Giving a View of (1) Femtosecond
Dynamics on the Upper Surface and
(2) The Shape of the Interaction
Potential of the Chemisorbed Molecule**

VI. Publications, Doctoral Dissertations, and Invited Presentations

Listed below are the documents that have resulted from our recent AFOSR sponsored activities. Section VI.1 lists the doctoral dissertations upon which most of this work is based, Section VI.2 lists the manuscripts that are due to our recent AFOSR sponsored activities, while Section VI.3 lists the invited presentations of the PI. The papers listed below are based upon the recent doctoral work of B. Gans, S. King, P. Knipp, D. Koleske, W. Menezes, G. Tisdale, and Y.W. Yang, as well as the postdoctoral work of J. S. Ha. Several additional manuscripts will be completed during the coming year which also come from the thesis work of these individuals.

VI.1 AFOSR Sponsored Doctoral Dissertations

Yaw-Wen Yang, Inelastic Atom Surface Scattering: LiF(001), Si(001) Surface Phonons, U. of Chicago- Chemistry, June, 1988.

Warren J. C. Menezes, Inelastic Electron Scattering Study of Ni(111) Surface Phonons, U. of Chicago- Chemistry, March 1990.

Barbara Gans, The Structure and Dynamics of Cu₃Au(001) Studied by Elastic and Inelastic Helium Atom Scattering, U. of Chicago- Chemistry, June 1990.

Daniel Koleske, Studies of Surface Vibrations and Structure Using Molecular Dynamics Simulations, Lattice Dynamics Calculations, and Helium Atom Scattering, U. of Chicago- Chemistry, December 1991.

Suzanne King, Helium Atom Scattering Studies of the Cu₃Au(001) Surface: The Order-Disorder Transition, U. of Chicago- Chemistry, March 1993.

Glenn Tisdale, Inelastic Electron Scattering and Lattice Dynamics Study of Ordered Oxygen Layers on Ni(111), U. of Chicago- Physics, expected completion March 1993.

[Please also note that the 1990 doctoral work of Peter Knipp under the guidance of Professor U. Fano in our physics department was stimulated by our AFOSR sponsored activities. Peter's thesis title was "Phonons on Stepped Surfaces".]

VI.2 AFOSR Sponsored Publications

Surface Phonon Spectroscopy of Ni(111) Studied by Inelastic Electron Scattering, Phys. Rev. B., 41, 5648 (1990), W. Menezes, P. Knipp, G. Tisdale, and S. J. Sibener.

Structure and Dynamics of Cu₃Au(001) Studied by Elastic and Inelastic Helium Atom Scattering, J. Electron Spec. and Rel. Phenom., 54/55, 333 (1990), B. Gans, S.K. King, P.A. Knipp, D.D. Koleske, and S. J. Sibener.

Temperature Dependence of Phonons on Stepped Surfaces Studied with Molecular Dynamics, J. Electron Spec. and Rel. Phenom., 54/55, 363 (1990), D.D. Koleske and S. J. Sibener.

Continued Next Page

Inelastic Electron Scattering Study of Ni(111) Surface Phonons, J. Electron Spec. and Rel. Phenom., 54/55, 373 (1990), W. Menezes, P. Knipp, G. Tisdale, and S. J. Sibener.

Measurement of Low Energy Frustrated Vibrational Modes of CO on Ni(111) via Inelastic Electron Scattering, Surface Science 256, 281 (1991), J.S. Ha and S. J. Sibener.

Surface Dynamics of Ordered Cu₃Au(001) Studied by Elastic and Inelastic Helium Atom Scattering, Surface Science 264, 81 (1992), B. Gans, P.A. Knipp, D.D. Koleske, and S.J. Sibener.

Generation of Pseudo-Random Sequences for Use in Cross-Correlation Modulation, Rev. Sci. Instrum. 63, 1 (1992), D. D. Koleske and S.J. Sibener.

Phonons on FCC (100), (110), and (111) Surfaces using Lennard-Jones Potentials: I. Comparison between Molecular Dynamics Simulations and Slab Technique Calculations, Surface Science 268, 406 (1992), D.D. Koleske and S.J. Sibener.

Phonons on FCC (100), (110), and (111) Surfaces using Lennard-Jones Potentials: II. Temperature Dependence of Surface Phonons Studied with Molecular Dynamics, Surface Science 268, 418 (1992), D.D. Koleske and S.J. Sibener.

VI.3 Invited Presentations by the PI: 1988-1992

1988

Symposium on Atomic and Surface Physics VI, La Plagne, France

University of California at Irvine, Department of Chemistry, Irvine, CA

UCLA, Department of Chemistry, Los Angeles, CA

University of Pittsburgh, Department of Chemistry, Pittsburgh, PA

Universität Erlangen-Nürnberg, 1988 Visiting Scientist and Guest Lecturer

Erlangen, Federal Republic of Germany

Adriatico Research Conference on the Application of Lasers in Surface Science,

International Centre for Theoretical Physics, Trieste, Italy

Ontario Laser and Lightwave Research Centre, University of Toronto

Toronto, Canada

1989

SPIE OE/LASE '89, Symposium on Photochemistry in Thin Films

Los Angeles, California

National ACS Meeting (April 1989), Symposium on Diffusion and Reactivity at Surfaces,

Dallas, Texas

Gordon Research Conference on Molecular Energy Transfer

Session Chair and Overview Presentation on Gas-Surface Interactions

Wolfboro, New Hampshire

Gordon Research Conference on the Dynamics of Gas-Surface Interactions

Andover, New Hampshire

International Workshop on Surface Dynamics, University of Texas-Austin

1990

Northwestern University, Department of Chemistry, Evanston, Illinois

University of California at San Diego, Department of Chemistry

San Diego, California

Florida State University, Department of Chemistry, Tallahassee, Florida

IBM Thomas J. Watson Research Center, Yorktown Heights, New York
Fifth Workshop on Interface Phenomena: Fundamental Concepts of
Interfacial Chemistry and Physics, Bar Harbor, Maine
200th National ACS Meeting (August 1990), Symposium on the Dynamics
of Gas-Surface Interactions, Washington, D.C.
American Vacuum Society Meeting, Fermilab, Naperville, Illinois
Symposium on Chemistry at Surfaces, University of CA at Irvine
Wayne State University, Department of Chemistry, Frontiers in Chemistry
Series, Detroit, Michigan
University of Illinois at Urbana, Department of Chemistry, Urbana, Illinois

1991

University of Notre Dame, Department of Chemistry, Notre Dame, Indiana
National ACS Meeting (April 1991), Symposium on Surface Science of
Catalysis: In Situ-Probes and Reaction Kinetics, Atlanta, Georgia
Surface Canada '91, Symposium on Surface Kinetics
Trent University, Peterborough, Ontario
Reactions in the Space Environment, Northwestern University, Evanston, IL
Conference on Molecule-Surface Interactions, Jülich, Germany

1992

Columbia University, Department of Chemistry, NYC, NY
Indiana University, Department of Chemistry, Bloomington, IN
APS March Meeting, Indianapolis, IN
National ACS Meeting (April 1992), Symposium on Intermolecular Forces:
From Simple to Complex Systems, San Francisco, CA
National ACS Meeting (August 1992)
Organizer, Symposium on "Surface Chemistry From Reaction Dynamics
Through Materials Growth", Washington, DC
University of Oregon at Eugene, Chemical Physics Institute Retreat Speaker, Coos Bay, OR
University of Wisconsin at Madison, Department of Chemistry, Madison, WI

VII. Curriculum Vitae - Steven J. Sibener

Born April 3, 1954; Brooklyn, New York

Education 1971-1975 University of Rochester, Rochester, New York.
Sc.B. in Chemistry awarded with High Distinction, 1975.
B.A. in Physics awarded with Distinction, 1975.

1975-1979 University of California, Berkeley.
M.S. in Chemistry, 1977.
Ph.D. in Chemistry, 1979.
Research with Professor Yuan T. Lee.

Professional Experience Eastman Kodak Research Laboratories, Photographic Research Division, Summer 1974: Electrostatic properties of polymers and polymer-metal interfaces.

Eastman Kodak Research Laboratories, Physics Division, Solid State Physics Research Laboratory, Summer 1975: Oxide growth on GaAsP for MOS fabrication.

Bell Laboratories Postdoctoral Fellow, September 1979 - August 1980. Research with Dr. M.J. Cardillo involving molecular beam scattering from single crystal surfaces.

The University of Chicago, The James Franck Institute and The Department of Chemistry:
Assistant Professor, August 1980 - June 1985.
Associate Professor, July 1985 - June 1989.
Professor of Chemistry, July 1989 - .

Honors and Awards Visiting Fellow, Joint Institute for Laboratory Astrophysics, University of Colorado, Boulder, 1992-93
Marlow Medal of the Faraday Division of the Royal Society of Chemistry, 1988.
IBM Faculty Development Award, 1984-86
Alfred P. Sloan Foundation Research Fellow, 1983-87
Camille and Henry Dreyfus Young Faculty in Chemistry Award, 1980.
Gulf Oil Research Fellow, University of California, Berkeley
American Institute of Chemists Award, University of Rochester
American Chemical Soc. Div. of Colloid and Surface Chemistry Undergraduate Thesis Competition Honorable Mention:
"The Shape of Liquid Interfaces," 1975.
Regional Scholar for New York City, University of Rochester

Associations Phi Beta Kappa
American Physical Society
American Chemical Society
Royal Society of Chemistry
Sigma Xi
AAAS

Curriculum Vitae - Steven J. Sibener

Invited Lectureships

Physikalisches Institut der Universität Erlangen-Nürnberg, 1988
 Chemical Physics Institute Retreat Speaker, University of Oregon at Eugene, 1992

Consulting

Dow Chemical USA (1982-1985)
 Teltech Resource Network (1985-)
 Institute for Defense Analyses (1985-)

Professional Activities

Vice-Chairman, 1985 Gordon Research Conference on the Dynamics of Gas-Surface Interactions
 Member, Defense Science Study Group--Institute for Defense Analyses (1985 - 1988).
 Member, Materials Research Laboratory Policy Committee, The University of Chicago (1987 -).
 Chairman, 1987 Gordon Conference on the Dynamics of Gas-Surface Interactions.
 Member, International Advisory Committee of the Vibrations at Surfaces V Conference (September 1987).
 Member, Board of Trustee's Visiting Committee for the College of Arts and Science, University of Rochester (July 1, 1987 -June 30, 1992).
 Member, Council of the University Senate, The University of Chicago (September 1989 - September 1992).
 Member, IQEC '90 Program Committee (May 1990).
 Member, Physical Electronics Conference Advisory Committee (1991).
 Member, Physical Electronics Conference Committee (1991-1994).
 Organizer, Symposium on "Surface Chemistry from Reaction Dynamics Through Materials Growth", August 1992, ACS National Meeting, Washington, D.C.

VIII. DoD Consulting of the PI

The PI was a charter member of the Defense Science Study Group of the Institute for Defense Analyses. He is currently a consultant for IDA.