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operation with beam energies of up to 240 eV. These new ultra-high vacuum instruments have performed at or exceeded their respective design goals, allowing experiments aimed at elucidating the structural and dynamical properties of surfaces to be pursued. In the future, the diverse capabilities of these scattering instruments will be used to study, at the atomic level, collision induced gas-surface and electron-surface energy transfer mechanisms. Another focus will be to continue studying the surface phonon dispersion relations for clean and adsorbate covered surfaces. Such measurements yield unambiguous information on the forces present at material interfaces.

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Summary Abstract

This research initiative has dealt with the interaction of atomic, molecular, electron, and optical beams with well-characterized single crystal surfaces. These studies were motivated by a desire to understand and control catalytic surface chemistry, 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. During the past grant period, two major new scattering instruments were completed. One is a high performance neutral particle scattering apparatus, which routinely achieves an energy resolution of ca. 300 micro-eV. It has successfully performed elastic and inelastic scattering measurements on alkali halide, semiconductor, and metallic surfaces. Results are presented in this final report for LiF(001), Si(001)-(2x1), and Ag(110). The Si phonon dispersion measurements differ markedly from theoretical calculations, and strongly suggest that the dynamical properties of partially *disordered* surfaces merit increasing attention in this program. The other instrument is a new electron energy loss spectrometer which has achieved, with high signal throughput, ca. 5 milli-eV energy resolution, and operation with beam energies of up to 240 eV. These new ultra-high vacuum instruments have performed at or exceeded their respective design goals, allowing experiments aimed at elucidating the structural and dynamical properties of surfaces to be pursued. In the future, the diverse capabilities of these scattering instruments will be used to study, at the atomic level, collision induced gas-surface and electron-surface energy transfer mechanisms. Another focus will be to continue studying the surface phonon dispersion relations for clean and adsorbate covered surfaces. Such measurements yield unambiguous information on the forces present at material interfaces.

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I. INTRODUCTION

AFOSR-84-0073 has been concerned with the design, construction, and use of two new scattering instruments for studying gas-surface and electron-surface interactions. Both of these new ultra-high vacuum instruments have been completed, and are performing at or exceeding their respective design goals, allowing experiments aimed at elucidating the structural and dynamical properties of surfaces to be pursued. A primary aim of this program was to develop the means of determining the surface phonon dispersion relations for a wide variety of clean and adsorbate covered surfaces. This has been accomplished. Such measurements yield unambiguous information on the forces present at material interfaces.

It is worth mentioning in this introduction that the neutral particle scattering apparatus described in this report represents a real advance in the field as it has been designed to simultaneously achieve an extremely low background in its detector, high angular (momentum) resolution, and, most importantly, excellent time-of-flight resolution. It achieves the above while maintaining its ability to determine surface phonon dispersion curves and inelastic scattering probabilities *without* varying incident kinematic conditions. This is accomplished with a novel rotating detector, and is especially important when comparisons are made between experimental data and theoretical scattering calculations. The new electron scattering instrument shared a similar design philosophy as it can also map out surface excitations as a function of final wavevector without varying the incident scattering geometry.

This Final Technical Report summarizes the major accomplishments achieved under the auspices of this grant. It also provides some background information on the motivation for this project. The reader can refer to earlier continuation proposals and progress reports for further information. The outline for the remainder of this Final Technical Report is as follows: it continues in Section II with relevant background material which describes the motivation for conducting single phonon inelastic scattering measurements, and discusses the complementary nature of neutral particle and electron scattering measurements. Section III then presents information on surface phonon spectroscopy which provides a general description of surface phonon physics, and a brief review of inelastic particle scattering kinematics. It also outlines in more detail some of the scientific questions this project has attempted to address. Section IV contains the important project accomplishments for both the neutral particle and electron scattering components of the project. Several sections then follow which summarize other aspects of this endeavor. Section VII deserves special mention as it lists the additional sources of financial support, including two Department of Defense - University Research Instrumentation grants, which contributed to the successful completion of this project.

II. INELASTIC PARTICLE - SURFACE SCATTERING: PROJECT MOTIVATION

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 [1-4]. Topics being explored cover elastic, inelastic, and reactive scattering, as well as laser induced desorption ("half-collisions"). These studies are motivated by a desire to understand and control catalytic surface chemistry, 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.

Elastic scattering experiments, including diffraction [5] and selective adsorption [6], are primarily concerned with the elucidation of static properties of the surface, such as the time-averaged structure [7] and interaction protential [8] for a given system. The combination of theory and experiment here is proving to be quite informative: after picking a given geometry, electronic structure theory can be used to generate a surface charge density distribution. This in turn can then be used to generate accurate gas-surface interaction potentials [9, 10]. These potentials can be used as the input for a quantum scattering calculation, whose results can be compared with experiment. Such studies are *extremely* sensitive to the assumed gas-surface interaction potential [11]. Excellent surface sensitivity is realized in these 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. In addition to probing the structure of clean and adsorbate covered surfaces, elastic scattering experiments can also yield information on chemisorbed and physisorbed island size distributions, surface defect densities (and roughening [12]), and two-dimensional phase transitions [13]. Studies involving partially disordered surfaces are currently assuming increasing importance in this area.

Inelastic scattering experiments can be grouped into two broad categories. One class deals with the topic of molecular "state-changing" collisions, such as recent investigations of translation-to-rotation, vibration (T → R, V) energy exchange involving a variety of diatomic and small polyatomic molecules such as H_2, D_2, NO, N_2, CO, HF, and, most recently, NH_3 [14-18]. Polarization measurements are also underway [19]. The scientific issues here center on the anisotropy of the gas-surface potential, and how energy is partitioned among the available degrees of freedom. The other class of inelastic scattering experiments is concerned with the exchange of energy and momentum between neutral particles and the vibrational modes of a surface [20]. Inelastic scattering experiments such as these allow one to study the dynamical properties of clean and adsorbate covered surfaces, and the microscopic energy transfer mechanisms which contribute to collision induced gas-surface energy exchange. It is this latter class of inelastic scattering experiments with which we shall primarily concern ourselves in this report. This is a new and very rapidly developing area of endeavor which holds the promise of high scientific payoff in a variety of areas.

Specifically, this project primarily deals with the experimental determination of the *surface phonon dispersion relations* for clean and adsorbate covered surfaces, including substrates covered with thin films of varying thickness and composition. These measurements are being compared with various theoretical calculations, including quantum scattering and lattice dynamics codes, in order to extract the desired physical information. Such measurements give unique information on the forces present at the surface of a material. Experience in the last few years has shown that virtually every system that has had its surface phonon dispersion relations experimentally mapped out has revealed major new insights into the forces present at interfaces. Studies on such seemingly simple materials as LiF(001) [21], the (111) faces of Ag, Cu, and Au [22], and Si(001) [23] all have shown that existing theoretical force field predictions (and hence surface charge density distributions) could not quantitatively account for the data. These few examples strongly suggest that this area is only just now beginning to yield the hoped for high scientific payoff, and that it will remain an extremely exciting area for many years to come.

These measurements are being accomplished using *either* angle and velocity resolved inelastic neutral particle scattering (usually He) or angle and energy resolved inelastic electron scattering as the dynamical probe. Experiments are being carried out in two recently completed scattering instruments. One of these is a novel neutral particle scattering instrument whose design 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 (≤ 300μeV is routinely being obtained at this time). The other instrument is a new inelastic electron scattering spectrometer which can operate at high sensitivity with high energy resolution (≤ 5meV), and incident beam energies of up to 240 eV. The measurements one can perform with these two types of scattering instruments are quite complementary in nature--the importance of having information from both neutral particle and electron scattering experiments will become apparent later in this report.

Inelastic neutral particle scattering experiments can be viewed as a two-dimensional analog to inelastic neutron scattering, which has been used with great success to elucidate the properties of bulk phonons. The surface phonon spectroscopy experiments discussed herein are exploring in great detail the lattice dynamics of clean and adsorbate covered surfaces, how the vibrational properties of epitaxially grown thin films evolve on a layer-by-layer basis towards those of bulk crystals, and how surface phonons interact with colliding particles, resonantly bound (metastably trapped) particles, and adsorbed molecules. Especial attention is being given to how, and with what probability, energy is transferred to a surface during collisional encounters. The goals in this regard include elucidating which modes actively participate in collision induced energy exchange, determining under which energy regimes single and multiphonon transitions dominate, and determining when electron-hole pair generation (with or without phonon participation) becomes a significant energy adsorption mechanism. The energy transfer questions being addressed here are central to a microscopic understanding of thermal accommodation, momentum accommodation (aircraft drag), and chemical adsorption (the primary event leading to surface chemical reaction). Furthermore, analysis of single-phonon excitation *lineshapes* may allow us to extract information on the dynamical couplings which lead to the decay of surface excitations (i.e., phonon lifetimes) [24-26]. 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. 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.

Finally, in addition to the aforementioned elastic and inelastic scattering measurements, this program will ultimately encompass photodesorption and chemical kinetics measurements which take advantage of the diverse capabilities of our new UHV instruments. In the future, the photodesorption experiments will focus on questions of energy flow and photochemical selectivity, topics of current interest in the field [27-29]. The chemical kinetics measurements will be conducted in our HREELS machine, with the focus being on the study of reaction intermediates, ultimately in a real-time mode of data acquisition [30, 31].

III. SURFACE PHONON SPECTROSCOPY

III.1 Background

Inelastic atom scattering is, in principle, a nearly ideal probe of 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. The latter condition dealing with momentum matching (i.e., the wavevector of a helium beam is comparable to that of a typical surface Brillouin zone) has extremely important consequences for the application of inelastic helium scattering as a surface spectroscopic tool. It implies that phonons can be probed across the *entire* surface Brillouin zone (SBZ). Thus "zone edge" (short wavelength) phonons can be detected which are an extremely sensitive probe of *surface* force constants, and as a direct consequence of this, of surface structure. The importance of zone edge phonons in surface physics can be qualitatively understood by noting that their group velocity ($d\omega/dK$) goes to zero at π/a, indicating that they behave as a standing wave at these locations. They are therefore an excellent probe of short range structure. In contrast to this, long wavelength phonons near the Brillouin zone center are well suited for probing the elastic continuum properties of a material--which can be adequately described using bulk (not surface) force constants.

High resolution inelastic electron scattering (HREELS) can also be used for probing excitations across the entire SBZ provided that relatively high energy electrons are employed [32-34]. Similarly, neutron inelastic scattering can also be used to probe surface phonons across the full SBZ. This technique unfortunately suffers from a lack of surface sensitivity. Brillouin inelastic light scattering is best suited for probing phonons near the zone center as it cannot exchange large quantities of momentum with the surface at the energies of interest. Electron and photon scattering techniques are quite complementary to inelastic atom scattering in that they can couple through electromagnetic interactions--and are therefore sensitive to optical phonons. Atom scattering is perhaps best suited for acoustic mode spectroscopy as it interacts via impact scattering resulting from charge density overlap with the surface (van der Waals repulsion). (It is worth mentioning here that recent inelastic scattering experiments on NaF(001) [35] and LiF(001) [36] have demonstrated that atom scattering can also detect surface optical modes.)

Inelastic atom scattering experiments are sensitive to the dispersion relations of surface phonons and to the surface projected densities of bulk phonons. Surface phonons are localized at the surface, and exist as a consequence of the new boundary conditions which arise when the translational symmetry of a material is broken by the introduction of a surface. Lord Rayleigh was the first to point out the existence of such surface waves (in a different context). These "Rayleigh waves" are well described by continuum theory in the long wavelength limit. They are sagitally polarized (i.e., they lie in the plane defined by the direction of propagation and the surface normal) and are the best known examples of macroscopic surface phonons.

At shorter wavelengths continuum theories break down, and dynamical calculations which take into account the nature of the individual atoms must be used to describe the surface. Two different theoretical approaches have been developed to treat these "dispersive" phonons: the multilayered slab technique of de Wette and co-workers [37], and the Green's function formulation of Benedek [38, 39]. The important point is that both of these calculation techniques provide high quality quantitative results. They each predict (correctly) that several new classes of acoustic and optical phonons should appear at the surface of a crystalline material.

Surface modes are described by discrete dispersion curves, in contrast to the broad bands of bulk phonons. Any mode whose frequency lies above or below the bulk subbands for its momentum, or falls in a gap between the bulk subbands, must be a surface mode [37]. For monatomic fcc crystals, a pioneering and very clear description of these modes is presented by Allen, Alldredge, and de Wette [40]. The authors of this article emphasize that dispersive surface modes can be described with a simple phenomenological model in which these modes are "peeled off" from the bulk bands. Their calculations further emphasize that "the qualitative features of the surface phonon spectrum are sensitive to changes in surface force constants." This suggests that studies of relaxed and reconstructed surfaces will be quite productive in giving the correct surface force constants of these interesting materials.

The preceding discussion has been limited to clean surfaces. However, one of the most exciting expectations for inelastic atom scattering is that it will evolve into a sensitive probe of the dynamical properties of adsorbate covered surfaces. Such high resolution experiments should allow for the investigation of lateral interactions within an adsorbate layer. These interactions are very important for understanding many aspects of physisorption and chemisorption, including two-dimensional phase transitions. Recent work from our group on rare gases physisorbed on Ag(111) [25, 41], from other groups on CO/Pt(111) [42], Xe/Pt(111) [43], and O/Pt(111) [44] indicate the ability to examine adsorbate covered surfaces. Inelastic scattering experiments involving adsorbate covered surfaces should also allow us to examine the probability of collision induced energy transfer to such a surface. Finally, studies involving epitaxially grown materials should reveal how the lattice dynamics of thin films evolve on a layer-by-layer basis towards those of a thick crystal [41].

III.2 Scattering Kinematics

The spectroscopy of surface phonons can be carried out by carefully measuring the final scattering angle and translational energy of inelastically scattered particles. For single phonon interactions the conservation equations for parallel momentum and energy are given by

$$\mathbf{K}_f = \mathbf{K}_i \pm \mathbf{Q} + \mathbf{G} \tag{1}$$

$$\mathbf{k}_f^2 = \mathbf{k}_i^2 \pm \frac{2m}{\hbar}\,\omega(\mathbf{Q}) \tag{2}$$

where + corresponds to phonon annihilation (deexcitation), - to phonon creation (excitation), $\mathbf{K}_i$ is the surface projection of the incident wave vector $\mathbf{k}_i$, $\mathbf{K}_f$ the surface projection of the outgoing wave vector $\mathbf{k}_f$, $\omega(\mathbf{Q})$ the phonon frequency, $\mathbf{Q}$ the phonon momentum, and $\mathbf{G}$ is a surface reciprocal lattice vector. For $\mathbf{G} = (00)$ and in-plane scattering, $\mathbf{k}_f$ can be eliminated from equations (1) and (2) to give an expression for $\omega(\mathbf{Q})$ in terms of the experimental conditions [45]:

$$\omega(\mathbf{k}_i,\mathbf{Q},\theta_i,\theta_f) = \frac{\pm\hbar}{2m}\left\{\mathbf{k}_i^2\left(\frac{\sin^2\theta_i}{\sin^2\theta_f} - 1\right) + 2\mathbf{k}_i\frac{\sin\theta_i}{\sin\theta_f}\mathbf{Q} + \frac{\mathbf{Q}^2}{\sin^2\theta_f}\right\} \tag{3}$$

This indicates that both the momentum and energy of a phonon can be determined by measuring the final velocity of the scattered particle at a well defined angle. By proceeding away from the specular reflection the phonon dispersion relation for each mode can be uniquely mapped out.

Phonon excitation probabilities have been calculated by Levi [46] and Benedek and Garcia [47], and are given by the following "differential one-phonon reflection coefficient" [47, 48]

$$\frac{d^2R}{d\omega d\Omega_f} = \frac{(\Delta k_z)^2}{2\pi^3} \frac{k_f}{|k_{i_z}|} \left| n^{\pm} \right|^2 g(\mathbf{K}\text{-}\mathbf{G})\ \rho(\mathbf{Q},\omega) \tag{4}$$

where Δk_z is the change in the normal momentum, $\mathbf{k}_{i_z}$ is the initial normal momentum, $n^{\pm}$ is a Bose weighting factor [48], g(**K**-**G**) is the scattering coupling coefficient (which is related to the scattering T matrix, and $\rho(\mathbf{Q}, \omega)$ is the surface projected density of states. Similar expressions have also been developed for scattering from adsorbate covered surfaces [49]. Single phonon processes should dominate when [50].

$$\frac{M_{beam}}{M_{surf}} \frac{E_{i_z} T_s}{k_B \Theta_D^2} < 0.01 \tag{5}$$

where Θ_D is the Debye temperature of the surface. This expression suggests that the use of light atoms, low surface temperatures, and low beam energies should favor the predominance of single phonon events. This is crucial as multiphonon events do not lead to discrete peaks in a time-of-flight spectrum (phonons can go, for example, backwards and forwards with differing momentum combinations to yield a broad band in an angle-resolved time-of-flight experiment.)

Phonons can also be probed by studying phonon mediated selective adsorption features in scattered particle angular distributions. In these experiments the usual diffractive selective adsorption conditions [2] are modified to include phonon participation:

$$(\mathbf{K}_i + \mathbf{G} + \mathbf{Q})^2 = \mathbf{k}_i^2 + \frac{2m}{\hbar^2}(\hbar\omega - \varepsilon_n) \tag{6}$$

where ε_n is a bound level of the particle-surface potential. Phonon assisted selective adsorption can be used (with difficulty and potential ambiguity) to probe surface phonons only when the bound state spectroscopy of the potential is completely understood [51-53].

IV. PROJECT OVERVIEW AND RESEARCH ACCOMPLISHMENTS

IV.1 Project Overview

In response to the many exciting scientific opportunities outlined in the preceeding two sections of this proposal, the Principal Investigator's group embarked with major financial support from the DoD on the construction of a new, very high resolution and sensitivity neutral particle scattering apparatus. DoD support came in three forms: this AFOSR grant (which is the primary continuing source of financial support for this research program) and two 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.) A new laboratory was completely renovated in the basement of the James Franck Institute in order to house this large instrument. A concrete foundation consisting of a special non-shrinking concrete was poured in this laboratory in January, 1985 to support the nearly two-ton rotating detector of the instrument. Inelastic single-phonon scattering was first observed in late August, 1986 (within a few days of turning on, the experimentally demonstrated energy resolution was already down to $\Delta E \approx 320$ μeV, exceeding the initial 400 μeV design goal that we hoped to meet during the first few months of operation). The instrument then successfully passed a final series of tests consisting of computer driven diffraction, selective adsorption, and surface phonon (time-of-flight) measurements. Illustrative results on LiF(001), Si(001), and Ag(110) are presented later in this report. In January, 1987 a second new laboratory was renovated for housing the new HREELS instrument. The electron optics passed all transmission tests during the summer of 1987, with computer driven spectra first being collected in December. Full operation was achieved during the summer quarter, 1988. (Note that in the original proposal this HREELS spectrometer was going to be installed in the same UHV chamber as the neutral particle scattering: severe spatial constraints, and instrument utilization (i.e., duty cycle) considerations caused us to abandon this idea early on and construct a second laboratory. With the advantage of hindsight, this was certainly the correct decision. Construction of this instrument proceeded quickly following the award of a second DoD-URIP grant.)

IV.2 Research Accomplishments - Neutral Particle Scattering

A schematic representation of the neutral particle scattering instrument is shown in Figure 1, while Figure 2 is a photograph of the completed instrument. The supersonic nozzle beam source (left side of the photo) is cryogenically cooled with a closed-cycle He refrigerator, giving us the capability to "dial up" a given nozzle temperature between ~ 40 - 300K (corresponding to wavevectors from 1.56-0.57 $Å^{-1}$; see the section on Ag(*110*) scattering for a further discussion of this point). The beamline routinely generates very intense cw He beams ($I \geq 2x10^{19}$ atoms / sr / sec) of extremely narrow velocity dispersion ($\Delta v/v \sim 0.75\%$, speed ratios of over 220). These beams are then chopped into short pulses by a mechanical chopper, and sent onto the target for scattering. The beamline can be connected in three different orientations, giving wide variability of incident scattering geometry. The crystal chamber (center of the photo) has a base pressure in the 10^{-11} torr range, and contains LEED, Auger, XPS, sputtering, and mass spectrometric (RGA) capabilities. The target mount has all necessary degrees of freedom, and can be cooled to cryogenic temperatures or heated with an electron beam heater. Finally, the detector (right side of the photo) is a massive, nearly 2-ton assembly which rotates ca. $\pm 22^{o}$ under computer control. Its position can be controlled to better than 0.05^{o} as monitored with an optical encoder. (The turntable that supports this rotation can be seen in the center of the photo just above the floor.) The crystal-to-ionizer flightpath can be varied, without giving up any differential pumping stages, from 100.5cm (typical arrangement) down to 64.8cm. Its background level of ≤ 10 counts per second at mass 4 corresponds to a He partial pressure in the low 10^{-14} torr range (representing a partial pressure drop of 18 orders of magnitude from the nozzle, which typically operates at 10 atmospheres pressure!). The triply differentially pumped detector is usually run with either 0.2° or 0.3° angular resolution. The importance of having an independently rotating detector is that scattering information can be collected over a range of final scattering angles *without varying the incident kinematics*--the ideal situation for facilitating comparison with scattering calculations.

Before going on to a discussion of results, it is worth mentioning that, although not discussed in detail, a large effort in the past few years was also devoted to the development of data collection and data analysis software. The successful completion of these tasks was crucial to the work that is described below.

Alignment of the instrument was confirmed by measuring the bound state scattering resonances for the He-LiF(001) physisorption potential. The four bound states for this potential were easily found, as shown in Figure 3. The peaks correspond to diffractive resonances mediated via the (11) G-vector. The important point to stress here is that the levels were easily seen (good S/N ratio) and agreed with literature values to within ca. 0.1meV. The machine's alignment and time-of-flight calibration were confirmed by these and other diffraction measurements.

We then moved on to a systematic study of the vibrational structure of the LiF(001) surface. The upper left panel of Figure 4 shows the superposition of the known LiF(001) Rayleigh wave with five "scan curves" (labelled a-e). These parabolic scan curves represent the allowed energy and momentum transfers that can be seen by our detector for a series of final LAB angles. The intersections of the Rayleigh wave with curves a-e indicate where inelastic scattering peaks should be observed in time-of-flight experiments at those detector settings. The five spectra in Figure 4 have peaks at the expected energies, with good intensity and resolution. The $\Delta E = 0$ peaks (near channel 150) are due to diffuse scattering from surface defects. The peaks all have widths on the order of a few tenths of an meV. The results of this study are shown in Figure 5, which gives our first experimentally determined surface phonon dispersion curve. The results are in excellent agreement with the Gottingen data, confirming the surprising mode softening found near the edge of the SBZ. Other interesting features are the points near $K = 0.3$ Å^{-1}, which are above the Rayleigh mode. They occur reproducibly, and are apparently due to some strong features in the surface projection of the bulk density of states.

Before moving on to a discussion of our results on Si(001), it is worth showing a few figures which illustrate how we currently process new experimental data. These analyses are based on a very detailed computer simulation program which took more than half a year to develop. This program allows us to extract accurate (deconvoluted) information about the positions, intensities, and true lineshapes for both diffraction and time-of-flight measurements. Figures 6-8 are of interest here. Figure 6 shows a time-of-flight spectrum for a 16.54 meV He beam specularly reflecting from LiF. It demonstrates that the instrument's time resolution is well matched to the quality of the incident beam's velocity distribution ($\Delta E_i \sim 200$ μeV). Figure 7 shows the initial steps in analyzing a time-of-flight spectrum--beginning with broad background subtraction, and followed by fitting of the residuals (phonon peaks). Note that the dashed line labelled "simulation" here does not provide a good fit for the lineshape of Peak 3. The simulation at this stage assumes only a delta function (single energy) phonon width. This indicates that phonon linewidth needs to be added to the simulation. This is done in Figure 8, where Peak 3 is found to have a FWHM Lorentzian width of 240 μeV. From such analyses we can extract accurate information on phonon energy <u>widths</u> (bounds on lifetimes), as further discussed in the proposed research section of this proposal.

We now turn our attention to experiments involving Si(001), with representative data and analyses being shown in Figures 9-12. This series of experiments was carried out in order to quantitatively determine the surface phonon dispersion relations for a reconstructed semiconductor surface. Figure 9 shows a He diffraction pattern measured along the <110> direction which clearly shows the half-order peaks characteristic of a (2x1) reconstructed surface. Also shown in the inset is the reciprocal lattice net for the corresponding two-domain (2x1) surface. Figure 10 shows Si diffraction runs taken with the detector in its long and short flightpath configurations. These runs illustrate that the higher acceptance angle of the short configuration raises the background levels between diffraction peaks, but does not appreciably alter the intensity of the (narrow) diffraction peaks. The shorter flightpath configuration was used for the Si phonon measurements in order to obtain higher signal levels from this highly disordered surface. Figure 11 shows both a specular and typical off-specular time-of-flight spectrum with a 16.3 meV beam. The upper panel demonstrates the high resolution of the experiment (220 μeV specular width) while the lower panel shows diffuse elastic scattering due to defects, and an energy gain (phonon annihilation) feature at about 10 meV. The source of the very broad background is still under investigation. Finally, Figure 12 shows the main results of this experiment. Panel (a) shows the scan curves and observed spectral features for a series of time-of-flight runs. The presence of a non-dispersing vibrational mode at ca. 10 meV is clearly indicated. Panel (b) shows the experimental results superimposed on the theoretical calculations of Mele and coworkers [69]. The three theoretical curves are for the Raleigh waves along each symmetry direction and for the dimer rocking motion. Panel (c) is a folded-zone representation of the results. The experimental results differ markedly from the theoretical calculations, which were done for a "perfect" (2x1) surface. Improved calculations are needed which take into account the effects of *surface disorder* and multiple domain structures. This result strongly suggests that the dynamical properties of partially disordered surfaces deserve increasing attention in this program.

Finally, in a recent set of experiments, we have started to examine Ag(110), a surface which is known to roughen at elevated temperatures [70]. (In the future we hope to study adsorbate phase transitions on this surface.) Figure 13 shows a diffraction spectrum for a poorly ordered Ag(110) surface. Specular reflectivities as a function of incident wavevector and incident angle are currently being measured to assess the nature of the disorder. However, the time-of-flight data in Figure 14 dramatically show that inelastic scattering contributions arise in the specular direction as a function of increasing incident beam energy (note how the reflected energy distributions at first develop wings, and then continue to broaden). The extent of this broadening is important: it implies that future "elastic" scattering and diffraction measurements on soft surfaces (or soft overlayers) with nozzle beams of ≥ 150K should be taken in a time-of-flight (i.e., energy dispersed) mode to ensure that the sought after elastic intensities are accurately obtained. (This figure also provides a nice demonstration of the tunability of our He beam source.)

To summarize the above, during the past grant period we have successfully brought on-line a novel high resolution neutral particle scattering apparatus. Diffraction, selective adsorption, and, most importantly, single phonon inelastic scattering measurements on a wide variety of substrates (alkali halides, semiconductors, and metals) confirm that the instrument is performing properly. Scientific projects on several different topics are now underway.

IV.3 Research Accomplishments - Electron Scattering

As was stated earlier, inelastic electron-surface scattering measurements provide complementary information to inelastic He scattering in that higher lying vibrational modes can also be interrogated (with, unfortunately, a factor of 20 poorer resolution). Carefully selected electron scattering conditions (chosen with the assistance of electron-surface quantum scattering codes) can also be used to study *in-plane* vibrations. Together, these two 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.

A schematic representation of the second level of the new HREELS spectrometer is shown in Figure 15, while Figure 16 is a photograph of the instrument. Note that several ports are available which focus at the electron scattering position. These will be used for a variety of photochemistry, chemical kinetics, and thin film experiments. This instrument is especially well suited for surface phonon measurements as it can operate with incident beam energies of up to 240 eV (important for impact scattering) with good transmission and ca. 5 meV resolution. The higher level of the chamber is equipped with an assortment of surface spectroscopic tools: LEED, Auger, XPS, and UPS, as well as a quadrupole mass spectrometer and a sample load-lock.

During the past grant period we have completed this instrument. Figure 17 shows an early direct reflection run which confirmed that the electron optics were performing as expected. The lower panel of this figure shows a computer controlled scan showing that data can be collected, at 5 meV resolution, with 100 msec sampling times. Recent results indicate that data can be collected with 20 msec sampling without spectral distortion. Such sampling is important for planned "beam-EELS" experiments which will attempt to observe reaction intermediates in real-time. Measurements on clean, O, and CO covered Ni(111) will be used to optimize performance of the instrument, and to assess the degree of force constant relaxation Ni(111) has with respect to bulk Ni.

V. FIGURE CAPTIONS AND FIGURES

Figure 1.	Schematic diagram of the high resolution neutral particle scattering apparatus.
Figure 2.	Photograph of the high resolution neutral particle scattering apparatus. The beamline is on the left, while the computer controlled detector is on the right.
Figure 3.	Experimental selective adsorption scan showing strong resonances due to the bound states of the He/LiF(001) potential. The peaks are coupled via the G=(11) lattice vector. The agreement of our level determinations (Eo = -5.7meV, E1 = -2.2meV, E3 = -0.6meV, and E4 = -0.1meV) with previous

measurements was one of several early indications that the instrument was correctly aligned.

Figure 4. Surface phonon dispersion curve for LiF(001) shown superimposed with five different scan curves for the time-of-flight runs shown in panels a-e. The scan curves (labelled a-e) indicate the energy and momentum values accepted by the detector at a given LAB angle of the detector. Intersections of the scan curves with the dispersion curve yield peaks in the experimental time-of-flight runs.

Figure 5. Results from our first surface phonon dispersion measurements on LiF(001) (open circles), which show excellent agreement with the 1983 Gottingen data in a folded zone representation. The agreement near the important softened zone edge is particularly striking. The squares are not phonons, but rather are energy dispersion features arising from the finite energy spread of the incident beam. Fascinating points above the Rayleigh wave at K = 0.3 Å-1 are reproducible, and are presumably due to unusual features originating in the surface projection of the bulk density of states.

Figure 6. Time-of-flight spectrum for an Ei = 16.54meV He beam specularly reflected from LiF(001). Note that the energy resolution is ca. 300μeV. The lines marked conv, vel. dist., and inst. res. are the results of a detailed computer simulation of the machine's performance. The lower panel shows the same data transposed to an energy resolved axis.

Figure 7. This figure, along with Figure 8, shows how a typical time-of-flight spectrum is processed. (a) Broad background subtraction. (b) Computer simulation and fitting of the residuals (sharp peaks). Note that Peak 3 is not well fit by the simulation which does not yet contain any energy broadening.

Figure 8. Time-of-flight and energy transfer representations which show computer simulations, including Lorentzian energy broadening, which fit the experimental data. From such analyses we can now extract information on phonon excitation probabilities, and phonon energy widths (bounds on lifetimes). (Peak 3 has a width of 240 μeV.)

Figure 9. Diffraction scan for Si(100) clearly showing the additional half-order peaks due to the (2x1) reconstruction of the surface.

Figure 10. Diffraction scans, and computer simulations, for Si(100) - (2x1) taken with the (a) long detector configuration (flightpath 100.47cm) and (b) shorter detector configuration (flightpath 64.82cm). Note the higher signal levels between the diffraction peaks in the lower panel, due to a higher acceptance angle. This configuration is used when necessary for higher sensitivity (but lower resolution) time-of-flight measurements.

Figure 11. Specular beam (upper panel) and off-specular (lower panel) time-of-flight runs for Si(001) - (2x1) with a 16.3 meV incident He beam. The broad inelastic feature at ca. 10.9meV is present at all final wavevectors. The sharp elastic peak in the lower panel is due to diffuse scattering from surface defects.

Figure 12. Surface phonon spectroscopic results for Si(001) - (2x1). (a) Experimental scan curves and principal energy transfer features (circles). (b) Calculations of Alerhand and Mele (solid lines) [69] superimposed on the experimental data. (c) Folded zone representation of the data superimposed on the calculation for a perfect (2x1) surface. The sharp disagreement suggests that a calculation including the effects of defects and disorder needs to be carried out.

Figure 13. He diffraction from a poorly ordered Ag(110) surface.

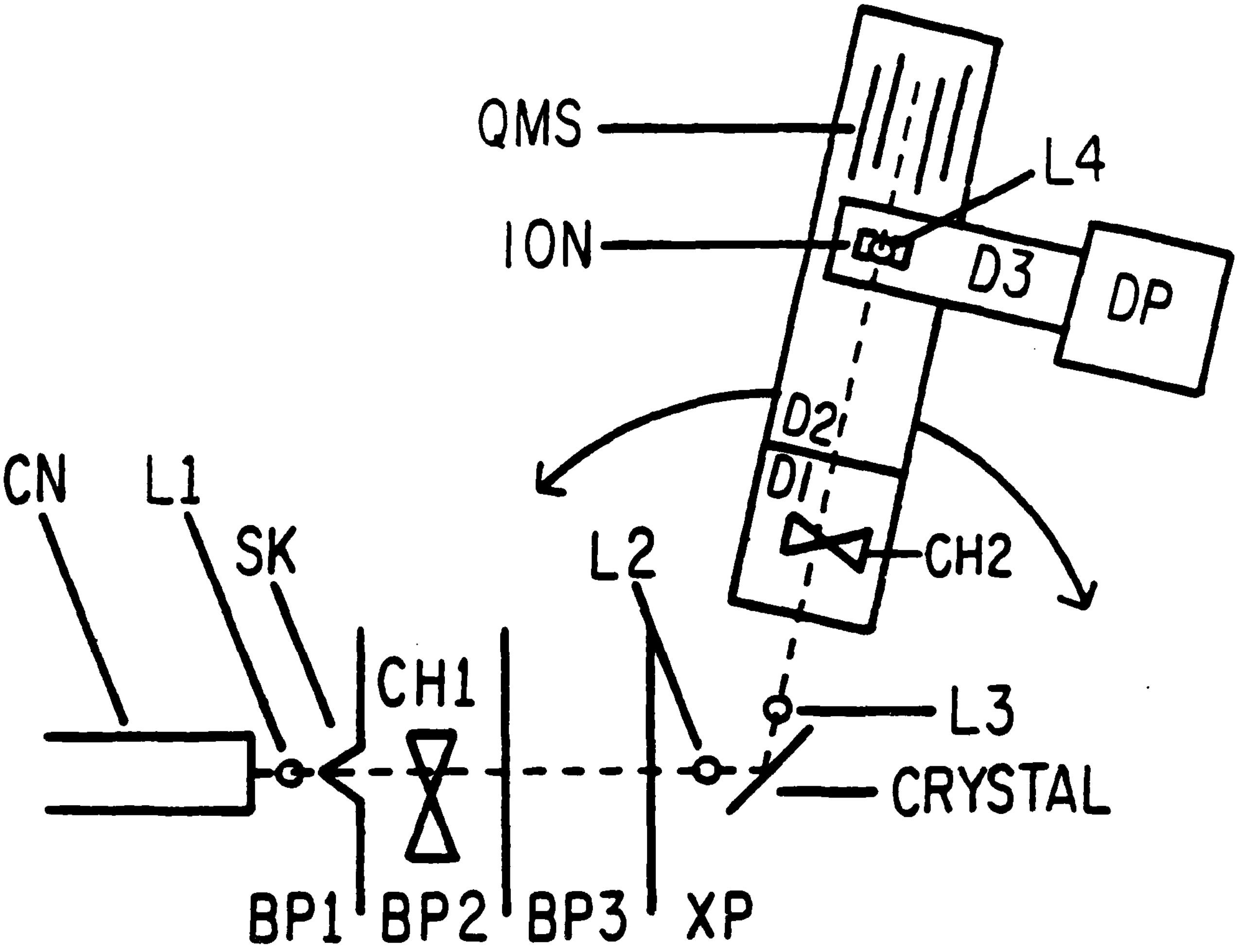
Figure 14. Specularly reflected time-of-flight distributions which demonstrate beam tunability from 1.56 - 0.57 Å^{-1}. Note the very surprising result that significant inelastic broadening grows in steadily with increasing beam energy. The extent of this broadening implies that future diffraction measurements on soft surfaces using beams with nozzle temperatures of ~ 150K should be taken in a time-of-flight (i.e. energy dispersed) mode to ensure that purely elastic intensities are obtained.

Figure 15. Schematic diagram of the second level of the new electron energy loss spectrometer. Provisions for other photochemical and time-resolved EELS measurements are indicated (see text).

Figure 16. Photograph of the new EELS instrument. The novel rotating lid can be clearly seen on the top of the chamber, below the long-stroke manipulator. Level one contains LEED, Auger, XPS, UPS, laser desorption, and quadrupole mass spectrometer capabilities. The second level (mu-metal shrouded) contains the EELS spectrometer.

Figure 17. (a) Early EELS spectrum (June 26, 1987) indicating successful performance of the electron optics. (b) First computer controlled scan showing data collected, at 5meV resolution, with 100 msec sampling times (Dec. 11, 1987). Operation with 20 msec sampling, without spectral distortion, has already been demonstrated.

Figure 1



Schematic representation of the ultra-high vacuum scattering apparatus. BP1, BP2, and BP3 are the three beam pumping stages, XP is the crystal pumping region, while D1, D2, and D3 are the three stages of differential pumping in the detector. D3 is pumped by a turbomolecular pump which is in turn backed by a diffusion pump. CN: cryogenic nozzle, SK: skimmer, CH1: incident beam chopper, CH2: post-collision chopper, L1-L4: laser-molecular beam intersection zones, ION: electron bombardment ionizer, QMS: quadrupole mass spectrometer. The instrument supports two beam sources which can be connected at five positions. The crystal-to-ionizer distance can be easily varied between 45 and 100 cm. The crystal chamber is equipped with a variety of surface analysis instruments which are not portrayed in this figure.

Figure 2

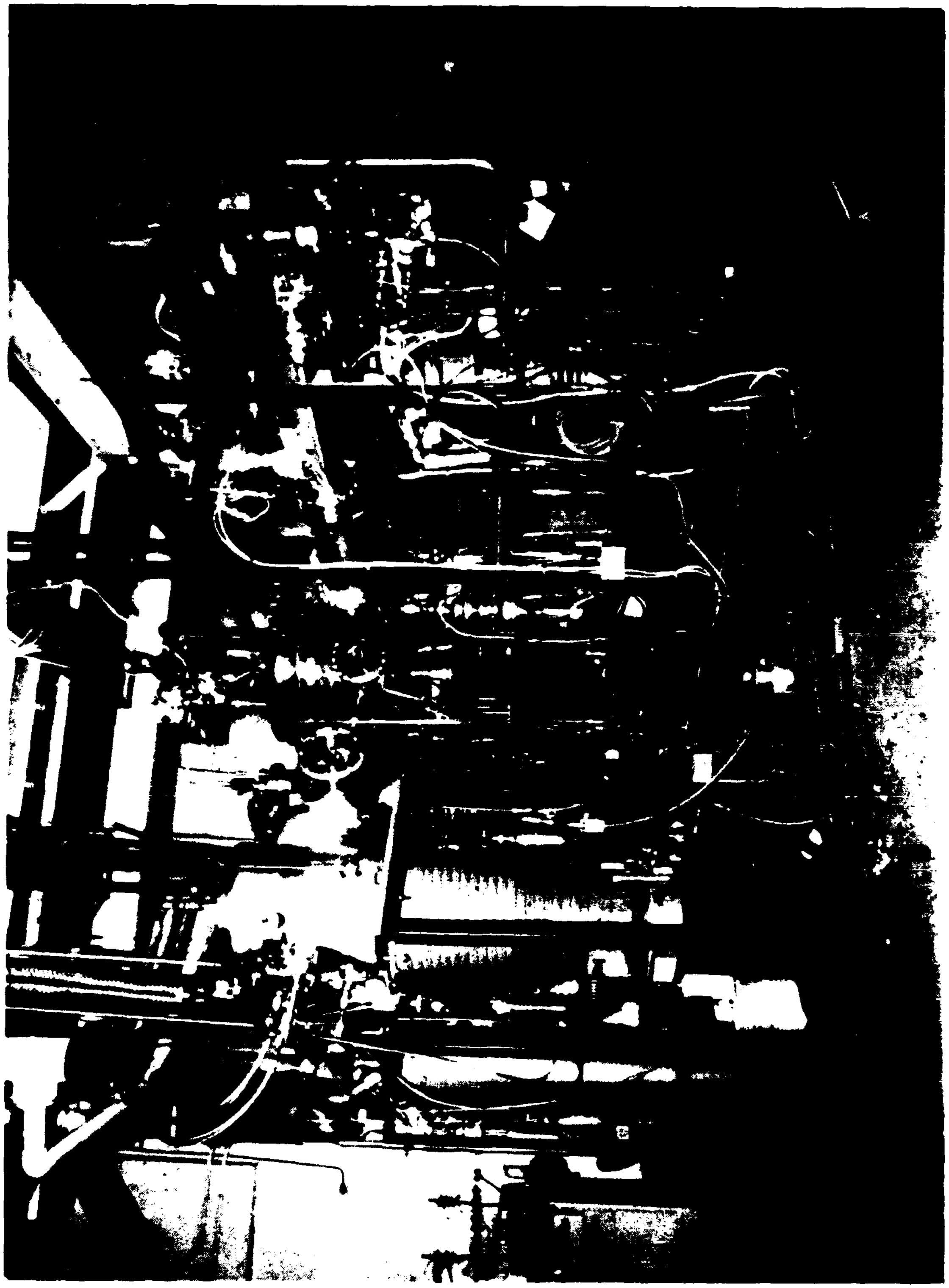


Figure 3

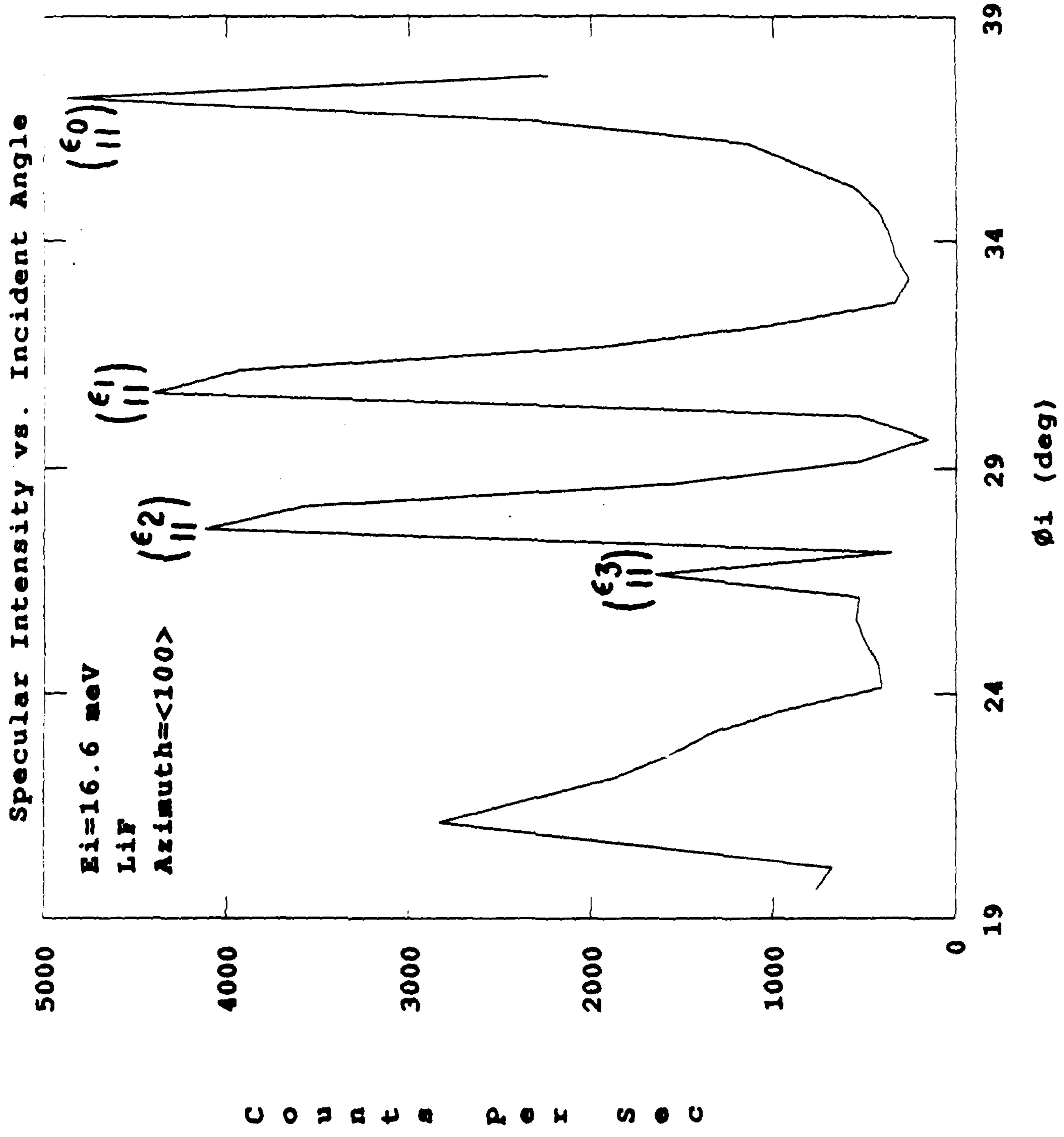

Specular Intensity vs. Incident Angle
Ei=16.6 meV
LiF
Azimuth=<100>
$\binom{\epsilon_0}{11}$
$\binom{\epsilon_1}{11}$
$\binom{\epsilon_2}{11}$
$\binom{\epsilon_3}{11}$
Counts per sec
5000
4000
3000
2000
1000
0
19
24
29
34
39
Ø1 (deg)

Figure 4

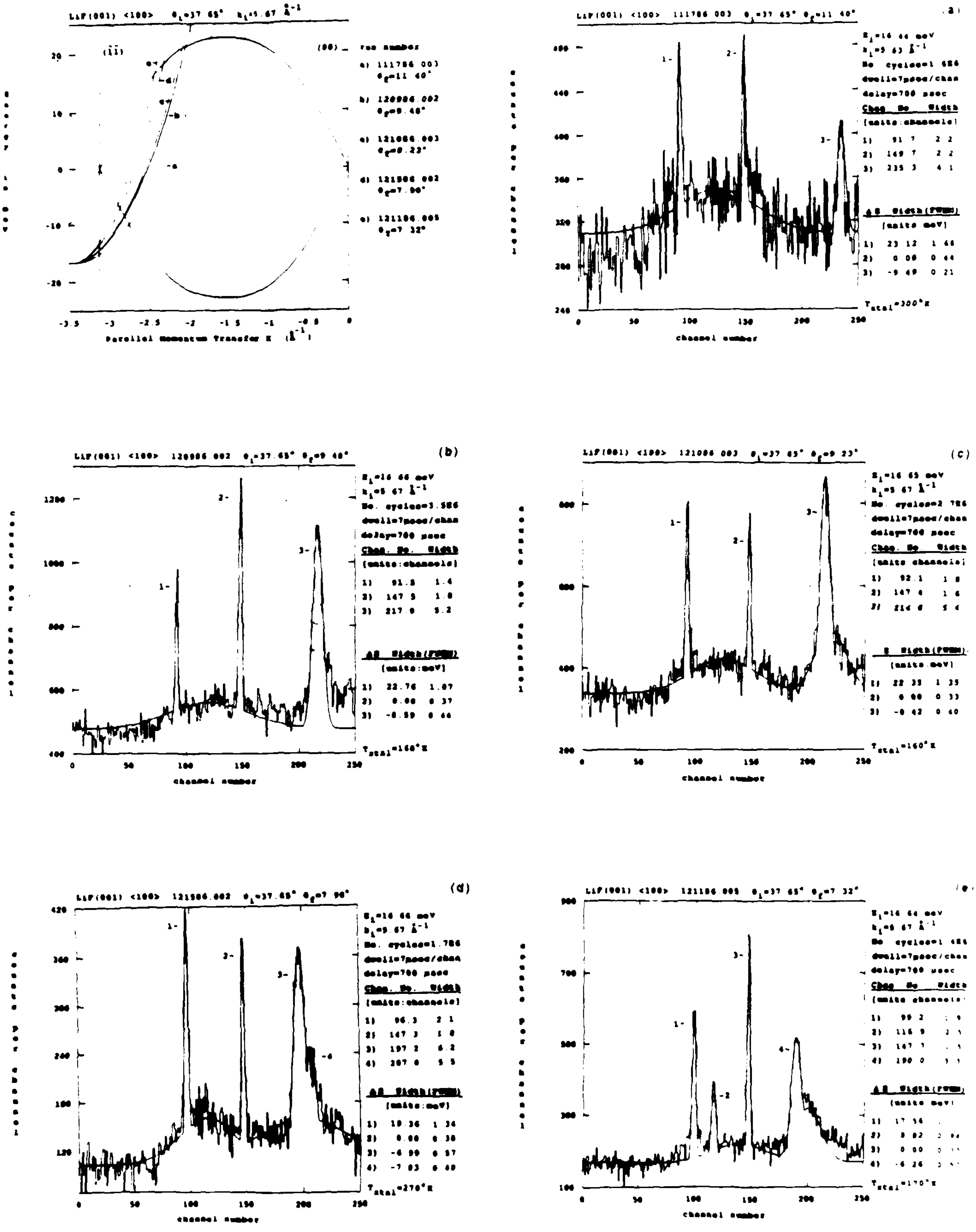

LiF(001) <100> θi=37.65° ki=5.67 Å-1
(1̄1̄)
(00)
run number
a) 111786.003 θf=11.40°
b) 120986.002 θf=9.48°
c) 121086.003 θf=8.23°
d) 121586.002 θf=7.90°
e) 121186.005 θf=7.32°
Energy Loss meV
Parallel Momentum Transfer K (Å-1)
(a)
LiF(001) <100> 111786.003 θi=37.65° θf=11.40°
Ei=16.66 meV
ki=5.63 Å-1
No. cycles=1.6E6
dwell=7μsec/chan
delay=700 μsec
Chan. No. Width
(units:channels)
1) 91.7 2.2
2) 149.7 2.2
3) 235.3 4.1
ΔE Width(FWHM)
(units meV)
1) 23.12 1.66
2) 0.00 0.44
3) -9.49 0.21
Txtal=300°K
counts per channel
channel number
(b)
LiF(001) <100> 120986.002 θi=37.65° θf=9.48°
Ei=16.66 meV
ki=5.67 Å-1
No. cycles=3.5E6
dwell=7μsec/chan
delay=700 μsec
Chan. No. Width
(units:channels)
1) 91.5 1.4
2) 147.5 1.8
3) 217.0 5.2
ΔE Width(FWHM)
(units:meV)
1) 22.76 1.07
2) 0.00 0.37
3) -8.59 0.44
Txtal=160°K
(c)
LiF(001) <100> 121086.003 θi=37.65° θf=9.23°
Ei=16.65 meV
ki=5.67 Å-1
No. cycles=2.7E6
dwell=7μsec/chan
delay=700 μsec
Chan. No. Width
(units channels)
1) 92.1 1.8
2) 147.6 1.6
3) 216.6 5.6
E Width(FWHM)
(units meV)
1) 22.33 1.35
2) 0.00 0.33
3) -8.42 0.40
Txtal=160°K
(d)
LiF(001) <100> 121586.002 θi=37.65° θf=7.90°
Ei=16.66 meV
ki=5.67 Å-1
No. cycles=1.7E6
dwell=7μsec/chan
delay=700 μsec
Chan. No. Width
(units:channels)
1) 96.3 2.1
2) 147.3 1.8
3) 197.2 6.2
4) 207.0 5.5
ΔE Width(FWHM)
(units:meV)
1) 19.36 1.34
2) 0.00 0.38
3) -6.99 0.57
4) -7.83 0.40
Txtal=270°K
(e)
LiF(001) <100> 121186.005 θi=37.65° θf=7.32°
Ei=16.64 meV
ki=5.67 Å-1
No. cycles=1.4E6
dwell=7μsec/chan
delay=700 μsec
Chan. No. Width
(units channels)
1) 99.2
2) 116.9
3) 147.7
4) 190.0
ΔE Width(FWHM)
(units meV)
1) 17.56
2) 8.02
3) 0.00
4) -6.26
Txtal=170°K

Figure 5

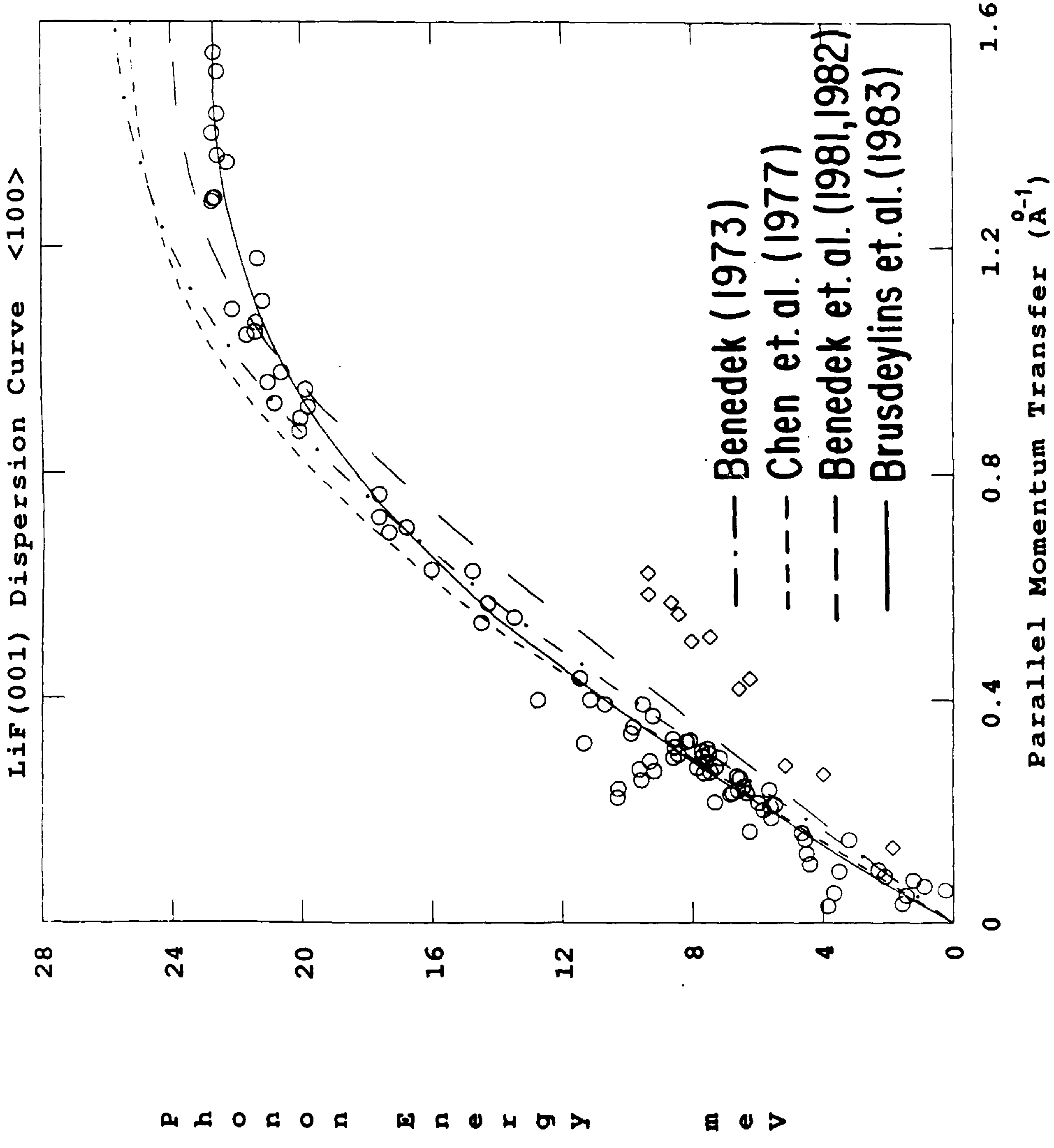

LiF(001) Dispersion Curve <100>
Phonon Energy meV
Parallel Momentum Transfer (Å^{-1})
0
4
8
12
16
20
24
28
0
0.4
0.8
1.2
1.6
Benedek (1973)
Chen et. al. (1977)
Benedek et. al. (1981,1982)
Brusdeylins et. al. (1983)

Figure 6

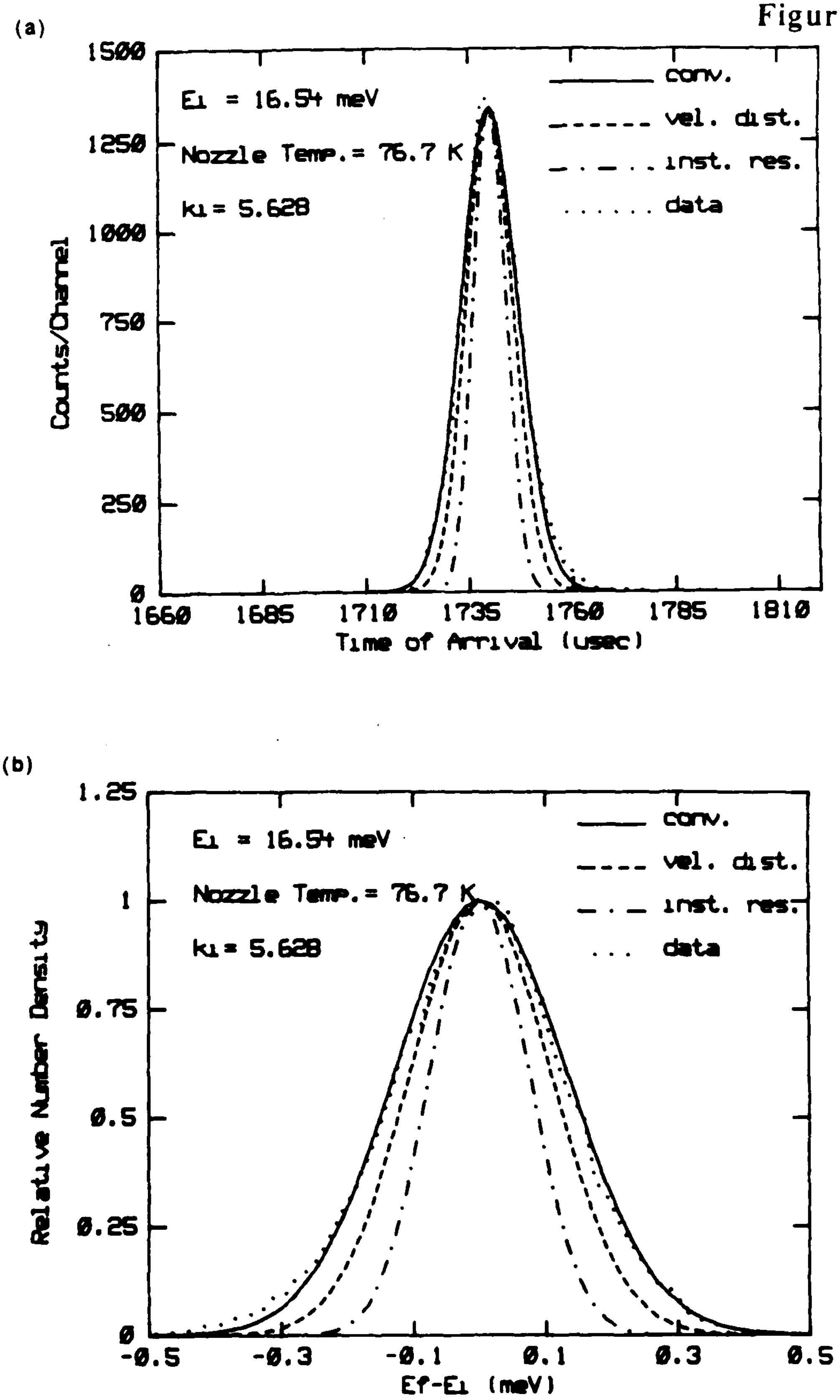

(a)
E1 = 16.54 meV
Nozzle Temp. = 76.7 K
k1 = 5.628
conv.
vel. dist.
inst. res.
data
Counts/Channel
1500
1250
1000
750
500
250
0
1660
1685
1710
1735
1760
1785
1810
Time of Arrival (usec)
(b)
E1 = 16.54 meV
Nozzle Temp. = 76.7 K
k1 = 5.628
conv.
vel. dist.
inst. res.
data
Relative Number Density
1.25
1
0.75
0.5
0.25
0
-0.5
-0.3
-0.1
0.1
0.3
0.5
Ef-E1 (meV)

Figure 7

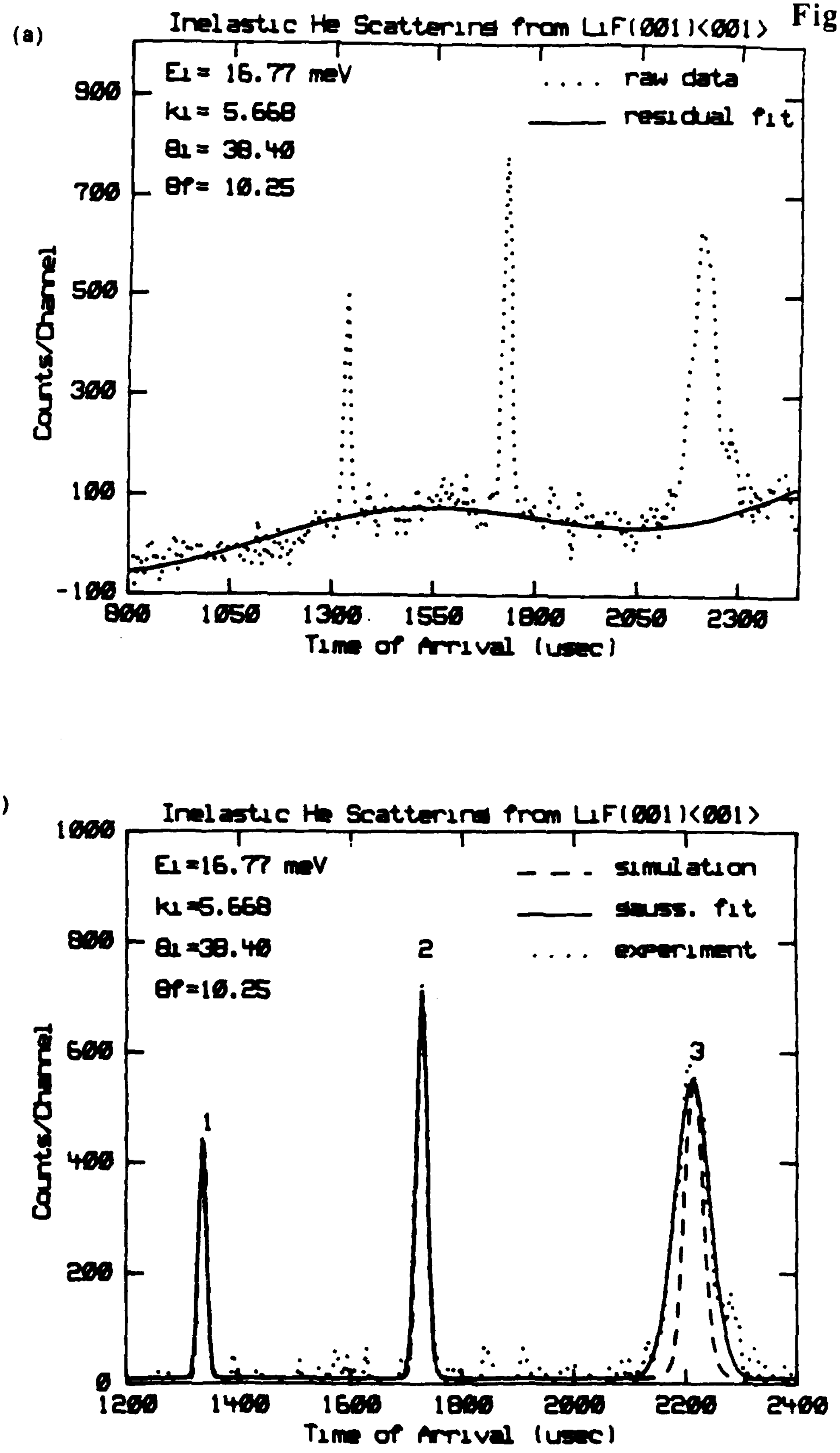
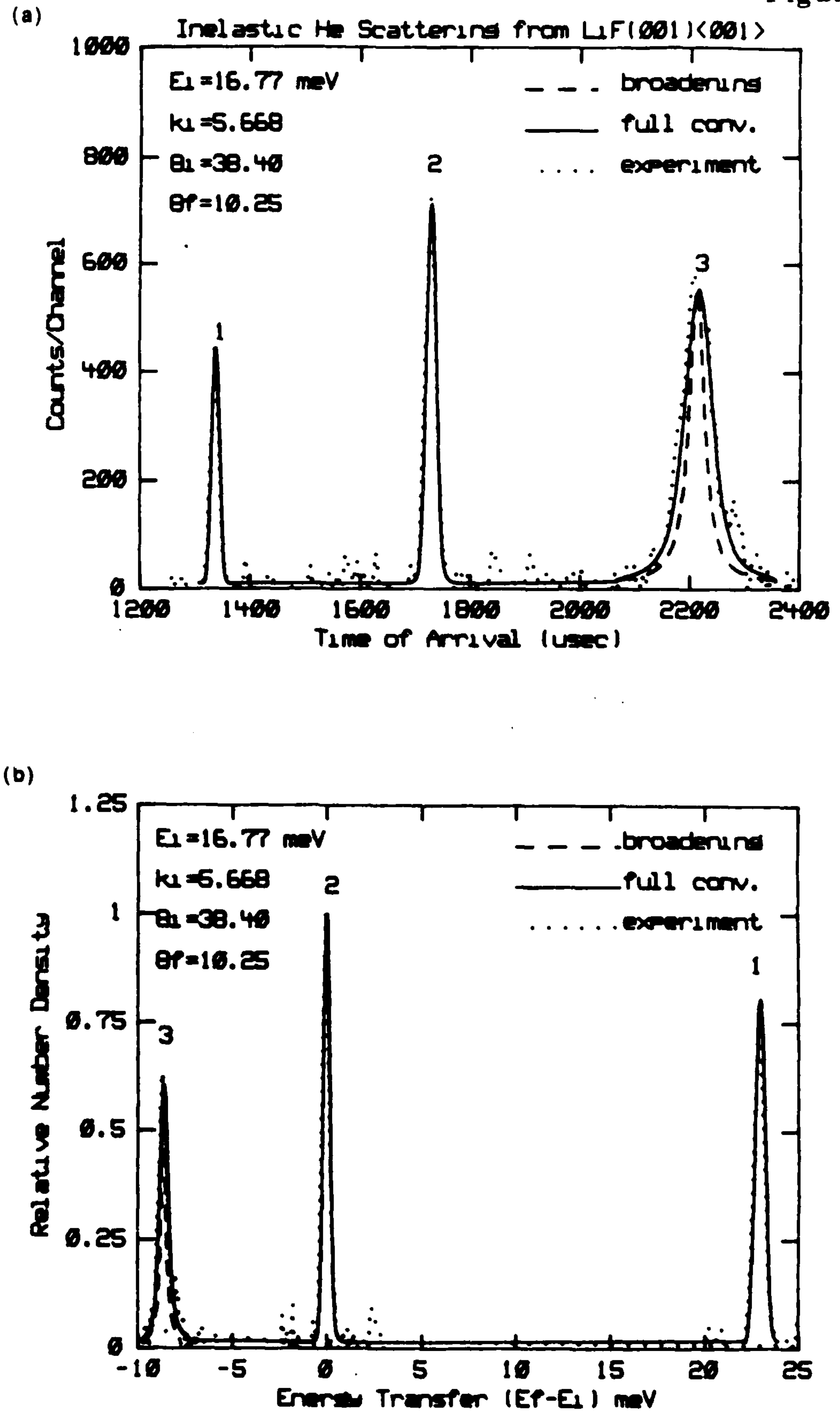

(a)
Inelastic He Scattering from LiF(001)<001>
Ei= 16.77 meV
ki= 5.668
θi= 38.40
θf= 10.25
.... raw data
—— residual fit
900
700
500
300
100
-100
Counts/Channel
800
1050
1300
1550
1800
2050
2300
Time of Arrival (usec)
(b)
Inelastic He Scattering from LiF(001)<001>
Ei=16.77 meV
ki=5.668
θi=38.40
θf=10.25
— — — simulation
—— gauss. fit
.... experiment
1
2
3
1000
800
600
400
200
0
Counts/Channel
1200
1400
1600
1800
2000
2200
2400
Time of Arrival (usec)

Figure 8


(a)
Inelastic He Scattering from LiF(001)<001>
Ei=16.77 meV
ki=5.668
θi=38.40
θf=10.25
broadening
full conv.
experiment
1
2
3
Counts/Channel
0
200
400
600
800
1000
1200
1400
1600
1800
2000
2200
2400
Time of Arrival (usec)
(b)
Ei=16.77 meV
ki=5.668
θi=38.40
θf=10.25
broadening
full conv.
experiment
3
2
1
Relative Number Density
0
0.25
0.5
0.75
1
1.25
-10
-5
0
5
10
15
20
25
Energy Transfer (Ef-Ei) meV

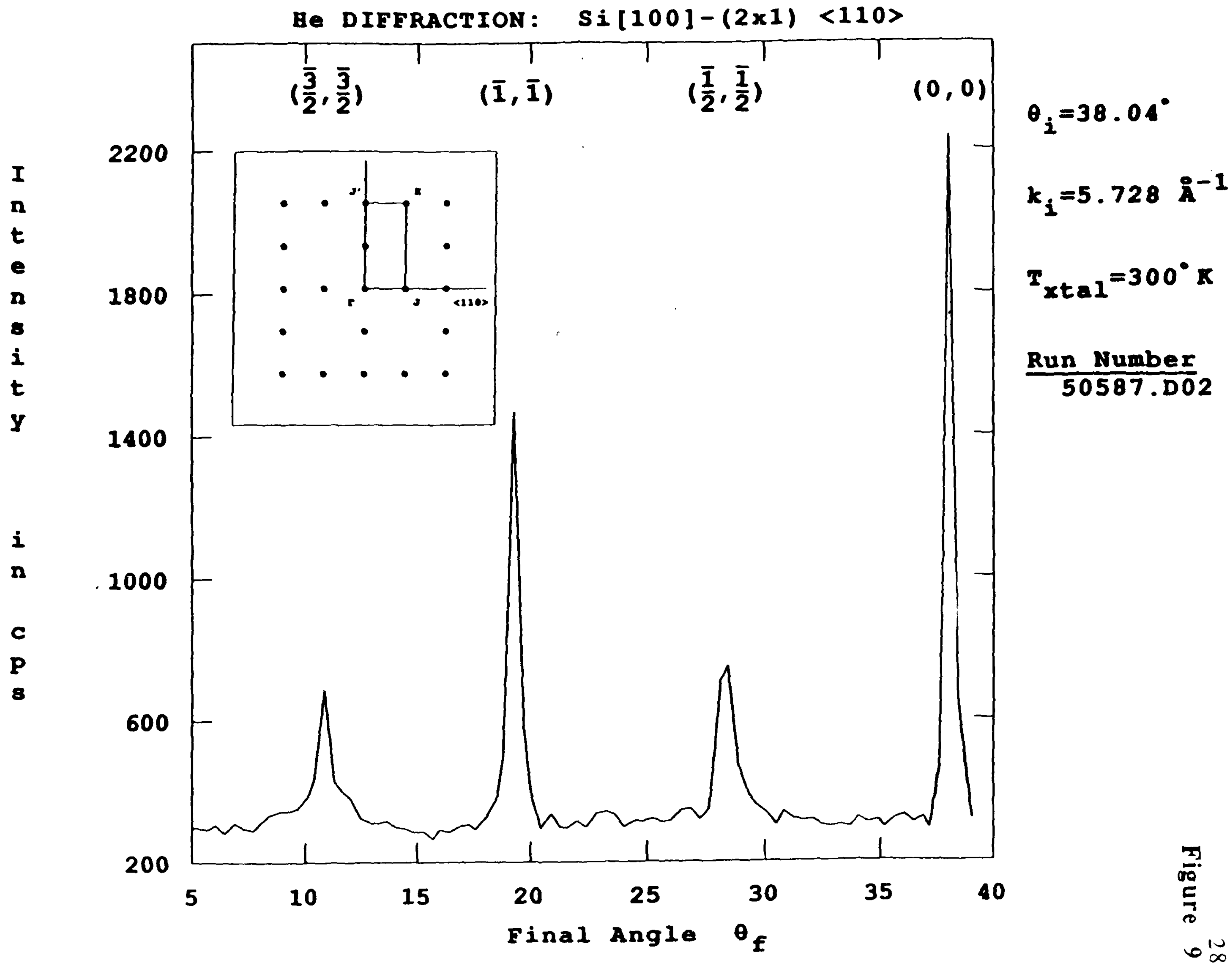

He DIFFRACTION: Si[100]-(2x1) <110>
$(\bar{\frac{3}{2}},\bar{\frac{3}{2}})$
$(\bar{1},\bar{1})$
$(\bar{\frac{1}{2}},\bar{\frac{1}{2}})$
(0,0)
θ_i=38.04°
k_i=5.728 Å^{-1}
T_{xtal}=300° K
Run Number
50587.D02
Intensity in cps
2200
1800
1400
1000
600
200
5
10
15
20
25
30
35
40
Final Angle θ_f
J'
K
Γ
J
<110>

Figure 9

Figure 10

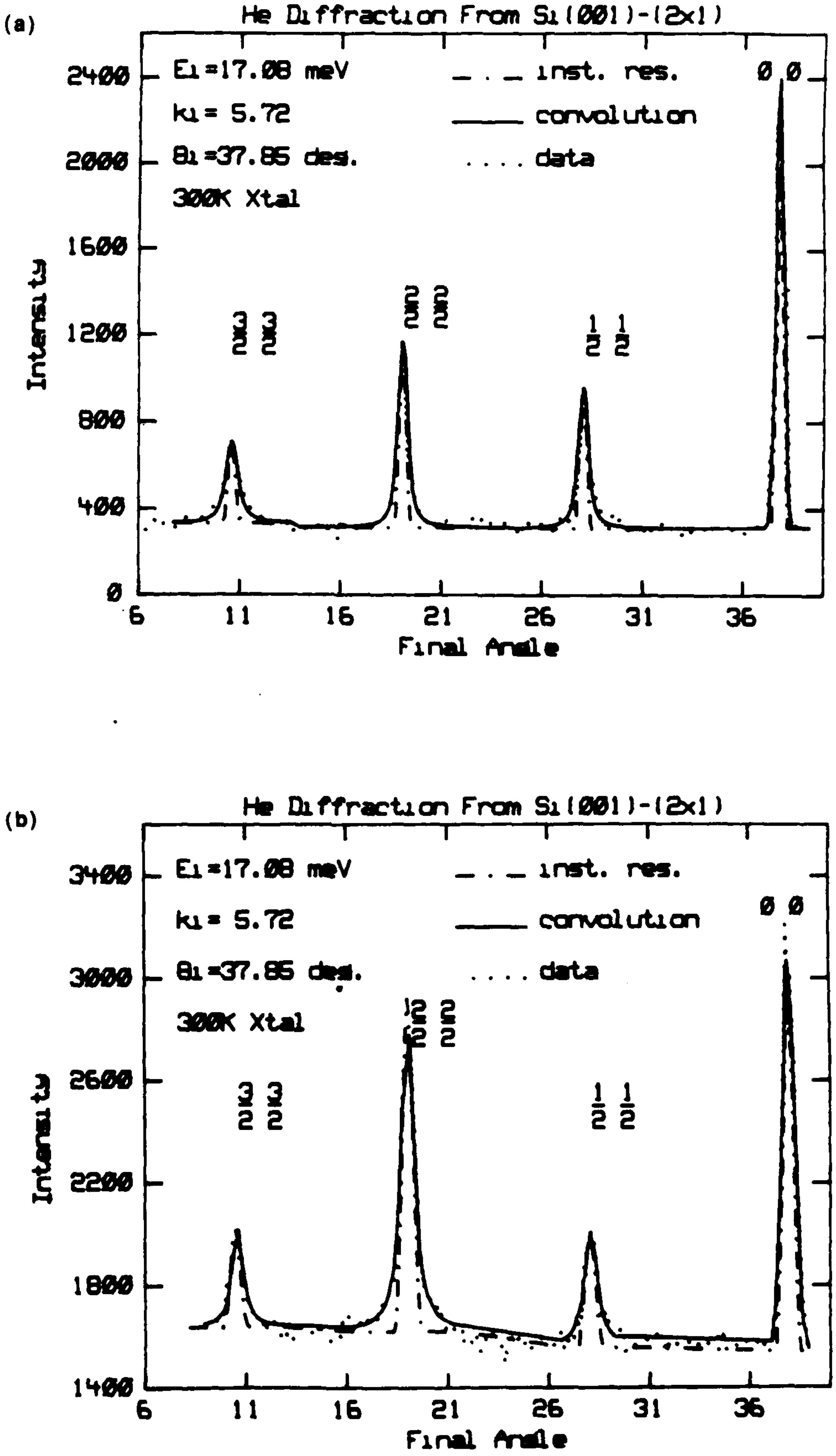

(a)
He Diffraction From Si(001)-(2x1)
Ei=17.08 meV
ki= 5.72
θi=37.85 deg.
300K Xtal
inst. res.
convolution
data
0 0
3/2 3/2
2/2 2/2
1/2 1/2
Intensity
0
400
800
1200
1600
2000
2400
6
11
16
21
26
31
36
Final Angle
(b)
He Diffraction From Si(001)-(2x1)
Ei=17.08 meV
ki= 5.72
θi=37.85 deg.
300K Xtal
inst. res.
convolution
data
0 0
3/2 3/2
2/2 2/2
1/2 1/2
Intensity
1400
1800
2200
2600
3000
3400
6
11
16
21
26
31
36
Final Angle

Figure 11

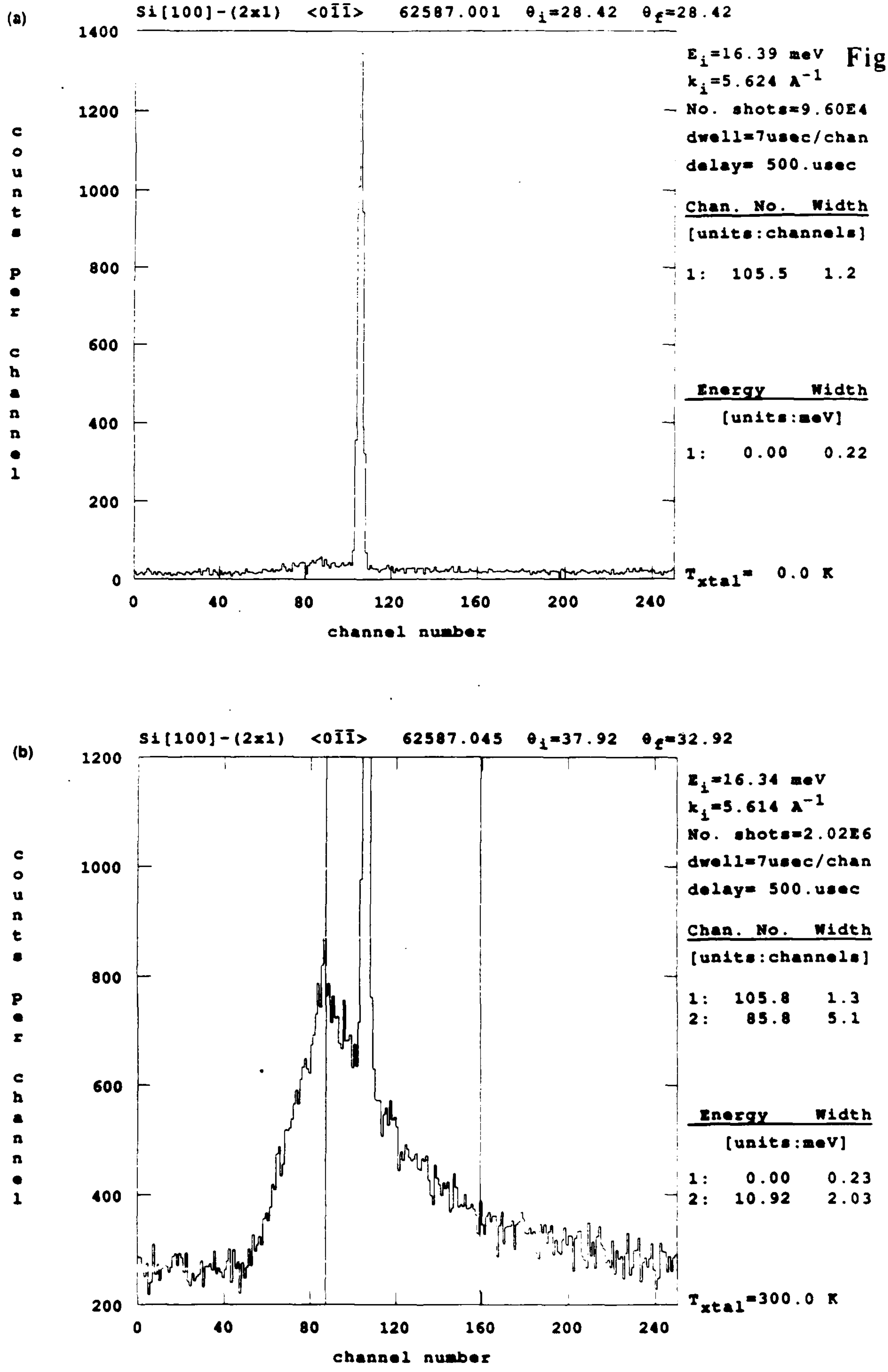
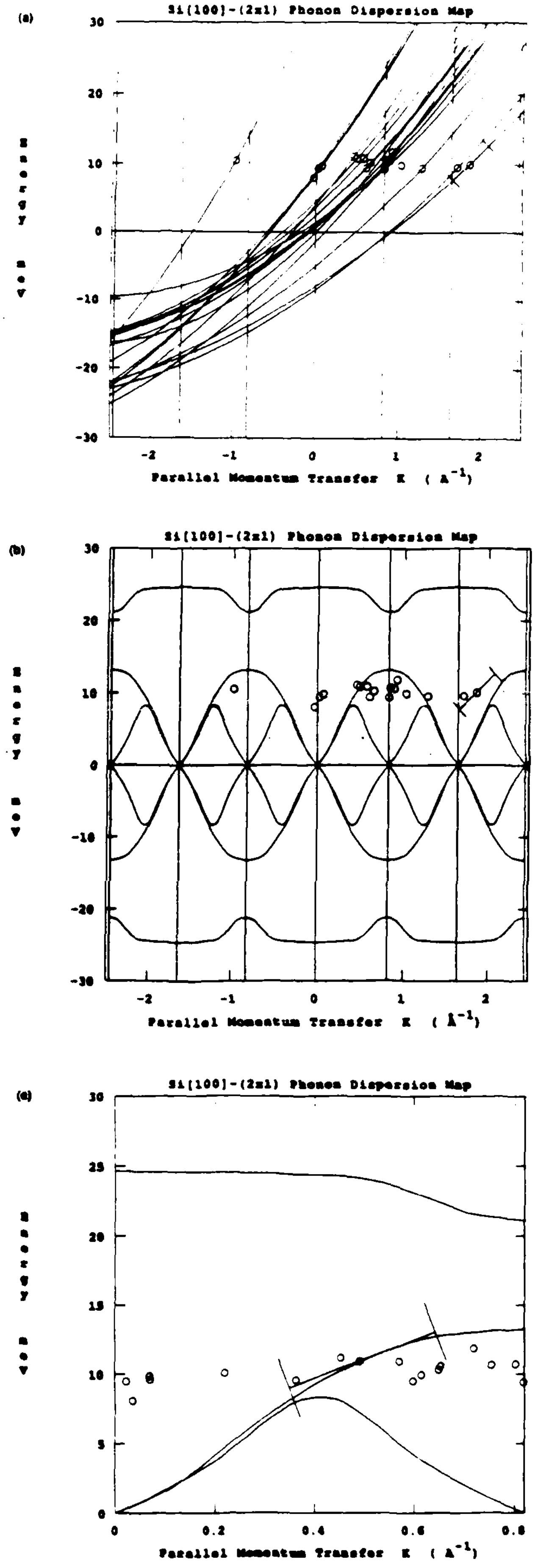

(a)
Si[100]-(2x1) <0$\bar{1}\bar{1}$> 62587.001 θ_i=28.42 θ_f=28.42
E_i=16.39 meV
k_i=5.624 Å^{-1}
No. shots=9.60E4
dwell=7usec/chan
delay= 500.usec
Chan. No. Width
[units:channels]
1: 105.5 1.2
Energy Width
[units:meV]
1: 0.00 0.22
T_{xtal}= 0.0 K
counts per channel
0
200
400
600
800
1000
1200
1400
0
40
80
120
160
200
240
channel number
(b)
Si[100]-(2x1) <0$\bar{1}\bar{1}$> 62587.045 θ_i=37.92 θ_f=32.92
E_i=16.34 meV
k_i=5.614 Å^{-1}
No. shots=2.02E6
dwell=7usec/chan
delay= 500.usec
Chan. No. Width
[units:channels]
1: 105.8 1.3
2: 85.8 5.1
Energy Width
[units:meV]
1: 0.00 0.23
2: 10.92 2.03
T_{xtal}=300.0 K
counts per channel
200
400
600
800
1000
1200
0
40
80
120
160
200
240
channel number

Figure 12


(a)
Si(100)-(2x1) Phonon Dispersion Map
Energy meV
30
20
10
0
-10
-20
-30
-2
-1
0
1
2
Parallel Momentum Transfer K (Å^{-1})
(b)
Si(100)-(2x1) Phonon Dispersion Map
Energy meV
30
20
10
0
-10
-20
-30
-2
-1
0
1
2
Parallel Momentum Transfer K (Å^{-1})
(c)
Si(100)-(2x1) Phonon Dispersion Map
Energy meV
30
25
20
15
10
5
0
0
0.2
0.4
0.6
0.8
Parallel Momentum Transfer K (Å^{-1})

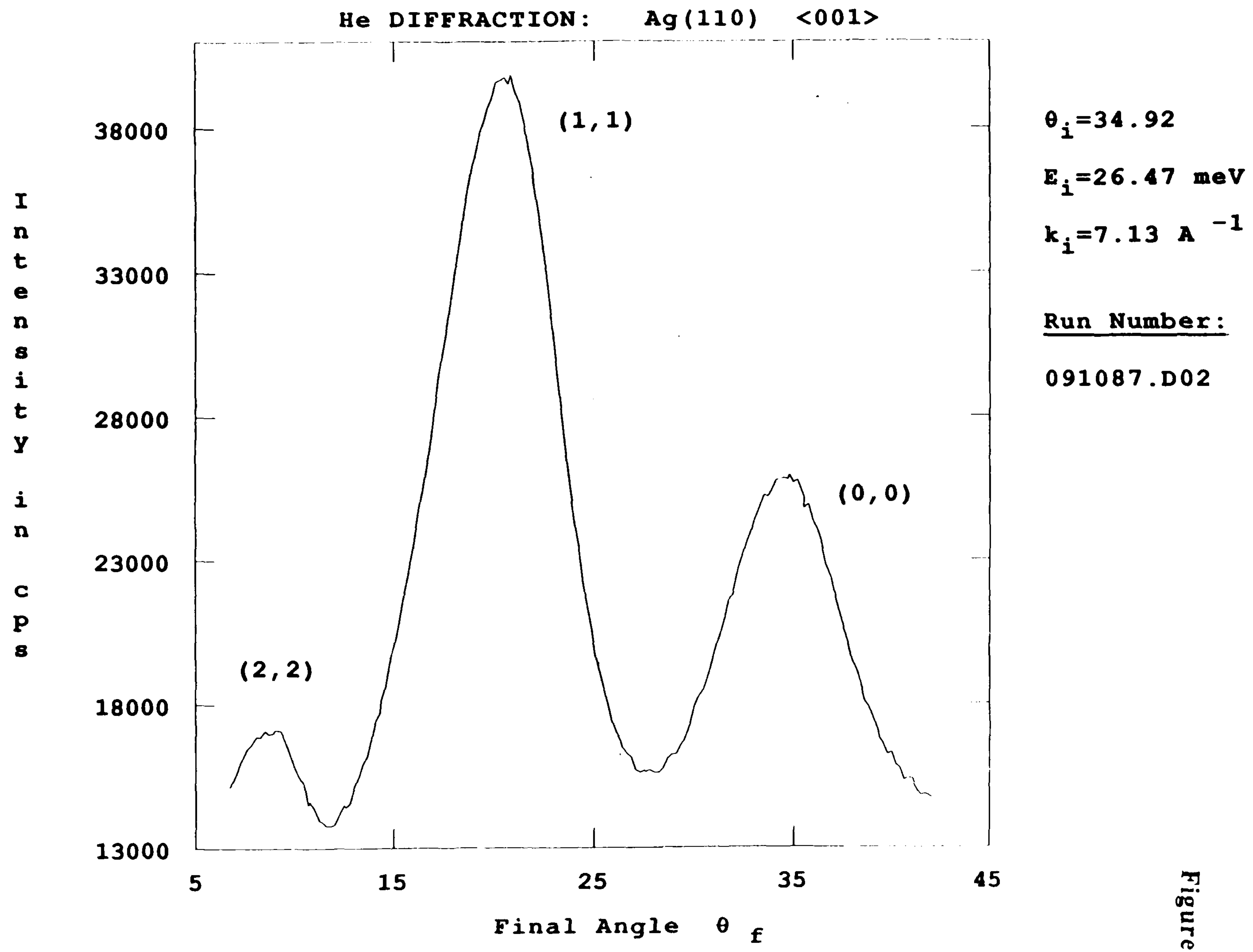

He DIFFRACTION: Ag(110) <001>
Intensity in cps
38000
33000
28000
23000
18000
13000
5
15
25
35
45
Final Angle θ f
(2,2)
(1,1)
(0,0)
θi=34.92
Ei=26.47 meV
ki=7.13 A -1
Run Number:
091087.D02

Figure 13

Figure 14

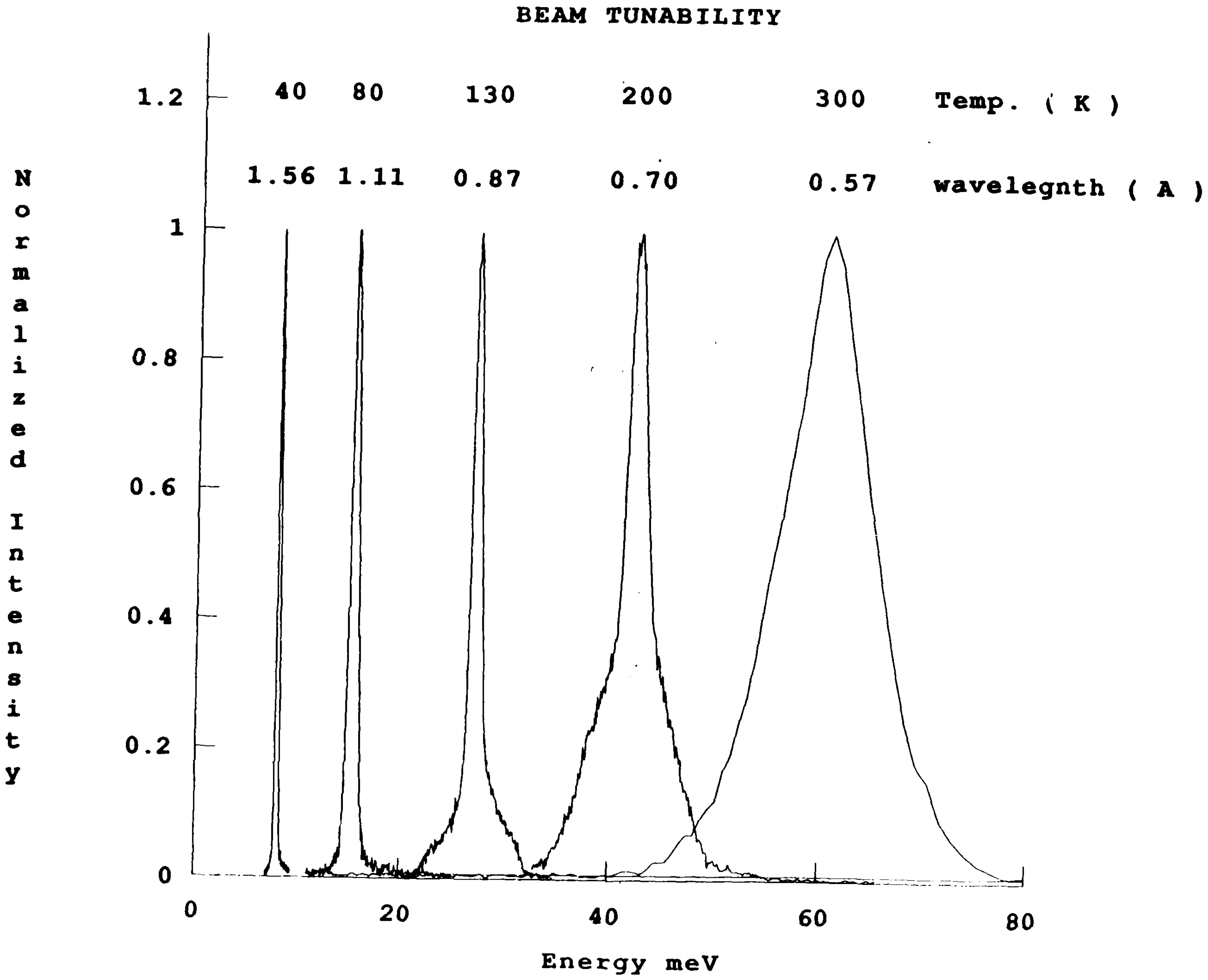

BEAM TUNABILITY
40
80
130
200
300
Temp. (K)
1.56
1.11
0.87
0.70
0.57
wavelegnth (A)
Normalized Intensity
1.2
1
0.8
0.6
0.4
0.2
0
20
40
60
80
Energy meV

Figure 15

Molecular Beam - EELS Instrument:
Electron Scattering Plane Schematic

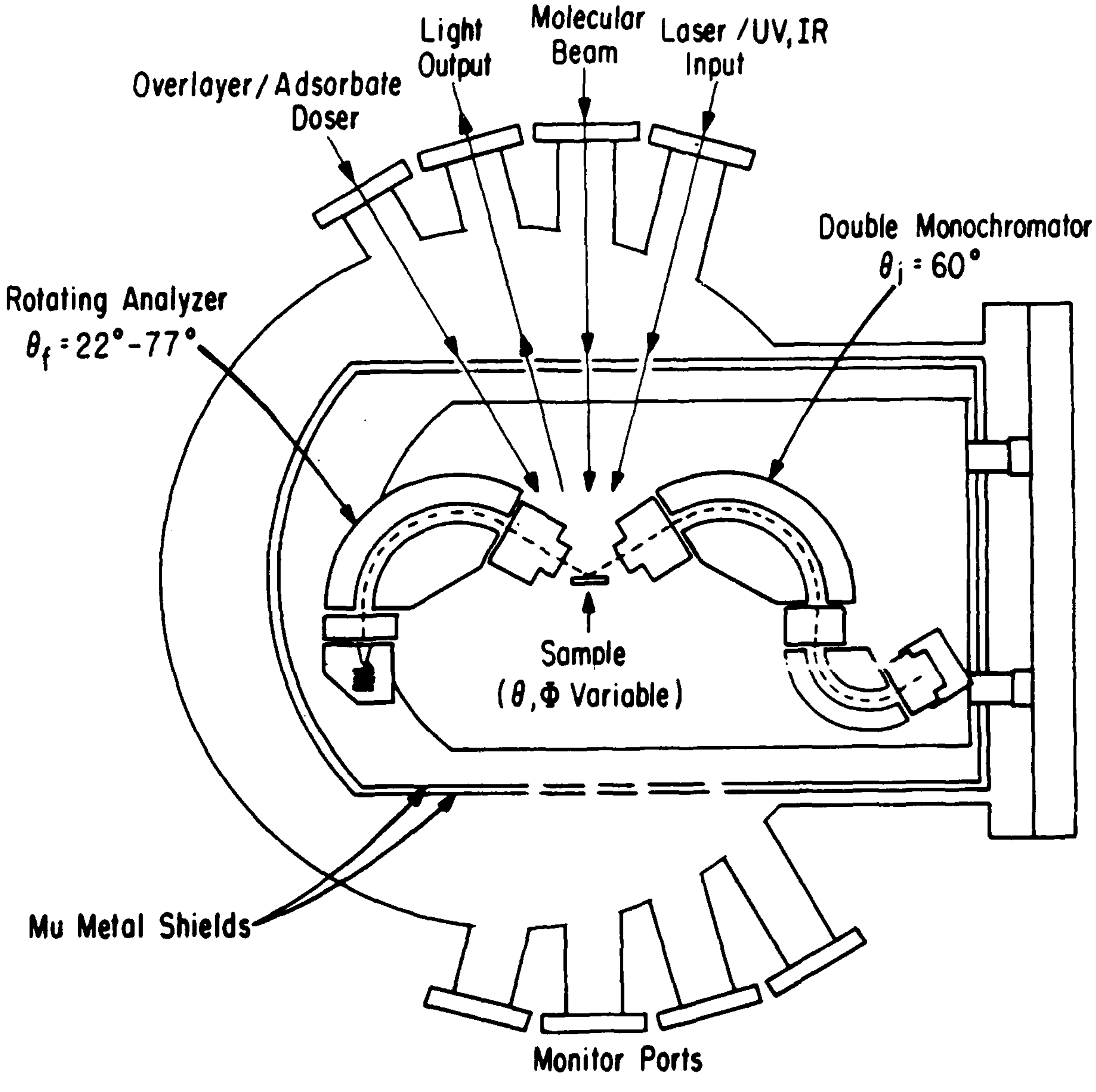


Figure 16

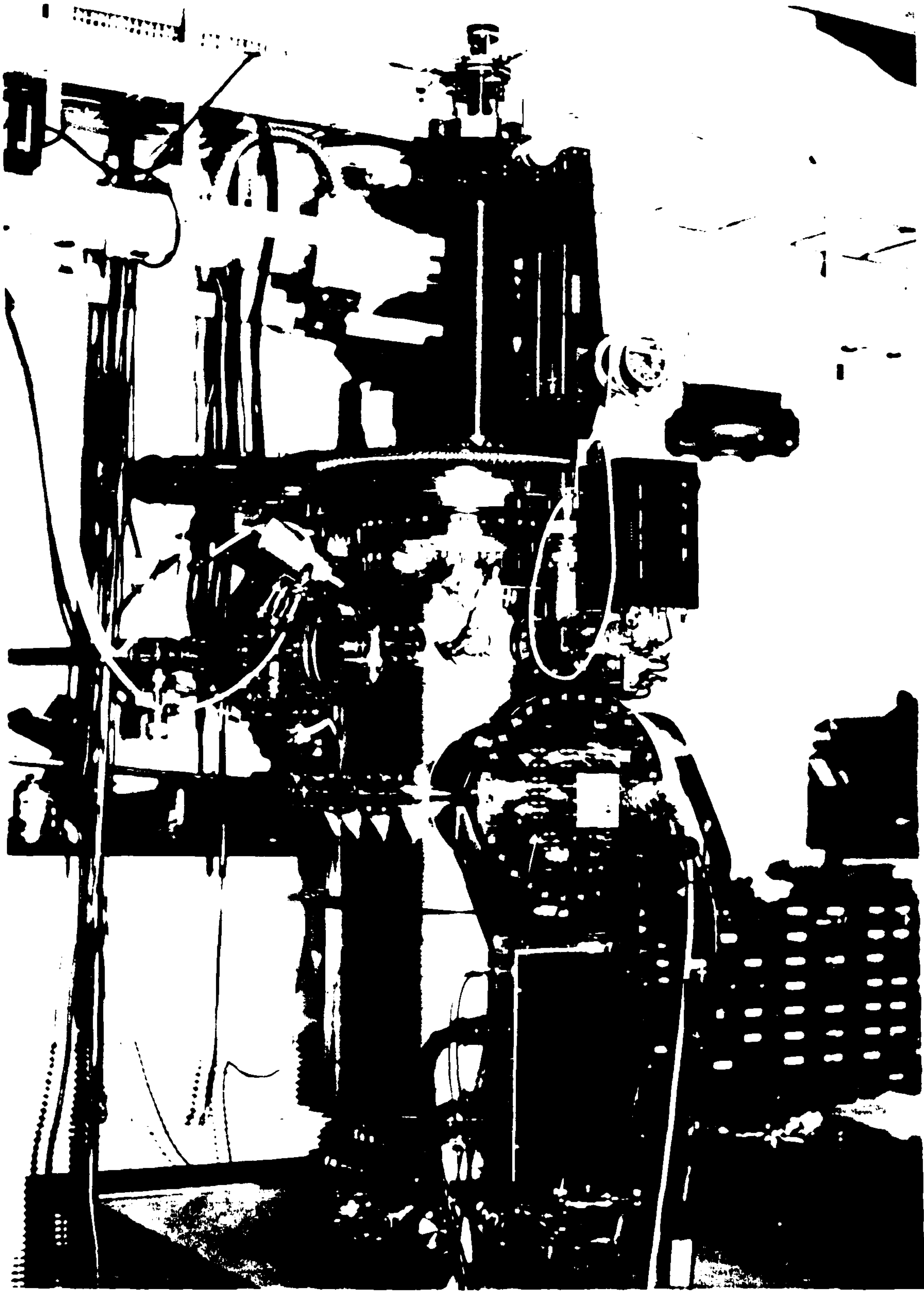
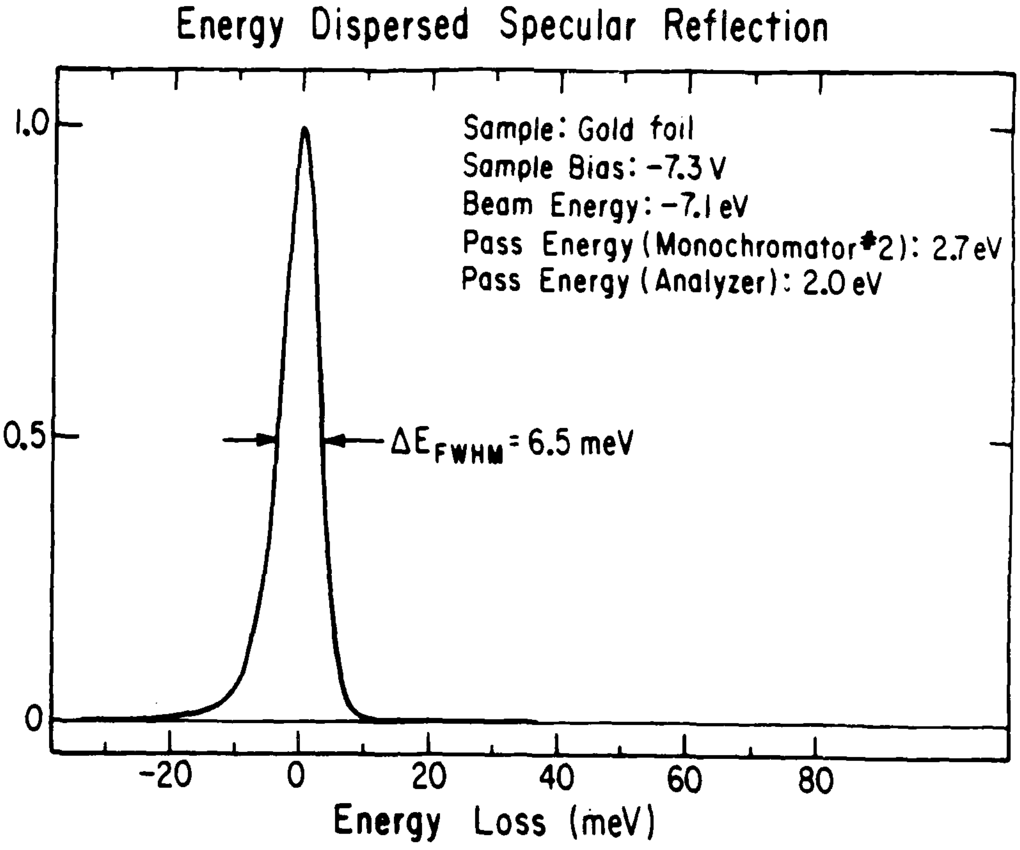
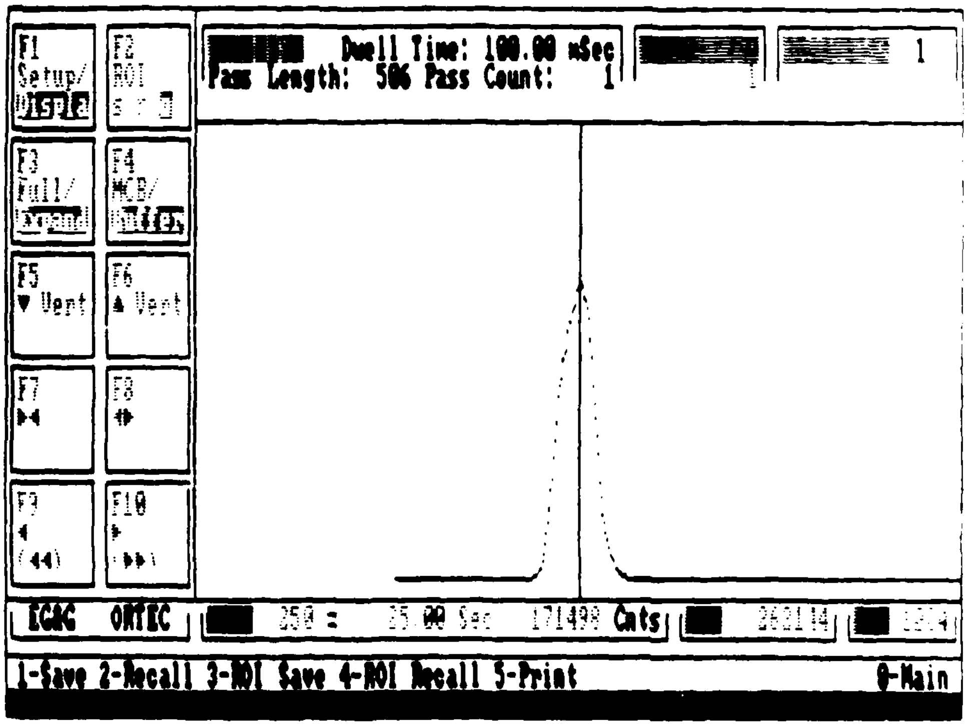


Figure 17

(a)



(b)



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Duell Time: 100.00 mSec
Pass Length:  506 Pass Count:    1
EG&G  ORTEC   250 =   25.00 Sec   171499 Cnts   260114
1-Save 2-Recall 3-ROI Save 4-ROI Recall 5-Print                0-Main
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VII. SUPPORT FOR INSTRUMENTATION

In addition to the AFOSR, which is the primary continuing source of financial support for the research program described in this proposal, several other sources contributed resources during the construction of the two new scattering laboratories. Other major DoD support came in the form of two Department of Defense - University Research Instrumentation Program grants:

Grant	Title	Period	Amount
DoD-URIP-AFOSR-85-0061	Instrumentation for Dynamics of Gas-Surface Interactions	01/01/85 - 12/31/85	$120,000 -Expended-
DoD-URIP-N-00014-86-G-0165	Instrumentation for Gas-Surface and Laser-Surface Interactions	07/15/86 - 09/30/87	$188,820 -Expended-

Partial support also came from the ONR for work in the EELS laboratory. Other non-DoD support came from The University of Chicago (support provided for complete renovation of two large rooms in the James Franck Institute), the NSF-Materials Research Laboratory at the University of Chicago, the Research Corporation, IBM in the form of a Faculty Development Award, the Camille and Henry Dreyfus Foundation in the form of a New Faculty Grant in Chemistry, the Louis Block Fund at the University of Chicago, and Dow Chemical USA (donation of an x-ray source for XPS studies).

VIII. PERSONNEL

In addition to the Principal Investigator, several undergraduates, graduate students, and postdoctoral fellows have particpated in this project during the past several years. The undergraduates were Mark Kramer, Joe Zwanziger, and Scott Silence. They went on to graduate school in chemistry at, respectively, Berkeley, Cornell, and MIT following their introductory research work at Chicago. The graduate students who have been in the PI's group during the of this project included, in order of seniority, Kevin Gibson, Yaw-Wen Yang (*N), Barbara Gans (*N), David Padowitz, Suzanne King (*N), Warren Menezes (E), Dan Koleske (*N), Kevin Peterlinz, and Glenn Tisdale (*E). [Note: (*) above indicates predominent support from this AFOSR grant; (N) denotes primarily associated with neutral particle scattering; (E) denotes primarily associates with electron scattering.] Postdoctoral fellows in the group during the past few years have included Dr. Wesley Natzle (now at IBM-Fishkill) and Dr. Larry Brown (now an Assistant Professor at Texas A&M). The first of several doctoral degrees to be awarded as a direct result of this AFOSR project was obtained by Yaw-Wen Yang in June, 1988. The title of this thesis was: "Inelastic Atom Surface Scattering: LiF(001), Si(001) Surface Phonons." Dr. Yang is presently a postdoctoral fellow with Professor Tom Engel in the chemistry department of the University of Washington at Seattle.

IX. OTHER DoD ACTIVITIES OF THE PI

The PI benefitted from technical discussions with several of the investigators in the AFOSR's surface science and chemical dynamics programs. He was also a charter member of the Defense Science Study Group at the Institute for Defense Analyses from 1985-1988. His background in gas-surface energy transfer and surface reaction kinetics, derived in part from this AFOSR project, proved to be quite useful in this DARPA sponsored program.

X. PUBLICATIONS AND INVITED PRESENTATIONS

X.1 Publications

Until last year, this AFOSR program consisted of a huge effort in apparatus design, fabrication, assembly, and testing which resulted in the successful construction of *two* novel surface scattering instruments. As can be seen from Section IV - Research Accomplishments, exciting scientific results are starting to come at a good and accelerating rate. A detailed manuscript on Si(001) is in final preparation for journal submission: Y.W. Yang, D.D. Koleske, and S.J. Sibener, "Observation of a Non-Dispersive 10 meV Surface Phonon on Si(001) - (2x1)", Phys. Rev. B., to be submitted. Other measurements on LiF(001), Si(001) - (2x1), Ag(110), and Ni(111) are being analyzed and readied for publication. Finally, a detailed paper describing the design and performance of the neutral particle scattering instrument is also being prepared at this time. Dr. Yaw-Wen Yang's Ph.D. thesis contains detailed information on this topic.

X.2 Invited Presentations

Invited presentations were presented by the PI at the following locations during the 1984-88 time period:

1984

1. University of Minnesota, Department of Chemistry
   Minneapolis, Minnesota

2. University of California at Berkeley, Department of Chemistry
   Berkeley, California

3. University of Maryland, Department of Chemistry
   College Park, Maryland

4. APS National Meeting; Symposium on New Advances in Surface Spectroscopy
   Detroit, Michigan

5. 17th Jerusalem Symposium on Quantum Chemistry and Biochemistry: Dynamics of Molecule-Surface Interactions
   Jerusalem, Israel

6. IBM Thomas J. Watson Research Center: Physical Sciences Colloquium
   Yorktown Heights, New York

7. First Bilateral US-Italy Symposium on Gas-Surface Interactions and Physisorption
   Charlottesville, Virginia

8. Gordon Conference on Atomic and Molecular Interactions, Brewster Academy
   Wolfeboro, New Hampshire

9. University of Chicago, Department of Chemistry
   Chicago, Illinois

10. Sandia National Laboratory
    Albuquerque, New Mexico

11. Iowa State University, Department of Chemistry
    Ames, Iowa

12. Cornell University, Department of Physics
    Ithaca, New York

13. University of Colorado at Boulder, Department of Chemistry
    Boulder, Colorado

1985

14. Tenth International Symposium on Molecular Beams
    Cannes, France

15. Dow Chemical U.S.A.
    Midland, Michigan

16. Faraday Discussion of the Royal Society of Chemistry: Physical Interactions and Energy Exchange at the Gas-Solid Interface, McMaster University
    Hamilton, Ontario, Canada

17. International Conference on Phonon Physics
    Budapest, Hungary

18. IVth International Conference on Vibrations at Surfaces
    Bowness-On-Windermere, England

19. Purdue University, Department of Chemistry
    West Lafayette, Indiana

1986

20. University of Illinois at Urbana, Condensed Matter Physics Colloquium
    Urbana, Illinois

21. University of Rochester, Department of Chemistry
    Rochester, New York

22. 41st Northwest Regional Meeting of the ACS,
    Symposium in honor of Dr. Paul Emmett
    Portland, Oregon

23. Aarhus University, Department of Physics
    Aarhus, Denmark

24. Jet Propulsion Laboratory, NASA Workshop on Atomic Oxygen Effects
    Pasadena, California

25. California Institute of Technology, Department of Chemistry
    Pasadena, California

1987

26. Loyola University, Department of Chemistry
    Chicago, Illinois

27. Texas A & M University, Department of Chemistry
    College Station, Texas

28. University of Texas at Austin, Department of Chemistry
    Austin, Texas

29. University of North Carolina at Chapel Hill, Department of Chemistry
    Chapel Hill, North Carolina

30. University of Pennsylvania, Department of Chemistry
    Philadelphia, Pennsylvania

31. 1987 Conference on the Dynamics of Molecular Collisions
    Olgebay Park, West Virginia

32. Gordon Research Conference on the Dynamics of Gas-Surface Interactions,
    Conference Chairman, Proctor Academy
    Andover, New Hampshire

33. National ACS Meeting:
    Symposium on Kinetics and Dynamics on Simple and Modified Surfaces
    New Orleans, Louisiana

34. Boston University, Department of Chemistry
    Boston, Massachusetts

<u>1988</u>

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

36. University of California at Irvine, Department of Chemistry
    Irvine, California

37. University of California at Los Angeles, Department of Chemistry
    Los Angeles, California

38. University of Pittsburgh, Department of Chemistry
    Pittsburgh, Pennsylvania

XI. BIOGRAPHICAL INFORMATION OF THE PRINCIPAL INVESTIGATOR

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.

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

Associate Professor of Chemistry, The James Franck Institute and The Department of Chemistry, The University of Chicago, July 1985 - .

Honors and Awards

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

Invited Lectureships

Physikalisches Institut der Universität Erlangen-Nürnberg, 1988

Consulting

Dow Chemical USA	(1982-1985, informal basis 1986-)
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 -).