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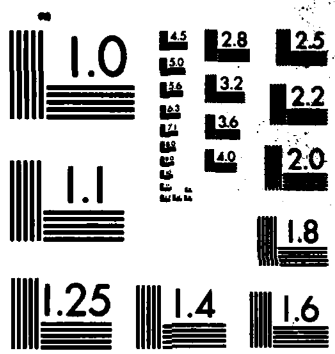
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ANNUAL REPORT

on

BASIC RESEARCH IN ELECTRONICS (JSEP)

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CONTRACTS F49620-82-C-0084
F49620-85-C-0078

JANUARY 1, 1985 TO DECEMBER 31, 1985

POLYTECHNIC INSTITUTE OF NEW YORK
MICROWAVE RESEARCH INSTITUTE
BROOKLYN, NEW YORK 11201

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER AFOSR-TR- 86-0078	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Basic Research in Electronics (JSEP)		5. TYPE OF REPORT & PERIOD COVERED ANNUAL REPORT 1 Jan. 1985 - 31 Dec. 1985
		6. PERFORMING ORG. REPORT NUMBER POLY-MRI-1446-85
7. AUTHOR(s) Arthur A. Oliner		8. CONTRACT OR GRANT NUMBER(s) F49620-85-C-0078
9. PERFORMING ORGANIZATION NAME AND ADDRESS Microwave Research Institute Polytechnic Institute of New York Brooklyn, New York 11201		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2305/A9
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Office of Scientific Research/NE Bolling Air Force Base Washington, D.C. 20332		12. REPORT DATE 31 December 1985
		13. NUMBER OF PAGES 86
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office) Same as #11		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Electromagnetics, microwaves, millimeter waves, waveguides and antennas, optics, x-rays, solid state interactions, solid state materials, information electronics, systems, image restoration

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This report presents a summary of the scientific progress and accomplishments on research projects funded by the Joint Services Electronics Program (JSEP) for the contract periods from 1 January 1985 through 31 December 1985. It does not contain information regarding accomplishments on research projects funded in other ways.

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20.

The Joint Services Electronics Program at the Polytechnic is the core of interdisciplinary research in electronics encompassing programs in the Departments of Electrical Engineering, Physics and Chemistry under the aegis of the Microwave Research Institute. The research encompassed by this program is grouped under three broad categories: Electromagnetics, Solid State Electronics and Information Electronics. The detailed projects (research units) comprising the complete program are listed in the Table of Contents.

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(December 31, 1985)

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1. A Theory for Optical Bistability in a Microparticle

Professor K.M. Leung

A theory was developed this past year that demonstrates that optical bistability can be exhibited by a resonant microparticle of nonlinear material. An optically bistable element of this type may yield an optical transistor that is the fastest and smallest, with the lowest switching power, of any to date.

Optically bistable or multistable devices have attracted much recent interest because of their potential applicability to the growing technology of ultra-high-speed optical computing and ultrafast optical image and signal processing. For applications in optical computing, they can be used as memory units or as switches and logic elements. For applications in optical signal processing, they can be used as pulse shapers, clippers or level slicers, discriminators and pulse amplifiers, analog-to-digital converters, and regenerative oscillators.

The basic ingredient for achieving optical bistability is a medium with a sufficiently high optical nonlinearity plus some kind of feedback mechanism. In general, it is highly desirable that the device consume as little power as possible. The switching power corresponds to the product of the area of the device and the incident light intensity, which must be close to the threshold value for the onset of optical bistability.

Our recent theoretical work shows that a microparticle with a size much less than the wavelength of the incident electromagnetic radiation is capable of exhibiting optical bistability and hysteretic behavior. Owing to the small size of the particle, the switching power is significantly reduced. In addition, one can take advantage of the Mie resonance within the particle to enhance the internal electromagnetic fields, thus reducing the required threshold intensity for the onset of optical bistability by as much as a few orders of magnitude. Switching occurs either by varying the input intensity at a fixed frequency detuned by about a linewidth away from the resonance, or by sweeping the frequency of the input light with the intensity fixed above some threshold value. It should also be pointed out that the relatively large surface-area-to-volume ratio in a microparticle will certainly ease the problem of overheating of the device. Moreover, switch-down times can be drastically reduced, for example, in cases where the carrier relaxation is due to exciton surface recombination. Our theoretical predictions of these novel optical devices are currently being tested experimentally in our Microparticle Photophysics Laboratory.

2. Complex Resonances for Fin-Like Target Features

Dr. H. Shirai and Professor L.B. Felsen

The discrete complex resonance frequencies of a scatterer, which correspond in the time domain to exponentially damped oscillations, are important elements in target classification and identification. By direct numerical techniques applied to an integral equation treatment of the scattering problem, it has been found that, for an $\exp(-i\omega t)$ time dependence, the resonances are distributed throughout the lower half of the complex frequency (ω) plane. For smooth convex target shapes, it has been shown that a grouping into "layers" that are essentially parallel to the real frequency axis is phenomenologically significant since the collective effect of the oscillatory resonances in each layer can synthesize a self-consistent wavefront field that travels around the object. This wavefront-resonance equivalence has important implications for constructing and interpreting the complex resonance map.

For fin-like scatterers as exemplified by thin flat plates or strips, wavefronts tracked self-consistently between the edges by the geometrical theory of diffraction (GTD) yield only the first layer of resonances. Conventional GTD, one of the most useful methods for analyzing high frequency scattering, therefore leaves unexplained the physical mechanism that generates the resonances in the other layers. This gap in understanding has now been closed by our discovery that such resonances result from previously ignored higher order edge diffraction phenomena, which lead to higher order surface rays. Incorporating these into a modified GTD has led not only to the accurate construction of the full resonance map for strip and disk model targets*, but has suggested that higher order edge diffraction GTD as a whole should be re-examined in the light of these modifications.

3. Microstrip Leaky Wave Strip Antennas

Professor A.A. Oliner

The theory has been developed for a new class of leaky wave antennas of particularly simple geometric configuration -- just a uniform length of microstrip line--but operating in its first higher mode near to cutoff.

The behavior of microstrip line higher modes near cutoff has been a source of confusion and controversy since the late 1970's, when it was found (by Ermert) that no real solutions for the propagation constant were possible in that region. That observation was correct, but incomplete, and the region was simply called a "radiation" region, with no further practical implications. Shortly thereafter, and independently, it was shown (by Menzel) that a traveling wave antenna of short length could be built using microstrip line fed in its first higher mode and operated near to cutoff. Menzel assumed that the propagation constant of that mode was real in the very region Ermert had said no such solutions exist. His approximate analysis and his physical reasoning were therefore also incomplete. No attempt was made by anyone to reconcile the discrepancy or to explain the relation between the two papers.

The theory developed this year clarifies the nature of this "radiation" region, explains why Menzel's antenna works as well as it does, and shows how that class of antennas can be designed to work properly. First, it is shown by means of a steepest descent procedure that the continuous spectrum in the "radiation" region is characterized

* H. Shirai won 2nd prize in the URSI Student Best Paper contest at the International URSI-AP/S Symposium, Vancouver, Canada, June 1985 (paper co-authored with L.B. Felsen, entitled "Modified GTD for Generating Complex Resonances for Flat Strips and Disks").

in a highly convergent manner by essentially a single leaky mode. Next, the power in that leaky mode is contained, over much of the range of operation, in both a surface wave and a space wave; however, the dominant portion of the power resides in the space wave, which results in horizontally polarized radiation at some angle. Then, once the relation between the "radiation" region and leaky modes becomes clear, it is evident that Menzel's antenna is indeed a leaky wave antenna that was made too short.

An accurate analysis based on a horizontal transverse resonance was developed to determine the properties of these leaky modes and to examine how a structure as simple as a uniform length of microstrip line would behave as an antenna. In addition to explaining all the performance features of Menzel's structure, the theory illuminates the advantages and limitations of this new class of antennas, and indicates what can be expected in terms of beam angle and beam width as a function of frequency and dimensional variations.

SECTION I

ELECTROMAGNETICS

SECTION I: ELECTROMAGNETICS

A. NEW PHYSICAL EFFECTS INVOLVING OPEN DIELECTRIC STRUCTURES

Professor A.A. Oliner

Unit EM5-1

1. OBJECTIVE(S)

This study is concerned with guiding, radiating and scattering effects involving open dielectric structures. Before our investigation, almost all of the published literature on these topics involved a surface wave incident on a dielectric junction or grating at normal incidence, where the resulting boundary-value problem is two-dimensional, and TE and TM modes do not couple to each other. In many open dielectric waveguides and antennas for millimeter-wave integrated circuits and for integrated optics, however, the surface wave is obliquely incident. The boundary-value problems then change from the scalar, two-dimensional ones to vector three-dimensional ones, and the TE and TM modes no longer remain independent but are coupled together. The vector nature of these problems introduces new mathematical challenges, but, more interestingly, the mode coupling produces a rich variety of interesting and sometimes unexpected new physical effects. In our studies so far, we have found that a number of such effects arise in potentially important guiding and radiating structures, either leading to possible performance problems or providing new opportunities if those effects can be properly utilized.

We propose to continue to explore these physical effects on old and new types of dielectric structure. It is, of course, necessary to first obtain the appropriate mathematical solutions; those solutions, or the approaches used to obtain them, are often of interest in themselves. We will then examine the physical consequences of those solutions, and, where appropriate, assess their implications for device performance in millimeter-wave integrated circuits and integrated optics.

2. SUMMARY OF RECENT PROGRESS

Major effort during the past year was placed on three topics, and some results obtained on these topics are discussed here. These topics are: (a) Two-dimensionally periodic grooved dielectric structures, (b) Dielectric image guide leaky wave antenna using periodic metal strips, and (c) Leaky higher modes on uniform microstrip line.

(a) Our earlier studies revealed that a very interesting variety of new physical effects occurs when a surface wave is incident obliquely on a dielectric waveguide that is grooved periodically in one dimension; those physical effects, which are absent when the incidence is normal instead of oblique, include extra stop bands due to TE-TM mode coupling, anisotropy effects such as beam steering, radiation at skew angles, and strong cross-polarization effects. A dielectric waveguide periodically grooved in two dimensions should offer increased flexibility in parametric dependences, and therefore the possibility of additional new effects.

SECTION I: ELECTROMAGNETICS

The first phase in the analysis of guidance by a two-dimensionally periodic dielectric waveguide involves the propagation of waves in an infinite medium that is uniform in height, say, but has periodic variations in the two orthogonal horizontal directions. That phase was largely solved earlier by us, and results for it were included in last year's annual report. The second phase, which changes the analysis from a scalar problem to a vector one, includes a variation along the axial (height) direction, and corresponds to a wave propagating at an arbitrary angle in such a medium. The third phase takes a slice of this periodic medium and places it between uniform regions, thereby creating a dielectric waveguide that is periodically modulated in two dimensions. The analysis requires mode matching at the interfaces between regions, and yields information with respect to wave scattering by such an interface or to the dispersion properties of these modulated waveguides.

The analyses for the second and third phases were completed during the past year, and results were obtained for the wavenumber curves for several different situations. Those wavenumber plots can become very involved because of TE-TM interactions as well as the two-dimensional nature of the geometry. If interpreted properly, the complexity offers new flexibility in performance. These results are reported in a recent Ph.D. thesis.[1]

(b) Although the literature contains many experimental papers on dielectric image guide leaky wave antennas using periodic metal strips, there is no theory available with which such antennas can be designed. Since this type of antenna is of significant interest for application to millimeter wavelengths, and since we have previously furnished the only successful theory for such antennas that use periodic grooves, we felt that we would be performing a service by undertaking this study. In fact, we had in mind a novel phrasing for the transverse resonance portion of this study, and we believed that the discontinuity evaluation portion of it would be relatively easy. Unfortunately, the technique we had in mind, small obstacle theory in a multimode context,[2] turned out be less accurate than expected. The discontinuity evaluation thus became the major focus of the effort, but we have produced some new solutions to the canonical consituent problem involved.

That constituent discontinuity problem is the scattering of an electromagnetic wave incident at an arbitrary angle on a metallic strip grating placed on a dielectric half space when the grating period is large enough to produce several propagating spectral orders. In microwave terms, the grating is multimode. To our knowledge, prior partial solutions in the literature are purely numerical and are therefore of little use to us since the grating is to be used as a constituent in a larger problem. We have used several analytical approaches, all related to integral equation techniques, that satisfactorily address the problem and yield numerical solutions that in combination cover all parameter ranges. These scattering results are of interest in themselves, but they will next be applied to the original antenna problem described above. Further details are presented in the next section.

(c) It is not generally recognized that higher modes on uniform microstrip line become leaky in the vicinity of cutoff. The first analysis of the behavior of such higher modes near cutoff[3,4] was incomplete and therefore confusing. It pointed out that no real solutions existed there, but it did not recognize that complex solutions did. Such complex solutions corresponds to leaky waves, which have important implications for antennas. During this past year, we have performed an accurate analysis of these higher modes and we have determined their leakage properties as a function of various parameter variations. We also show that the continuous spectrum in this range is given essentially by a single leaky wave, which is non-spectral but has important practical significance.

We also show that an antenna structure[5] that was proposed as a traveling wave competitor to microstrip patch antennas, and was therefore made short, is in reality a leaky wave antenna. Our analysis explains why the antenna worked as well as it did, despite its insufficient length, and how its performance can be readily improved.

3. STATE OF THE ART AND PROGRESS DETAILS

A. Two-Dimensionally Periodic Grooved Dielectric Structures

It was mentioned in the previous section that many interesting new physical effects were found in the earlier study of waves incident obliquely on dielectric waveguides grooved periodically in one dimension. For one of these effects, extra stop bands due to TE-TM mode coupling, our calculations agreed extremely well[6] with careful measurements made by Ulrich and Zengerle on an optical guiding structure.[7]

Ulrich and Zengerle, in this paper[7] and especially in Zengerle's Ph.D. thesis,[8] of which we have a copy, also took careful measurements on optical waveguides that were grooved periodically in two orthogonal directions. They found additional interesting physical effects, such as weird-looking dispersion diagrams, and the focusing of a divergent light beam. These were determined experimentally; they did not have any theory available. The possibility of finding additional physical effects, and the availability of the Ulrich-Zengerle measurements, were the motivating factors in this new study of a two-dimensionally periodic grooved dielectric waveguide.

The model chosen for the periodic modulation was a cosinusoidal variation in the dielectric constant in both the x and y directions. The first phase of the analysis, involving propagation in the xy plane, with no variation of the geometry or the field in the z direction, shows that the harmonic amplitudes of the Floquet solution are determined by a five-term recurrence relation. The solution of this recurrence relation, and the wavenumber curves for propagation in this periodic medium, were discussed in last year's annual report.

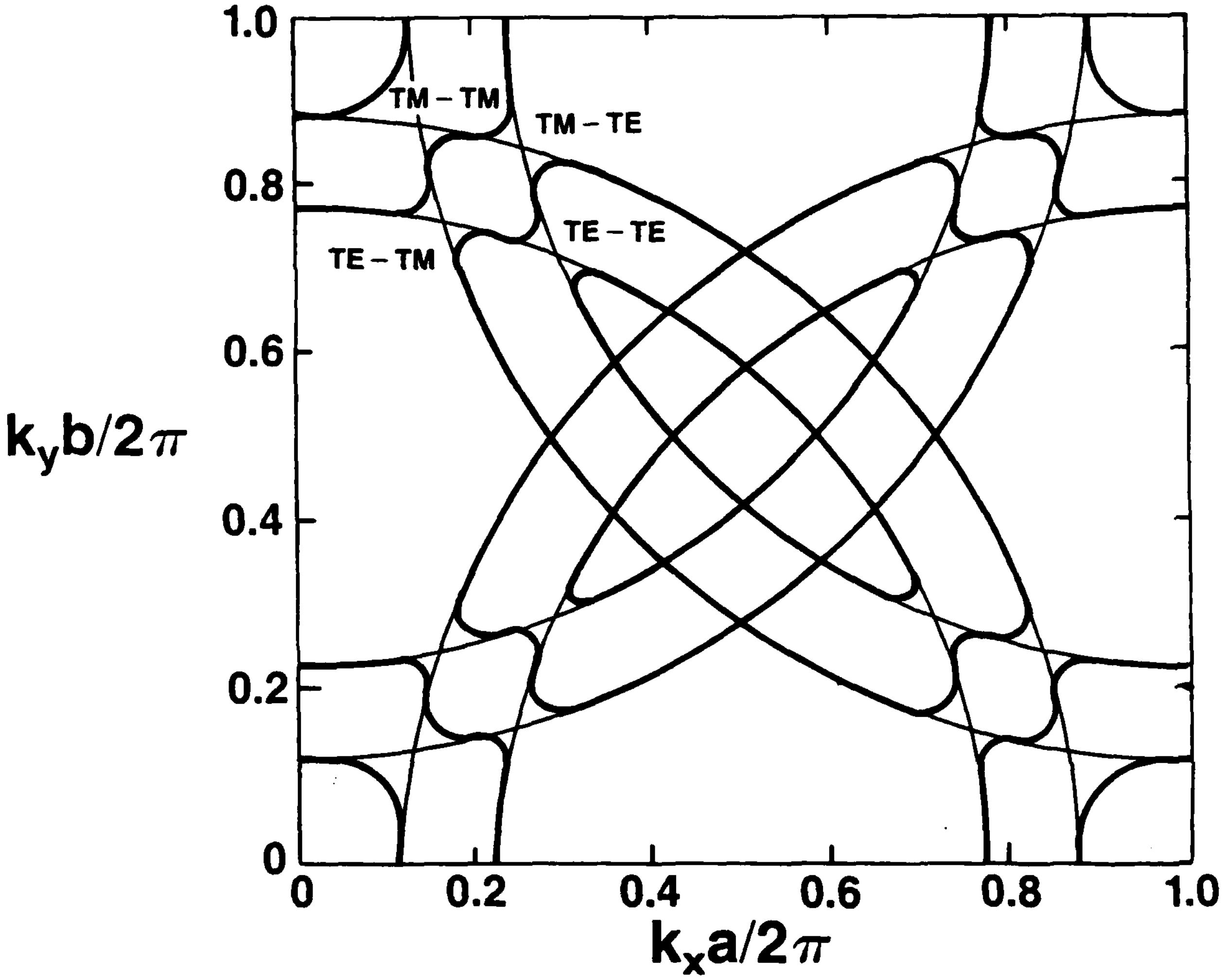
When the fields also vary in the z direction, meaning that the wave is incident at an oblique, or arbitrary, angle in the two-dimensionally modulated medium, the problem becomes vector in nature and all the modes become hybrid with six field components. The same general mathematical procedures are followed in arriving at a solution, but with the above complications (including $k_z \neq 0$) present. The wavenumber plots now take on an additional flexibility, with the "unperturbed" circles becoming smaller in diameter as k_z increases, meaning that the incident wavenumber is more oblique, with a larger component in the z direction. The effects are interesting in themselves. For example, in one sequence of wavenumber plots where only the value of k_z is changed, we begin with a plot, for k_z very small, in which there are stop bands in both the k_x and k_y coordinates and a pass band between the stop bands. As k_z is increased, the pass band decreases in size until it disappears, so that the stop bands on both sides coalesce, leaving a very wide stop band. This stop band is wide in both k_x and k_y, and is therefore unusual. Then, as k_z increases further, this stop band becomes narrower until it also disappears, and the whole region becomes a pass region.

In the third phase, a modulated dielectric waveguide is formed by placing a slice of the infinite medium discussed above between uniform regions. The simplest configuration of this type then consists of a layer of this modulated medium placed on a metal ground plane, with air above. For the guidance of waves by such a two-dimensionally periodic waveguide, a boundary-value problem must be solved in which the eigenfunctions found for the above infinite medium are employed to form the general solutions in both the periodic and uniform regions. The continuity of tangential field components at the interfaces is then imposed, and the equivalent of a transverse resonance is then used to obtain the dispersion relation. Those solutions have been obtained for the model chosen originally for the periodic layer, namely, a cosinusoidal variation in dielectric constant along the two orthogonal directions in the layer. For the case of a modulated layer on a ground plane, applicable to millimeter wavelengths, numerical values have been obtained for wavenumber plots in the Bragg regime. A typical plot is shown in Fig. 1, where it is seen that TE-TM mode coupling helps to make the plot even more complicated. At this stage, it is unclear how to use this plot for practical applications. In addition, it is likely that the crossings of lines that occur in the middle region (rather than couplings between them) are an artifact of the particular model, and that a different model would result in couplings there as well. The study discussed above forms the content of a recent Ph.D. thesis.[1]

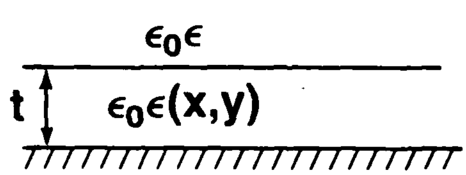
B. Scattering by a Multimode Metal Grating Placed on a Dielectric Half Space

It was stated in Sec. 2 that the structure mentioned above is a key constituent of dielectric image guide leaky wave antennas that use metal strips to produce the periodic variation. The solution for the scattering by such a periodic strip grating is then employed in a transverse resonance solution, involving more than one transverse mode, that yields the α and β needed for the design of leaky wave performance. In this overall study, the effort so far has been concentrated on the constituent scattering problem of a wave incident at an arbitrary oblique angle on a metal strip grating placed on a dielectric half space, but with the additional vital complication that the grating period is large enough to permit several propagating spectral orders.

We first derived a reference solution, against which we can compare the accuracy of our actual solutions. This reference solution is



$$\epsilon(x,y) = \epsilon_{ave}(1 + 4\delta \cos 2\pi x/a \cos 2\pi y/b)$$



$\epsilon_{ave} = 4.09$
$\epsilon = 1.6$
$t = 4.453(a/2\pi) = 0.327\lambda$
$a = b = 0.461\lambda$
$\delta = 0.05$

Fig. 1 Wavenumber diagram for two-dimensionally periodic dielectric waveguide, where the dielectric constant in the periodically modulated layer varies cosinusoidally in the two orthogonal directions, x and y, as indicated on the figure.

rigorous in principle, but it is valid only when the dielectric medium is the same on both sides of the grating. That solution employed a Riemann-Hilbert approach, and permitted checks in special cases.

The actual scattering problem, which is complicated by the simultaneous requirement of asymmetry in the dielectric media and the presence of several propagating spectral orders, was attacked in several ways, all using integral equation techniques in the context of an equivalent circuit so constructed that the kernels of the integral equations represent sums of "static" modes. Within this context, we have obtained solutions in the small aperture range and in the small obstacle range, and we also derived a rigorous solution via a reduction to a Fredholm equation of the second kind. In principle, this last solution is valid everywhere, but it contains infinite sums that are very slowly convergent in certain parameter ranges (particularly for narrow strips). These solutions taken together cover all relevant ranges of parameters. We will next compare numerical values obtained from these solutions with results for various special cases presented in the literature.

C. <u>Leaky Higher Modes on Microstrip Line</u>

During the late 1970's, a paper presented by H. Ermert at the European Microwave Conference stimulated instant controversy. The paper was devoted to the properties of higher modes on microstrip line, and one of its conclusions was that a "radiation" region exists close to the cutoff of those modes. Because the description of this region, made in that talk and in published papers,[3,4] was incomplete and therefore unclear to many, confusion persisted and certain practical consequences remained hidden. Also in this general period, a paper by W. Menzel[5] presented a new traveling-wave antenna on microstrip line fed in its first higher mode and operated near to the cutoff of that mode. Menzel proposed his structure as a competitor to a microstrip patch antenna, and he therefore made his antenna short in terms of wavelength. He also assumed that the propagation wavenumber of the first higher mode was real in the very region where Ermert said no such solutions exist; since his guided wave, with a real wavenumber, was fast in that frequency range, Menzel presumed that it should radiate. His approximate analysis and his physical reasoning were therefore also incomplete, but his proposed antenna was valid and his measurements demonstrated reasonably successful performance.

Ermert selects a spectral description for the modes of microstrip, and he rejects any inclusion of leaky modes as nonspectral (true) and therefore "no longer of importance" in his analysis (untrue). We have shown now that the continuous spectrum in the "radiation" region is characterized in a highly convergent manner by essentially a single leaky mode and that the power in that leaky mode may be contained in only a surface wave in part of the frequency range and in a combination of a space wave and a surface wave in the remainder of the range. Simple conditions define the relevant portions of the range. These conditions are well known in other contexts but are shown to apply here.

Once we recognize the relevance of leaky modes to the "radiation" region of microstrip line higher modes, the application to leaky wave antennas becomes evident. In particular, it is clear that Menzel's traveling-wave patch antenna is a leaky wave antenna in principle, even though he did not recognize this fact and did not discuss the antenna's design or behavior in those terms. What is puzzling at first is why the antenna radiated so well in traveling-wave fashion even though it was so short ($2.5\lambda_0$); leaky wave antennas are usually longer than $20\lambda_0$. Employing a rigorous (Wiener-Hopf) solution derived by D.C. Chang and E.F. Kuester[9] for the reflection from one side of that microstrip line, we derived an accurate transverse resonance formulation for the propagation characteristics of the first higher mode on microstrip line, both in its purely bound range (real wavenumbers) and its "radiation" range (complex wavenumbers). As a check, we obtained very good agreement with special cases in the literature (Ermert, for the real wavenumber cases, and J. Boukamp and R.H. Jansen,[10] for a complex wavenumber case). We made a parametric dependence study of the leakage and phase constants in the "radiation" range, and found that the leakage constant is very large for the Menzel antenna structure, thus explaining why so much power can leak out despite the antenna's small length. Other characteristics of the antenna's performance also readily follow from the leaky wave analysis.

We also find that Menzel's antenna is not very efficient, radiating only about 50% of the power in the forward direction and producing a large back lobe. A proper leaky wave design would require that he double the antenna length to $5\lambda_0$; 90% of the power would then be radiated into the forward direction and the back lobe would essentially disappear.

A difficulty associated with this type of antenna is that a part of the leakage goes into a surface wave on the dielectric layer (as with microstrip patch antennas). We therefore performed an accurate analysis of the same structure but with the dielectric present only under the metal strip itself. All leakage then corresponds to space wave radiation. We found that the leakage constant becomes somewhat reduced in this modified structure, but, by and large, the parametric dependences are similar and narrow beams are still difficult to achieve. Nevertheless, this modified structure is novel and may be of interest in some applications.

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B. BEAM-WAVE PROPAGATION AND INTERACTIONS IN OPEN LAYERED MEDIA

Professor T. Tamir

Unit EM5-2

1. OBJECTIVE(S)

This investigation aims to provide a new and systematic approach to the propagation, scattering, guiding and coupling of beam waves in open layered structures, particularly of the thin-film variety. In the past, problems involving wave progression through different media have been treated mostly in terms of plane waves of infinite extent, or in terms of strongly localized rays that connect a source to an observation point. However, an increasing number of application areas utilize fields that propagate by means of well-bounded beams, such as those provided by lasers. Because they occupy an intermediate position between unbounded plane waves and rays of infinitesimal cross-section, beams exhibit propagation characteristics that are different in many respects from either plane waves or rays. For example, they are subject to non-geometric lateral displacements, peculiar focal phase shifts, angular deviations, anomalous absorption effects, and other recently recognized phenomena that have not as yet been investigated except in a few special cases. It is thus desirable to study these phenomena and other related aspects in terms of beam fields, which are realistic and meaningful representation of many practical electromagnetic (and other) fields.

To achieve results that are relevant to a wide spectrum of applications areas, this study addresses basic aspects of beam propagation through, and guidance along, open layered configurations that are typical of a very broad variety of situations. For this purpose, we consider beams of the Gaussian form because they are more easily tractable from mathematical points of view and, fortunately, they are also of greatest practical application.

The configurations of interest are first expressed in terms of canonic models consisting of a single layer placed between two open media having different electromagnetic properties; structures with multiple layers can thereafter be treated as composite configurations made up of several individual canonic models. While the first phase of the investigation focuses on lossless passive media, the projected work will consider media with arbitrary absorption (or other) losses and media having active properties. Some of the specific aspects to be explored include: the peculiar but possibly strong lateral, focal and angular shifts of the propagating beam profile; the interaction of beam waves with other (surface, leaky, etc.) waves; and the conversion of beam fields into other characteristic field types. Although phrased in electromagnetic terms, the results of this basic investigation are applicable also to other areas, such as acoustic waves along interfaces or layers, elastic waves along geophysical strata, plasmon waves in metal films, and other configurations involving waves and beams through or along layered media.

2. SUMMARY OF RECENT PROGRESS

During the past year, we have obtained interesting results for three different phases of the present investigation. In the first one, we have completed the development of a unified approach which describes and quantifies the peculiar beam-shifting effects; these occur when a beam is incident on a layered structure so that it is phase-matched to a leaky wave supportable by that structure. This approach has made it possible to characterize and correlate the three separate effects, namely, the lateral displacement, the focal shift and the angular deviation of the beam axis. In addition, we have found the presence of a novel fourth effect, which manifests itself as a reduction or increase of the beam width. A quantitative analysis of these effects has shown that all of them can be quite strong, so that each of the four effects is a candidate for applications using beams interacting with thin films.

In a second phase, we have examined the types of leaky waves that are responsible for the above beam interactions in a variety of canonic thin-film geometries, which include duct, gap and transition configurations. In particular, we have found a new type of leaky-wave field which leaks into only the rarer of the two exterior media, thus behaving in a manner that is opposite to the leaky wave that is responsible for the beam-coupling process produced by prism couplers. Part of this study was extended to TM modes, but most of the results have so far been restricted to TE modes.

The results outlined above, as well as other results obtained for plasmon waves guided by thin metallic films, indicate that the number of leaky-wave fields supported by layered media is larger than was known hitherto. We have therefore undertaken a systematic investigation to determine all of these possible varieties of waves. The results show that a total of eight leaky-wave field types may exist having different leakage properties and different forward or backward traveling behavior. However, by examining whether any of these waves can actually be excited by realistic sources, such as beams, we have shown that only four out of those eight waves can be generated. Thus, while the four excitable waves have physical significance, the other four appear only as mathematical solutions of the pertinent boundary-value problem which do not provide measurable quantities.

Papers have been written for each of the three study phases listed above and they have been accepted for publication in the professional literature.

3. STATE OF THE ART AND PROGRESS DETAILS

The interest in beam fields was stimulated by applications in laser technology, fiber optics, ultrasonic diagnostics and other areas which have generated a number of fundamental studies of beam propagation through a variety of media. However, most of the studies have dealt with beams propagating over long distances through uniform or "slowly varying" media. Thus, comparatively few investigations have been carried out on beam fields interacting with abrupt transitions and/or multiple boundaries separated by distances of the order of a wavelength, such as occur in his film configurations.

SECTION I: ELECTROMAGNETICS

Because lasers generate beam fields, a considerable number of investigations on beams inside laser cavities were undertaken in the early sixties. These studies viewed the beams primarily in terms of ray optics and considered their interaction with mirror reflectors or thin lenses.[1,2] The fields of beams that are emitted by lasers into free space have also been studied, mostly in terms of their Hermite-Gaussian modes,[1-3] and interest into the fine structure of those propagating fields is continuing to this day.[4,5] However, all of those studies are concerned primarily with a beam that propagates basically through a single uniform medium.

When the medium inside which the beam propagates is not uniform, the usual assumption has been that the medium properties change slowly over a distance of a wavelength, i.e., one deals with a slowly varying medium. The treatment has then involved a variety of techniques, which include complex rays,[6,7] or the propagating-beam method,[8] which relies heavily on numerical computations.

In contrast to the above, our study is concerned with beam fields that propagate through media that can change rapidly and are therefore characterized best by boundaries that separate media having different electromagnetic properties. In this context, most recent studies have dealt almost exclusively with the lateral Goos-Haenchen shift of beams incident under total reflection conditions at a single interface between different media.[9-15] Only a very few investigations have examined incidence of beams on layered configurations having two are more interfaces.[18,19] Of these, a considerable amount of basic work was carried out by us;[17,19] in this context, we have also shown that electromagnetic beam phenomena on layered configurations have analogous counterparts in acoustics,[20,21] thus stimulating investigations in that area which are still continuing.[22,23]

The major topics investigated by us during the past year include the following phases:

A. Unified Treatment of Beam-Shifting Effects

In addition to the (Goos-Haenchen) lateral displacement of the beam axis, recent studies have shown that the beam may also exhibit an angular deviation,[11,26] and/or a focal shift.[24,25] However, those effects were examined only for beams incident from a denser medium onto a single interface to a rarer medium under total-reflection conditions. By extending an approach recently developed by us, we have obtained qualitative and quantitative results for all of these effects for arbitrary incidence on multilayered structures. This unified approach has revealed a hitherto unknown phenomenon, which manifests itself as a reduction or increase in the effective beam width.

To appreciate these aspects, consider a Gaussian beam of the form $\exp[-(x_i/w)^2+ikz_i]$ incident on a layered configuration, as shown in Fig. 1. The reflected field can then be expressed as

$$E_r(x,z) = \frac{w}{2\sqrt{\pi}} \int_{-\infty}^{\infty} r(k_x)\, e^{-(k_x w/2)^2}\, e^{i(k_x x_r + k_z z_r)}\, dk_x, \qquad (1)$$

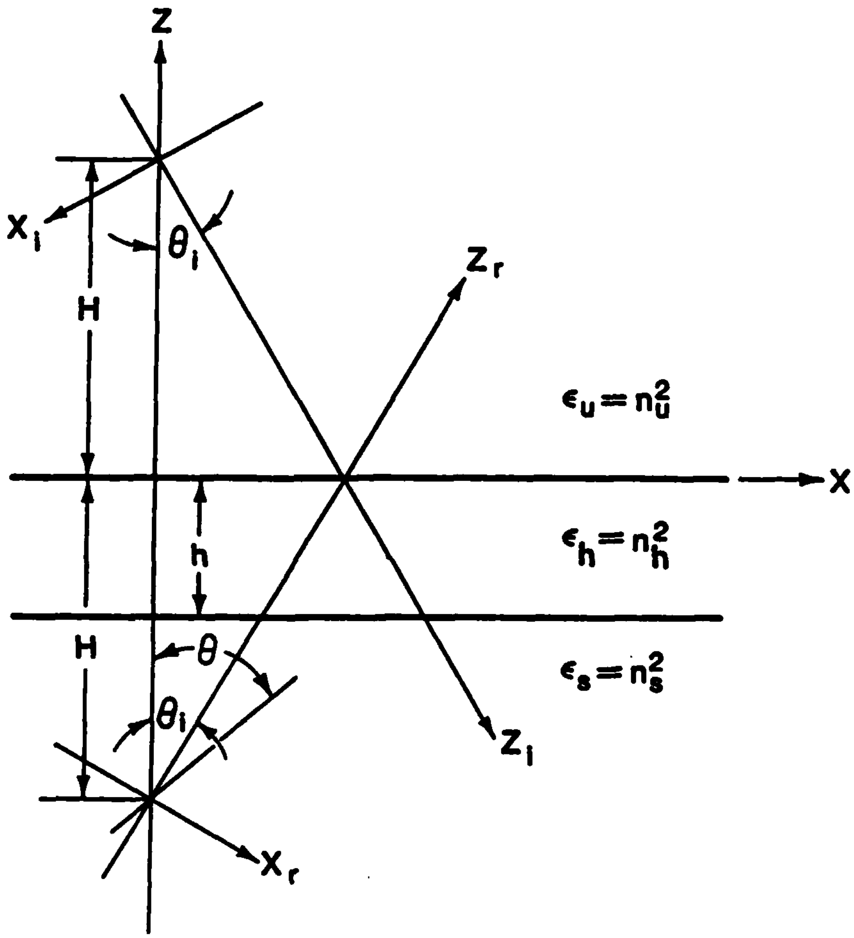

Fig. 1 Geometry showing coordinates of the incident beam (x_i, z_i) and the reflected beam (x_r, z_r). In general, the layer at $-h<z<0$ may have an arbitrary variation $\varepsilon_h = \varepsilon_h(z)$ along z.

where $r(k_x)$ is the plane-wave reflectence at the z=0 plane, and

$$k_x = k \sin(\theta-\theta_i). \tag{2}$$

By expanding $r(k_x)$ into a power series and retaining the first three terms only, and by taking a Fresnel expansion for k_z, Eq. (1) yields:

$$E_r(x,z) \simeq \frac{w}{w_r}\, r(\theta_i) \exp[-(\frac{x_r-L}{w_r})^2+ikz_r], \tag{3}$$

where

$$w_r{}^2=w^2\,[1 + i\,\frac{2(z_r-F)}{kw^2}]\,. \tag{4}$$

Here L and F are complex quantities given in terms of derivatives of $r(k_x)$. It is thus evident that L and F appear directly as beam shifts if Eqs. (5) and (6) are compared with those for propagation in free space (wherein L = F = 0). In particular, if we take

$$L = L' + iL'' , \tag{5}$$

$$F = F' + iF'' , \tag{6}$$

so as to separate real and imaginary parts, we find that:

(a) L' denotes a lateral shift of the beam axis, which was already studied by us[17,19,28-33] extensively in the past.

(b) L" is proportional to an angular deviation α of the reflected beam axis, which was identified by others[11,26,27] in the case of a single dielectric interface only.

(c) F' is a longitudinal shift of the beam waist along the propagation direction; this was called focal shift by Carniglia et al.[24,25] because a convergent beam could have its focus displaced by a distance F'. However, as for L', the shift F' was found only for incidence at a single dielectric interface.[24]

(d) F" is proportional to a modification μ of the beam waist w. This is a novel effect which predicts that the reflected beam-width will be given by a modified parameter w_m obtained from

$$w_m{}^2 = w^2\,(1+\mu). \tag{7}$$

Hence, depending on whether μ is positive or negative, the reflected beam-width w_m will be increased or decreased, respectively.

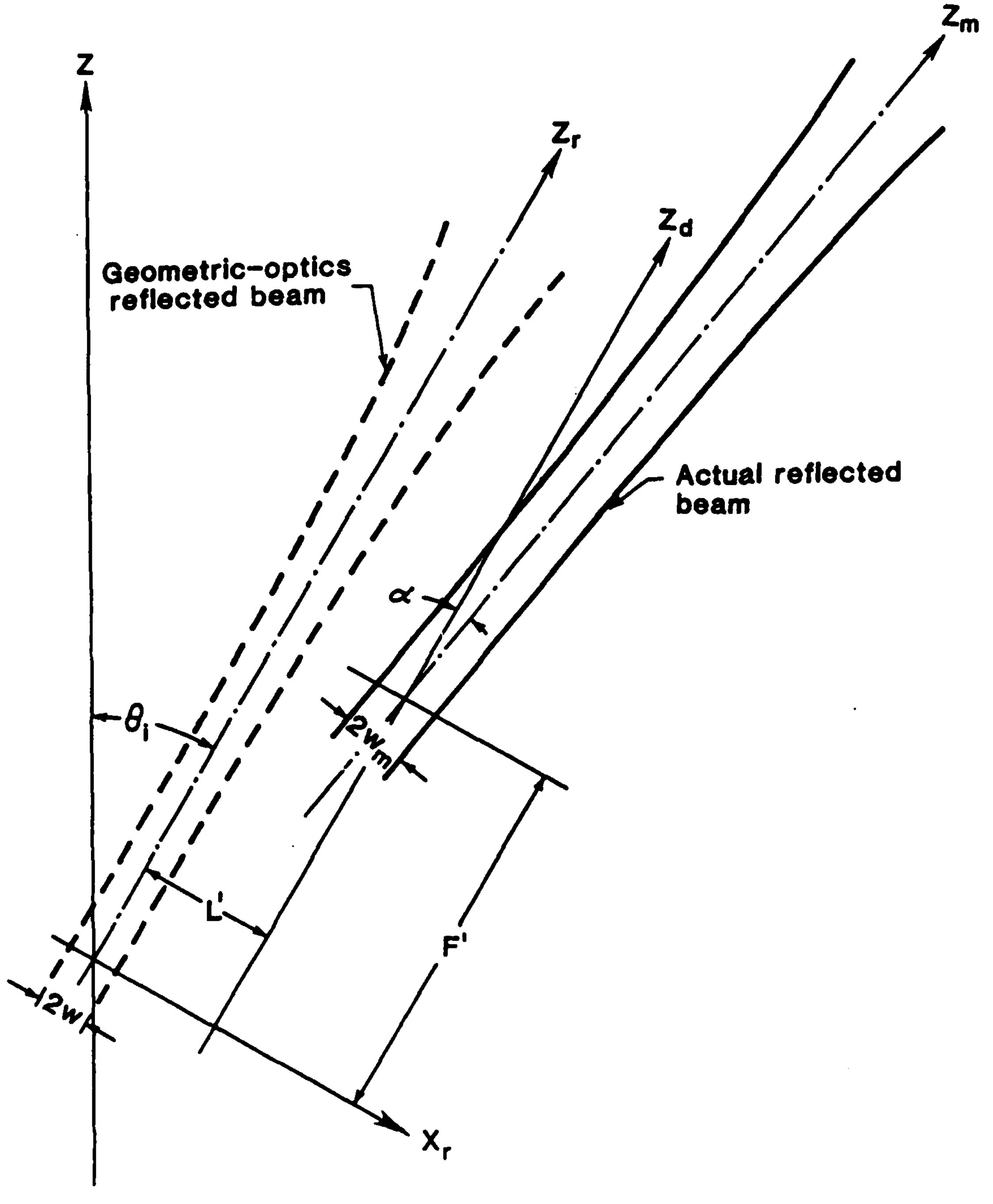

Fig. 2 Profile of the actual reflected beam (solid lines) and the geometrical-optics beam (dashed lines). Note the lateral displacement L', the focal shift F', the angular deviation α and the modified beam waist $2w_m$.

All of the above effects are illustrated in Fig. 2, which shows that the actual reflected beam (solid lines) is obtained from the geometric-optical reflected beam (dashed lines) by: (a) shifting the beam axis laterally through a distance L'; (b) rotating that axis through an angle α; (c) shifting the beam waist over a longitudinal distance F'; and (d) modifying the half beam-width w to a value w_m.

By taking suitable approximations of $r(k_x)$ in the form

$$r(k_x) = R \frac{k_x - k_n}{k_x - k_p} \quad , \tag{8}$$

where R, k_n and k_p are constants, we have derived formulae for all of the above effects and have obtained quantitative results for layers of the type shown in Fig. 1. We have thus found that $F' \gg L' \gg \lambda$ for layers having heights of a few wavelengths, provided that the incidence angle is phase-matched to the leaky-wave field corresponding to the term k_p of $r(k_x)$ in Eq. (8). In those cases, L' can be of the order of $10\text{-}100\lambda$ and F' can be of the order of $10^2\text{-}10^4\lambda$, so that the focal shift is generally larger than the lateral displacement. On the other hand, the angular deflection and the beam modification factor μ can be large only for relatively small values of the beam-width parameter w.

The above quantitative results hold for configurations of the duct type, i.e., $\varepsilon_h > \varepsilon_u, \varepsilon_s$ (see Fig. 1). Preliminary results indicate that L' and F' can be considerably larger for configurations of the gap type, i.e., $\varepsilon_h < \varepsilon_u, \varepsilon_s$. A first paper on these aspects has been accepted for publication[34] and our study continues to evaluate all of these effects for possible application to beam-control devices.

B. Evolution of Leaky Waves Guided by Layered Media

In the above item A, as well as from results obtained by us in the past[17,20,28-32], it is known that beams interact strongly with layered structures if they can couple energy to leaky waves guided by such structures. The dispersion and guidance properties of these leaky waves are therefore important and they have been studied in the recent past.[34,35] It was thus found that, in addition to the leaky waves that have been known to propagate along symmetric ($\varepsilon_u = \varepsilon_s$) configurations, a new type of leaky-wave field can exist if the configurations are not symmetric, i.e., $\varepsilon_u \neq \varepsilon_s$ in Fig. 1.

Specifically, the older known leaky-wave fields are shown in Fig. 3(a), which describes a field that is basically guided by the central layer but leaks energy into both the exterior (upper and lower) regions. In the case of symmetric configurations, the leakage occurs symmetrically also, i.e., $\theta_0 = \theta_2$ in Fig. 3(a). In contrast, the newer type of leaky wave is shown in Fig. 2(b) where leakage occurs only into the denser of the two open regions, i.e., into the lower (substrate) medium for the case shown. Although rather unexpected, this leaky wave is the one that accounts for coupling of beams into surface waves in beam couplers of the prism type.[17]

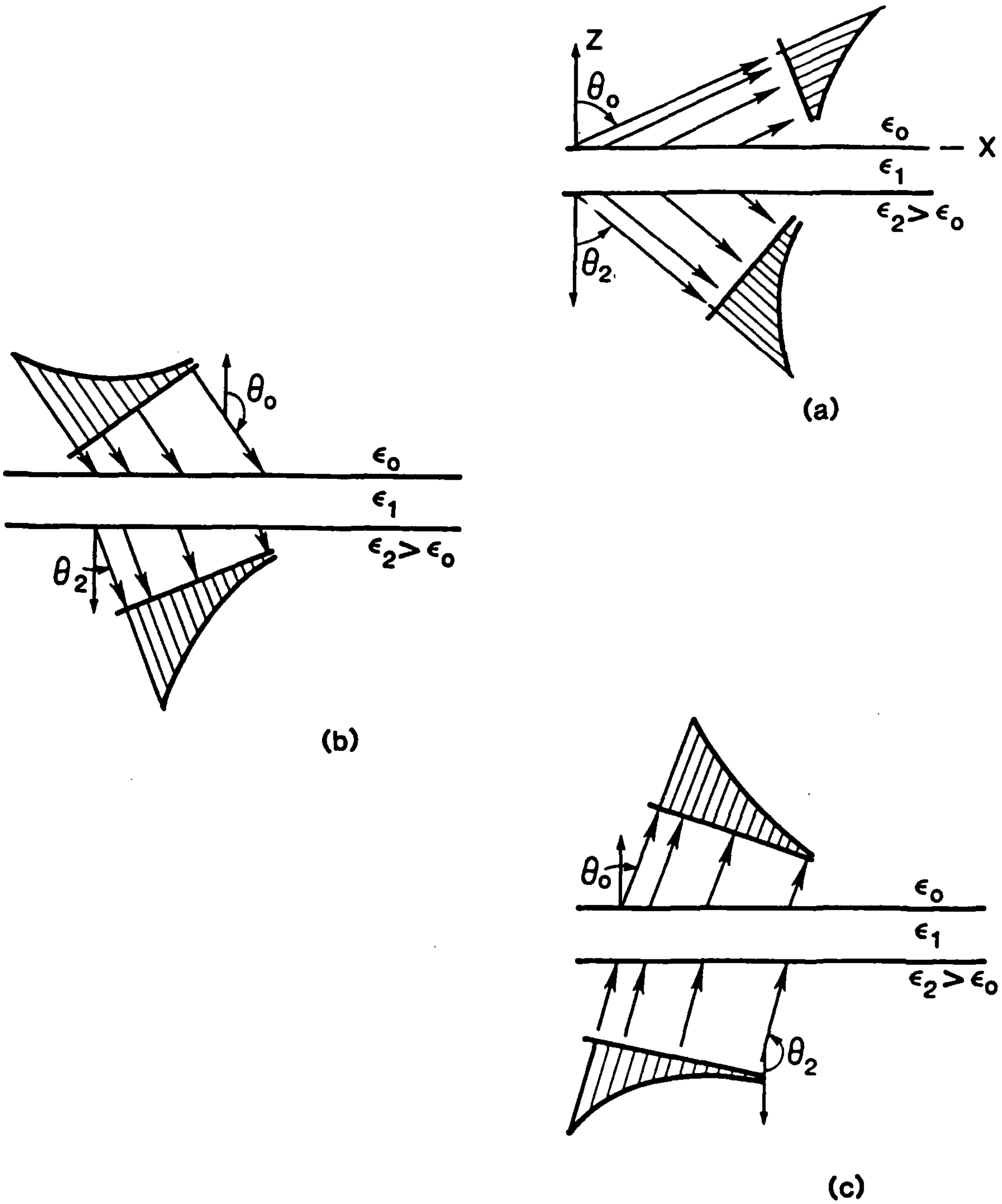

Fig. 3 Leaky-wave fields: (a) Leakage into both exterion regions; (b) leakage into the denser exterior medium only; (c) leakage into the rarer exterior medium only. Arrows show power flow direction, shading indicates amplitude variation.

However, the above results were restricted to TE modes along ducts (i.e., $\varepsilon_h > \varepsilon_u, \varepsilon_s$). We have therefore extended the analysis also to TE gap ($\varepsilon_h < \varepsilon_u, \varepsilon_s$) and transition ($\varepsilon_u < \varepsilon_h < \varepsilon_s$) geometries, with the results being given in a Doctoral dissertation.[37] In addition, we have carried an analysis also for TM modes on a duct geometry, and the results have been summarized in a recent paper.[38] These results have revealed the presence of a third type of leaky wave, which is shown in Fig. 3(c). In that case, leakage occurs only into the rarer of the two exterior media, so that this third leaky-wave field behaves in a manner that is the opposite of that in Fig. 3(b). However, the leaky wave in Fig. 3(c) has, so far, not found any application. This is consistent with the more general considerations developed in the study described below.

C. Varieties of Leaky-Wave Fields and Their Excitation

The study phase B outlined above has indicated that leaky waves of several types can be supported by dielectric layers. Work done by us in the past on plasma layers[39] and more recent work on metal films[40,41] has revealed additional such types, some of which have a backward-traveling behavior instead of the more conventional forward-traveling one. Because of the interest generated in these areas and, in particular, because of questions concerning the physical significance of the various leaky-wave fields, it is important to clarify the possible presence of these waves, in general, and their excitation in suitable configurations, in particular.

We have therefore carried out a general study on the types of leaky waves that may be supported by an arbitrarily stratified layer bounded by two half spaces having different dielectric constants $\varepsilon_u \neq \varepsilon_s$. Thus, the permitivity of the layer $\varepsilon_h = \varepsilon(z)$ can accommodate either a continuously varying medium or any number of sub-layers. Furthermore, the layer region may be either lossy or lossless. Our results reveal that, under these rather general conditions, a total of eight different types of leaky waves can be supported. Three of these are shown in Fig. 3, while the other five exhibit various differences in their leakage behavior; also, four of the eight waves have forward-traveling and the other four have backward-traveling fractures. The latter can occur only in the presence of plasma or metallic layers.

While thus showing that only eight leaky-wave field types can exist unde the general conditions assumed, the question remains as to whether any of these eight fields have physical significance. We have therefore explored this question by examining the field excited by realistic sources, such as beams or small (point-like) radiators. This analysis was based on a field representation that expressed the total field in terms of individually measurable field constituents, some of which are leaky waves. We have thus found that, of the four forward-traveling leaky waves, only three can be excited; similarly, only one of the backward-traveling leaky waves can be excited by realistic sources. This result is of very general application and should provide a simple and useful tool in assigning physical significance to leaky-wave fields that are theoretically identified in problems involving isotropic planarly stratified media.

These considerations have been summarized in a paper[41] dealing with metallic films and in another paper[42] dealing with the more general problem involving arbitrary media.

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C. MIXED SPECTRAL TECHNIQUES FOR WAVE PROPAGATION AND DIFFRACTION

Professor L.B. Felsen

Unit EM5-3

1. OBJECTIVE(S)

High frequency or transient propagation in, or transmission through, layered media, and high frequency or transient scattering by impenetrable and penetable targets, usually requires synthesis in terms of a large number of basic wave processes. For the guiding or ducting problem, these wave processes are either normal (discrete and continuous) modes or ray-optical fields. For the transmission problem, the basic wave processes are traveling waves which undergo multiple internal reflection at the layer boundaries. For the transient scattering problem, the wave processes involve multiple wavefront and resonance fields. Because descriptions by multiple propagation events are often poorly convergent and do not provide physical interpretation in compact form, it is desirable to seek collective descriptions of multiple phenomena.

Thus, the objective of this fundamental study is the construction of a new theory of propagation, transmission and scattering that has broad implications for a general class of electromagnetic and other wave problems. The approach is to seek suitable spectral representations in the spatial and temporal domains and to adapt these by arguments of asymptotic localization to successively more complicated environments. The basic spectral building blocks are time harmonic and transient local plane waves, and the spectra may be real or complex. Localized spectra can represent ray fields, true and local mode fields, hybrid ray-mode forms, wavefront-resonance phenomena, and, in more fleshed out form, also transitional effects where these simple compact spectral formulations may fail. The tools involve the theory of spectral representations and asymptotic treatment of integrals and partial differential equations.

2. SUMMARY OF RECENT PROGRESS

This section presents a brief summary of recent progress; more detailed descriptions of selected portions are contained in the next section.

1) Time-Harmonic Fields

(a) Singularity-free field tracking

Asymptotic ray theory (ART) analysis of high-frequency propagation may fail in a highly overmoded waveguide that has an inhomogeneous refractive index profile in the transverse direction x. If the refractive index decreases monotonically from the perfectly reflecting top boundary to the bottom boundary, which separates the waveguide from an exterior semi- infinite medium with (lower) constant refractive index, one encounters the following categories of rays originating at the source: a) rays which are continuously refracted toward the top without encountering the bottom; b) rays which encounter top and bottom but are totally reflected at the bottom; c) rays which encounter top and bottom but are refracted into the exterior. ART incorrectly predicts infinite fields in the following transition regions: near the caustics formed by the surface guided rays in category a); near the bottom-glancing ray that separates categories a) and b); near the critically incident ray that separates categories b) and c). By the ray-mode equivalent, spectral intervals surrounding these transitional rays can be filled with modes.

The theory for time-harmonic line source excitation has previously been developed and implemented numerically for a model waveguide with exponentially varying index profile[1] (see previous Annual Report). The calculations are now being extended to high frequency sound pulse propagation in an underwater acoustic channel.

(b) Complex ray techniques

This technique continues to be applied to transmission of beam type fields through plane and curved dielectric structures, with emphasis on simplifying paraxial approximations.

2) Transient Fields

(a) Hybrid wavefront-resonance formulation of transient scattering

By extending the concept of rays, modes and their equivalents into the transient domain, we have developed a new theory of transient scattering that combines wavefronts (rays) and complex resonances (modes) in a self-consistent framework for efficient analysis of a target response at all observation times.

The theory is now being applied to strip obstacles, where the multiple wavefronts arise from edge diffraction. Results for the complex resonances, derived by collective treatment of multiple wavefront fields, have already been reported (previous report).[2,3] New results for the scattered fields are discussed in Section 3.

(b) Spectral theory of transient fields

Work has continued on the general spectral theory of transient propagation and scattering which reverses the conventional procedure, whereby one first solves for a source-excited field in terms of a wavenumber spectral integral in the frequency domain and thereafter, by Fourier inversion, passes to the time domain.[4] The theory utilizes the concept of weakly dispersive propagation processes, and relies heavily on complex spectra in the spatial and frequency domains. The formulation has now been completed and its implications are being studied.

SECTION I: ELECTROMAGNETICS

3. STATE OF THE ART AND PROGRESS DETAILS

A. Background

Many electromagnetic propagation environments, whether natural or man-made, are so complicated that direct solution of the field equations to determine signal characteristics is beyond the scope of present analytical and computational capabilities. At high frequencies, propagation can be localized and approximated as ray fields which undergo reflection, refraction and(or) diffraction on their path from a source at S to an observer at P. While ray theory provides a fundamental view of the propagation process by tracking local plane wave fields emanating at the source, such tracking becomes cumbersome when many ray paths exist between S and P. It would therefore be desirable to deal with multipath effects collectively. In guided propagation along a refracting channel, rays may form caustics (convergence or focusing zones of enhanced field strength) where simple ray theory fails. When these caustics are sufficiently distinct, one may correct ray theory by uniform asymptotic transition functions, but situations arise for rays with many reflections where an accumulation of caustics makes such corrections impractical and even impossible. Here, again, a collective alternative to multiple ray reflections - for example, by employing guided modes - is desirable or actually necessary. However, the modal approach to ducted propagation is beset with similar difficulties when the required number of modes is large. It would then be useful to express the interference properties of clusters of modes collectively in terms of simpler events.

The preceding discussion makes evident the importance of collective treatment of mode or ray fields when many of these are required to synthesize the signal in a particular transmission or guided propagation channel, or when failures in approximate mode or ray theory make these descriptions inapplicable. Substantial progress in this direction has been made through the new hybrid ray-mode theory developed by us.[5] It has been shown how clusters of ray fields excited by a localized source can rigorously be converted into clusters of guided mode fields plus a (usually small) remainder, and vice versa. The theory has been applied to a series of "canonical" problems involving guided electromagnetic propagation along concave surfaces (here, the guiding mechanism is provided by "whispering gallery" effects), in tropospheric ducts, in plane parallel homogeneously filled waveguides, and in graded index waveguides. The theory has also had impact on other fields such as underwater acoustic propagation and, with generalization to time-dependent signals, the modeling of seismic events. Concern in these applications has been with the greater computational efficiency of the hybrid formulation, with the avoidance of singular regions in ray fields or mode fields by filling these regions with mode fields or ray fields, respectively, and also with the penetrating physical insight of the propagation mechanism provided by the hybrid method. The collective approach linking ray fields and mode fields has been applied also to the complex spectra emitted by a source at a complex location. Such a source generates in physical space a Gaussian beam,[6] and therefore makes the important class of beam propagation and diffraction problems amenable to the hybrid format. These accomplishments have been documented in a comprehensive series of publications, cited in previous reports.

B. Selected Results

Although various facets of the spectal theory have received attention during the past year, we have selected here for presentation new results obtained from the wavefront resonance formulation of transient scattering. We have shown[2,3] (see previous report) how the high frequency constructs of the geometrical theory of diffraction (GTD), when applied to collective treatment of multiple diffracted rays for a flat perfectly conducting strip obstacle, can generate accurate data for the complex resonances, even at the low frequency end where the validity of GTD is being strained. Calculations have now been performed for the scattered fields excited by an incident plane pulse.[7] Evaluating the fields per se poses a more severe test of the applicability of GTD than their integrated (smoothed out) effect that generates the resonances. Indeed we find that the multiple diffracted GTD fields in the time domain are accurate only near their wavefronts but tend tc diverge at later times when the low frequencies in the spectrum predominate. Nevertheless, the results demonstrate the internal consistency of the hybrid wavefront-resonance mix and the flexibility afforded thereby although the actual field values are inadequate. In support of this assertion, we show in Fig. 1 the H-polarized multiple diffracted fields $U_{j,n}(t)$ where n denotes the number of diffractions and j=1 to 4 denotes the ray species ordered according to the edge excited by the incident ray and the edge emitting the diffracted ray to the observer, respectively. Figure 1 pertains to species j=1, with the details of the diffraction mechanism and corresponding wavefront arrivals indicated by the sketches on the bottom. The plots show the first few individual ray fields (dashed) and their sum (solid). By the collective treatment, the sum of ray fields is equal to the sum of resonances (triangles) plus a continuous spectrum (dots). The latter, attributable to the two dimensional nature of the infinite strip scatterer, has strong low frequency content and is therefore poorly represented by the GTD analysis; it dominates by far the contribution from the resonances. The numbers next to the triangles denote the number of resonances included in the sum to achieve accuracy to within 1%. The good agreement between the ray sum and the sum of resonances plus continuous spectrum demonstrates the validity of the collective treatment although, for the reasons stated, the field values as such are inaccurate. Similar conclusions emerge from the other ray species j=2,3,4. Adding all species and including as well the primary diffracted fields $U_{1,3}$ from each edge yields the results in Fig. 2. The crosses now represent resonances (their included number being shown) plus continuous spectrum.

When the exciting pulse spectrum has a low frequency cutoff, the damaging effect of the low frequencies in the GTD approximation is expected to be minimized. This is now being tested on a raised cosine pulse waveform which meets these requirements.

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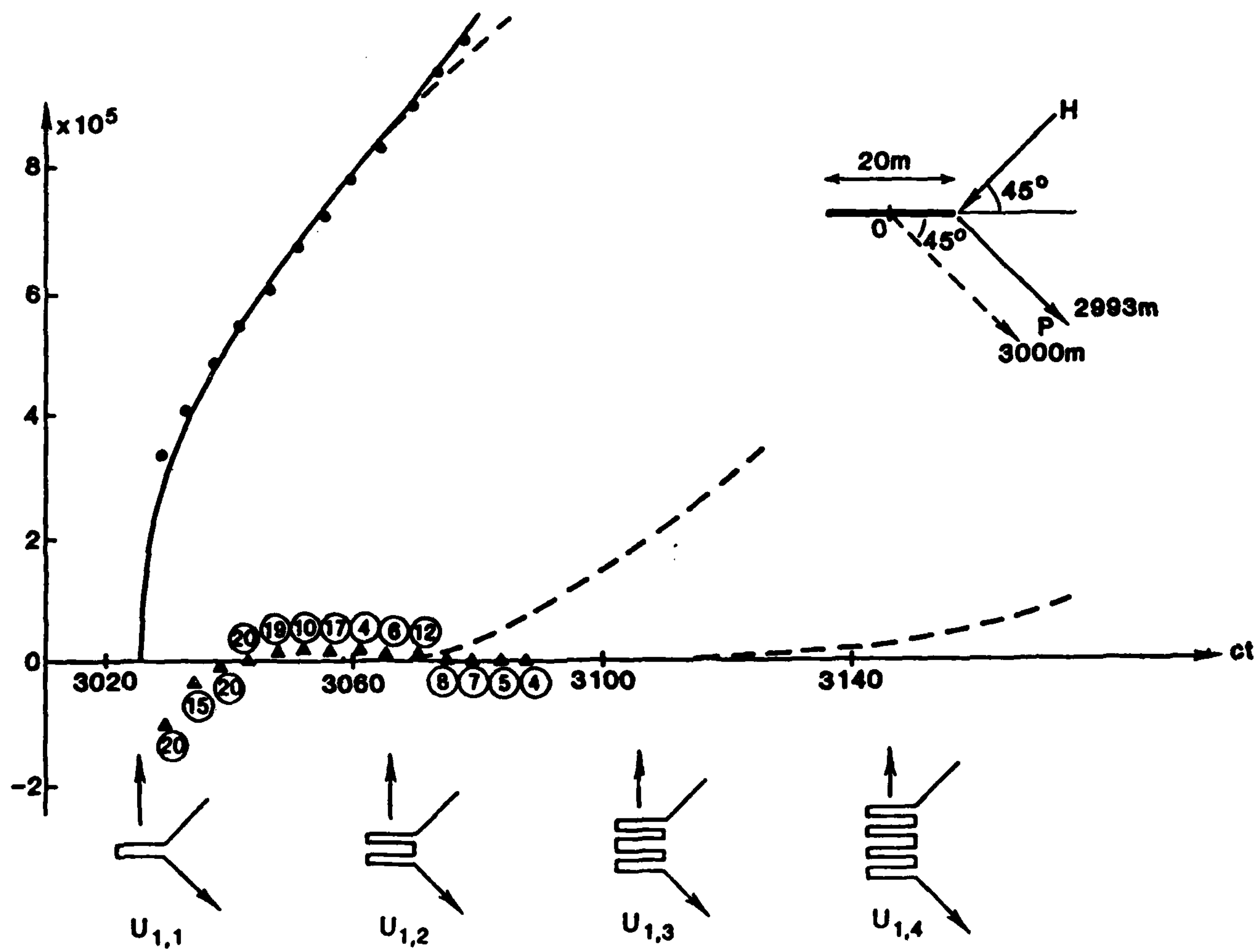

Fig. 1 H polarized impulsive plane wave scattering by a perfectly conducting flat strip. Ray species j=1. Incidence, observation and strip parameters are shown in the upper inset. Curves and symbols are explained in the text.

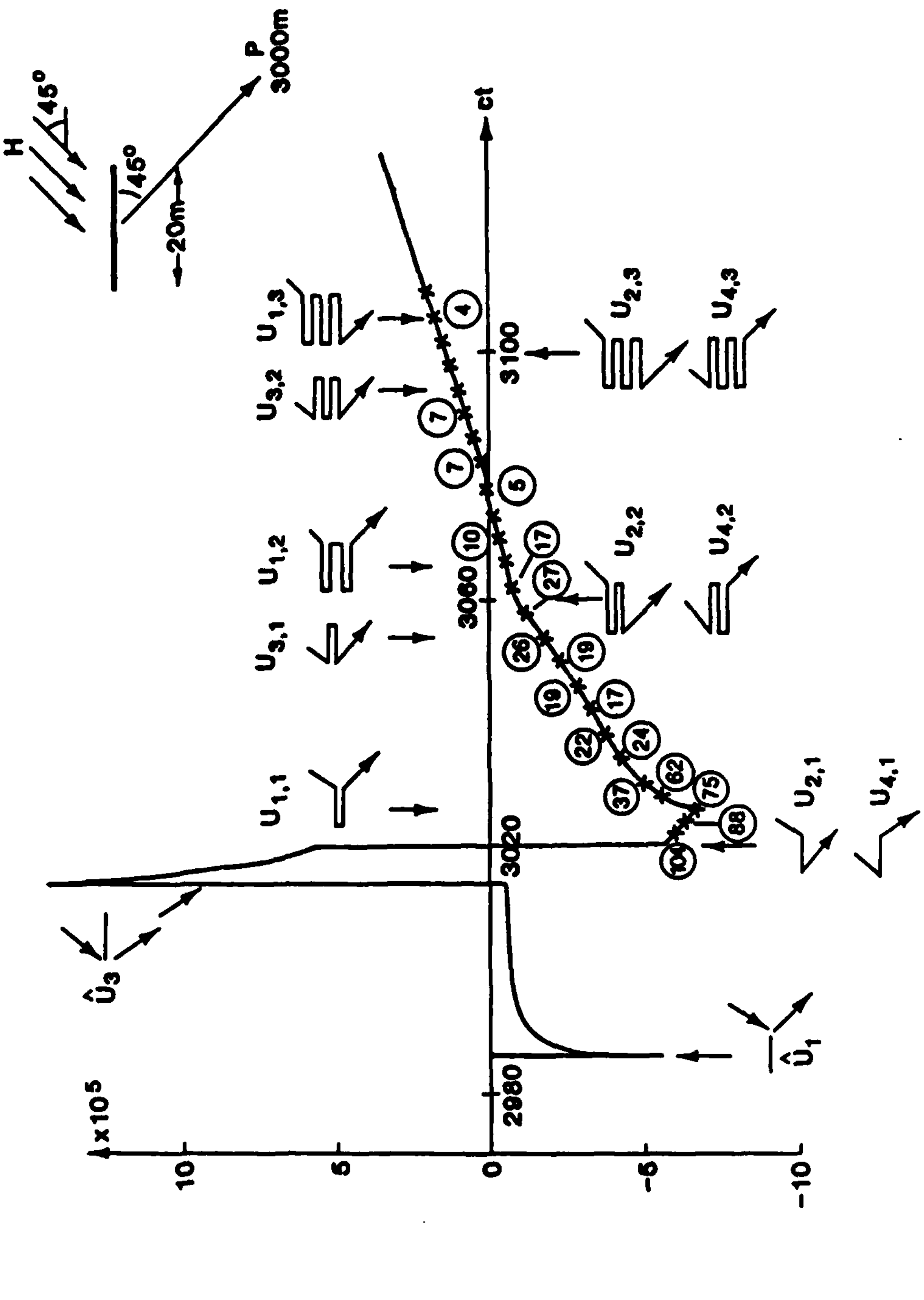

Fig. 2 As in Fig. 1, but for total field.

SECTION II

SOLID STATE

SECTION II: SOLID STATE

A. X-RAY COUPLED WAVE INTERACTIONS AT CRYSTAL SURFACES

Professors H.J. Juretschke and B. Post

Unit SS5-1

1. OBJECTIVE(S)

To use the multiple interaction of x-rays in a Bragg geometry in order to develop simple and compact methods for obtaining direct phase information about the crystal scattering factors, and for characterizing the mode structure; to extend the interactions to include coupling to other waves that can modify the mode structure, and that can be used to explore non-linear interactions of x-rays; and to understand the local x-ray fields in the immediate surface region of the solid, as well as the effect of stringent boundary conditions on all modified x-ray waves, especially those originating in the interior. High resolution x-ray diffraction experiments will be supported by theoretical studies of the predictions of n-beam dynamical theory, and by rigorous extensions of the theory to include the coupling with other waves.

2. SUMMARY OF RECENT PROGRESS

Professor H.J. Juretschke has been on sabbatical leave for the calendar year 1985, at the University of Melbourne and the Royal Institute of Technology, in Melbourne, Australia. Since both institutions have a strong interest and capability in the areas of diffraction, and since the same holds for the nearby Chemical Physics Division of CSIRO (Commonwealth Scientific and Industrial Research Organization, Australia) the year has turned out to be one of very fruitful interaction and accomplishments, largely centered around activities in this research unit. Following the same order of listing as in the last progress report (December 1984), the work will be summarized in sections A and B below.

An extensive effort was undertaken this past year to apply the theory published last year,[1] of a simple analytical formulation of the onset of many-beam interactions, to a variety of specific situations, and to show that this theory gives a satisfactory, and also very simple, account of experimental findings in this area, and that, furthermore, it predicts that these experiments often contain additional information. Four particular cases have been examined in detail this past year and are discussed in the next section.

The experimental phase of this program is summarized below in Sec. 3. A detailed experimental study of 4-beam simultaneous diffraction effects in germanium has been completed. A manuscript describing the work has been acceptance for publication.[13]

In a related investigation, we observed phase indications due to "forbidden" germanium reflections whose intensities are sensitive functions of the aspherical character of the atomic electron distribution. This work is continuing.

Analyses of phase effects observed in n-beam diffraction patterns of gallium arsenide and phosphide are underway. Additional studies by us of experimental phase effects in acentric, ferroelectric, lithium niobate will begin in February 1986 at the Brookhaven x-ray synchrotron.

3. STATE OF THE ART AND PROGRESS DETAILS

A. n-Beam Interactions

1) The sign of structure factors of 'forbidden' reflections. Forbidden reflections are, in many cases, the result of anharmonic thermal motions of the atoms in the unit cell, which, because they have a different symmetry, will allow diffraction in directions for which the normal diffracted intensity vanishes. The sign of the 'forbidden' structure factor then determines the sign of the anharmonic coupling constant, which has traditionally been inferred from other physical reasoning rather than the direct information given by x-ray scattering. We have shown in the specific example of the 301 reflection in Zn that this information actually contains the desired sign. The integrated intensity curve of this reflection in a Renninger scan has a pronounced asymmetry, and from the neighboring peaks of this Renninger scan the geometry of the reflection can be determined uniquely, and this then allows fixing the sign of the phase of the interaction.[2]

2) Pendellosung shifts near n-beam points. The interference between two modes excited in a thin crystal gives rise to a fringe pattern of intensities as a function of position in a wedge-shaped crystal. These so-called Pendellosung fringes have been used for precision determination of structure factors. In the neighborhood of an n-beam point the fringes are displaced in a systematic way, which only very recently was confirmed theoretically by elaborate computer-based computations. We have shown that our theoretical formulation yields these shifts in simple analytical form, and that this can be applied with equal ease to 3-,4-, or higher-beam interactions. The theory was worked out quantitatively to confirm earlier qualitative interpretations of a famous 4-beam experiment.[3] The results when applied to the 4-beam interaction in Ge are shown in Fig. 1. In addition, the theory was able to point to other specific aspects of the interaction, such as the surprisingly large range of multiple beam interactions, and the interference of the fringe patterns due to the separate polarizations, for which there had not been any theoretical guidelines.[4]

3) Anomalous asymmetries in the interaction of π-modes near an n-beam point. One of the predictions of the original theory was that under certain geometric conditions the σ-mode and the π-mode would show asymmetries of the opposite direction. The detailed content of this prediction has now been worked out for all multiple interactions in Ge, using copper radiation, and a large number of cases have been identified where this anomalous asymmetry of the π-mode is actually realized. The most important of these involves the $222/13\bar{1},513$ 4-beam case, for which experimental data are, in fact, available. The theory has been able to reproduce the experimental data in full detail, and has also been able to show that in this particular case the Renninger scan in the neighborhood of the interaction under discussion has very differing features for the two polarizations, something that has not been appreciated nor looked for till now. Some calculated results and corre-

sponding experimental data taken earlier are shown Figs. 2 to 4. In all cases examined in Ge, the asymmetry observed with the use of unpolarized incident radiation is that of the σ-component, though the sharpness of the features is reduced so that, in the unavoidable presence of noise, the final asymmetry may not be clearly observable.[5]

4) First-order asymmetries for a strong primary reflection interacting with a weak secondary one. One of the experimental results alluded to in the last progress report showed that under certain conditions, such as those mentioned in the heading, the reversal of asymmetry expected with structure factors of differing sign does not occur. We have shown that this result also follows directly from the theoretical formulation. When a weak reflection interacts with a strong one, the predominant contribution to the first order asymmetry comes from modifications in the absorption coefficient near the multiple interaction point. This modification depends on the square of the contributing structure factors, and is therefore independent of their sign. Hence the absence of sign reversal is fully predicted, and the magnitude of the resulting first order asymmetry can be evaluated explicity for different interactions. This situation is illustrated in Fig. 5. It is of the order of a few percent for Ge 311/222, and is partially masked experimentally by second-order (symmetric) contributions.[6]

B. Interactions of X-rays with Other Waves.

1. Dynamical therimal diffuse scattering of x-rays. In a revised version of two manuscripts prepared last year[7] on this topic, we have now shown that all previous theories of this effect had used incorrect free modes to satisfy the boundary conditions for all signals generated inside the crystal, and that the major conclusion that the traditional divergence of TDS as the phonon wavevector q approaches zero is suppressed by dynamical contributions is fully confirmed. The papers are to appear late in 1985.

2. Laser-induced phonon polariton coupling with x-ray. This extension of the same theoretical approach as for TDS to optical phonons, where both energy and momentum conservation have to be accounted for explicitly, has now been worked out for various crystals, and in both the reflection and transmission geometry. In the former arrangement, the effect is strongly suppressed by the same factors that eliminate the divergence discussed above, but in the latter, anomalous propagation (Borrmann effect) of the phonon-excited mode produces enhancement. Among the crystals considered as hosts for this interaction, SiC is more promising than MgO, at a typical infrared wavelength, while InSb is expected to show a very large effect, but only in the far infrared where competition with thermal processes becomes important.[8]

3. Phonon scattering in n-beam interactions. In a coupling of the two main areas of investigation, we have studied the coupling of x-rays to phonons under the conditions where the first-order theor of n-beam modifications of a 2-beam mode applies. It is found that TDS does not vary with the effective structure factor of this mode, but remains controlled by the actual uncoupled structure factor. This opens the possibility of studying phonon effects in the absence of a coherent background. But the details and practically of a realizable arrangement for this situation remain to be studied.

C. Experimental Studies of the Structure Factors of Centrosymmetric and Acentric Crystals

The experimental investigation of simultaneous n-beam diffraction of x-rays within crystals has been continued during the past year. That aspect of our research is aimed primarily at the development of simple and efficient procedures for the direct experimental determination of the phases of the crystal structure factors of perfect and mosaic crystals.

It has been shown by us previously[9-11] that the phases of x-ray structure factors are lost in the diffraction process when conventional 2-beam x-ray techniques are used (i.e., involving "incident" and "diffracted" beams). The phases are, however, preserved and displayed in the diffracted intensities when three or more beams diffract simultaneously within the crystal. The utilization of that method has led to the successful experimental determination of the phases of large numbers of structure factors of centrosymmetric perfect and relatively imperfect crystals.[11,12]

The phase angles of centrosymmetric structure factors are restricted by symmetry to 0 and π. Their determination is clearly much simpler than the corresponding determination of acentric phases. The phase angles of the latter range from 0 to 2π. Work during the coming year will be concentrated on such acentric crystals.

A substantial part of the experimental effort during the past year has been devoted to investigations of apparently anomalous results observed in the course of determinations of the phases of 4-beam interactions displayed by germanium crystals. Those involved the display of different phase indications by a given 4-beam interaction when the crystal was rotated about different axes. The causes of the apparent anomalies have been established and the work is described in a manuscript recently accepted for publication in Acta Crystallographica.[14]

A second investigation involved the unexpected observation of apparently non-centrosymmetric character in selected ultra-weak interactions in germanium crystals. In each case, one of the structure factors in the n-beam interactions represented a so-called "forbidden" reflection, i.e., one whose intensity would vanish completely if the germanium atoms possessed spherical symmetry. Packing of atoms in crystals results in aspherical distortions of the arrangements of the bonding electrons and gives rise to weak, but observable, "forbidden" reflections in diamond-type crystals, such as germanium, silicon and diamond. The resultant reflection intensities are at least four orders of magnitude weaker than those of normal, "permitted" reflections. It had been assumed, at the outset of this investigation, that the phases, if any, displayed by such weak interactions could not be detected. Nevertheless, unambiguous phase indications have been observed. The analysis of the observations is now in progress.

Several sets of n-beam data have been collected for acentric crystals of gallium arsenide and gallium phosphide. In those crystals, reflections with even indices have phase angles of 0 or π, i.e., they display centrosymmetric character. The phases of reflections with odd indices display the ranges of phase angles characteristic of acentric reflections.

It was found that, though it was possible to establish the "signs" of the interactions, the resolution of our experimental arrangement was not high enough to permit the assignment of adequately precise phase angles to the acentric reflections.

Our experimental setup has been rebuilt to permit improved resolution. Measurements of both crystals will be repeated within the next two months.

Arrangements have been made to conduct some of our research at the x-ray synchrotron at the Brookhaven National Laboratory. Work will be begun in February 1986 on the analysis of the phases of structure factors of ferroelectric lithium niobate crystals. Emphasis will be placed on the determination of the phases of weak interactions and of the effects of applied electric fields on the phases of those interactions.

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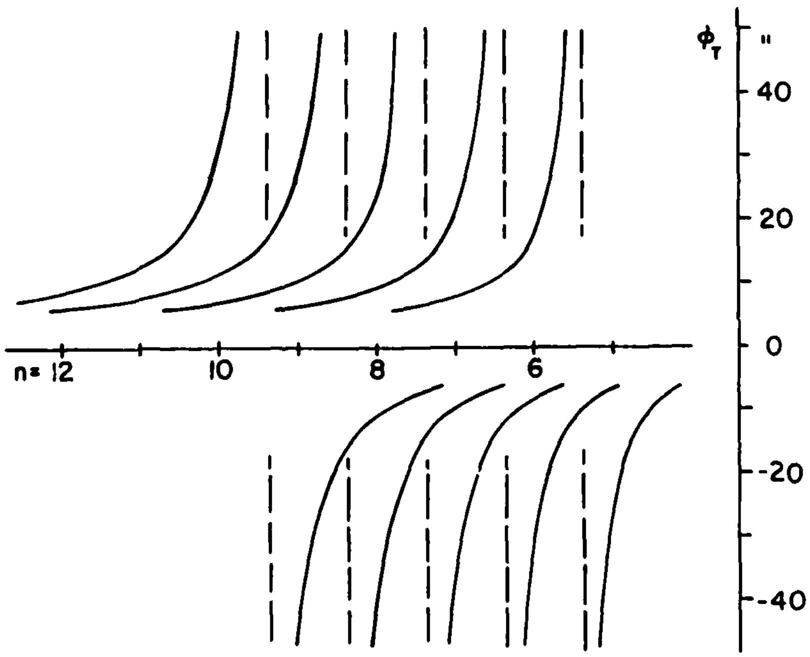

Fig. 1 Pendellosung fringes due to a wedge predicted by the modified 2-beam formulation of the 4-beam interaction Ge $\bar{2}20/(3\bar{1}\bar{1},11\bar{1})$. The location of the asymptotic 2-beam fringes is given by dashed verticals. The wedge thickness increases towards the left. n is the asymptotic fringe order.

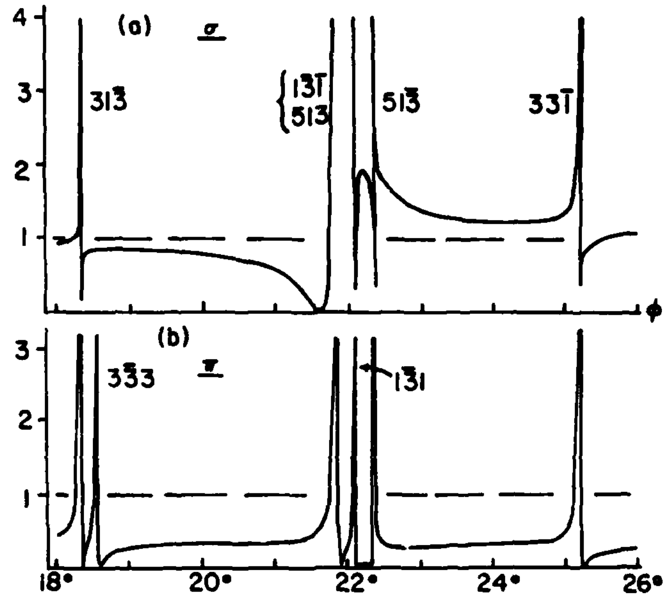

Fig. 2 Calculated Renninger scans for Ge 222/1$\bar{3}\bar{1}$ and neighboring 3-beam points, assuming a symmetric primary reflection, for σ- and π-polarizations, relative to the strict 2-beam intensity I_H^{σ}.

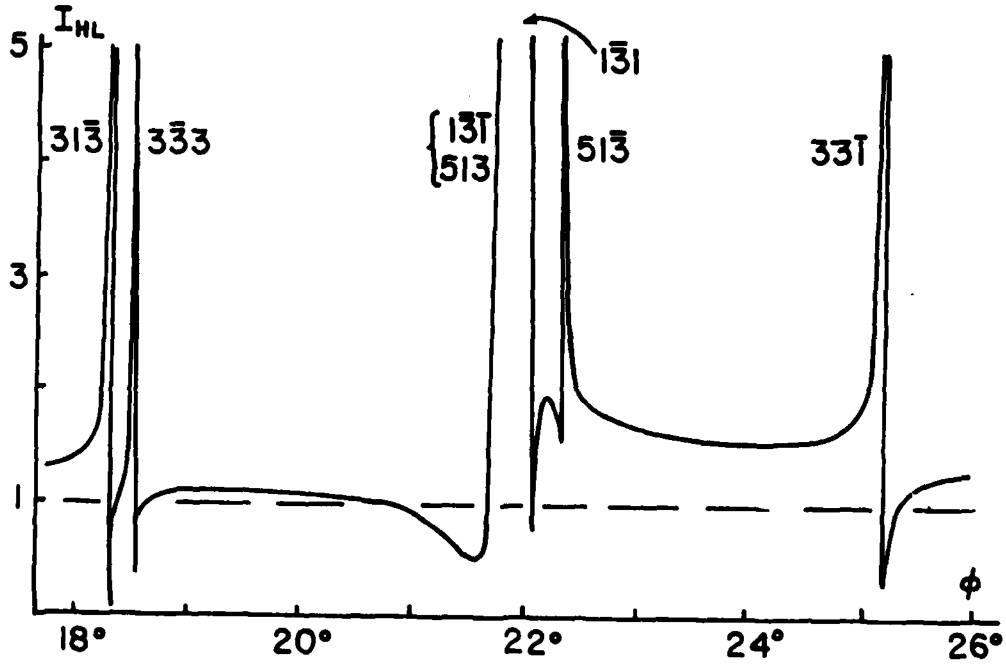

Fig. 3 The sum of the intensities of Fig. 2, for unpolarized incident radiation.

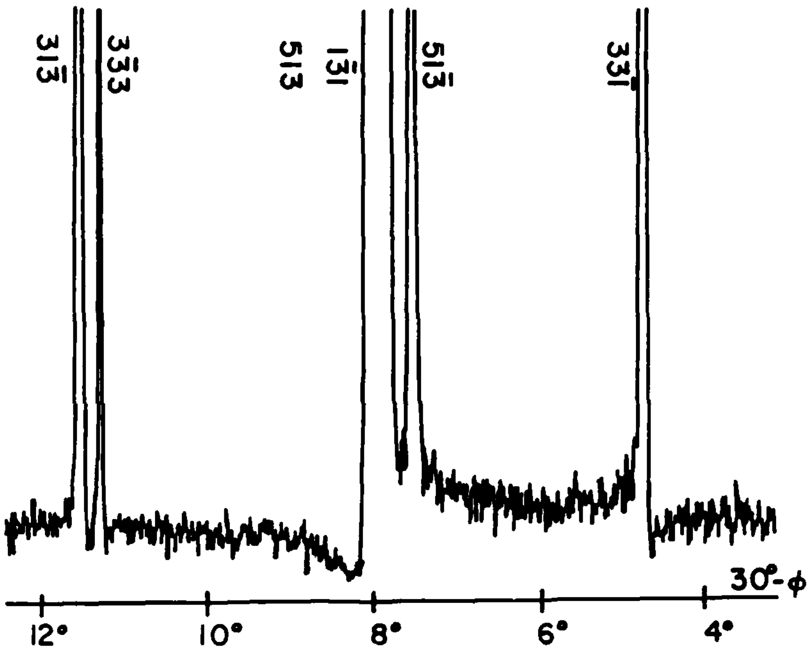

Fig. 4 Experimental Renninger scan of Ge 222/L, from J. Nicolasi, "Experimental Procedures for Determining the Invariant-Triplet Phases of X-ray Reflections," Ph.D. Thesis, Polytechnic Institute of New York, June 1982.

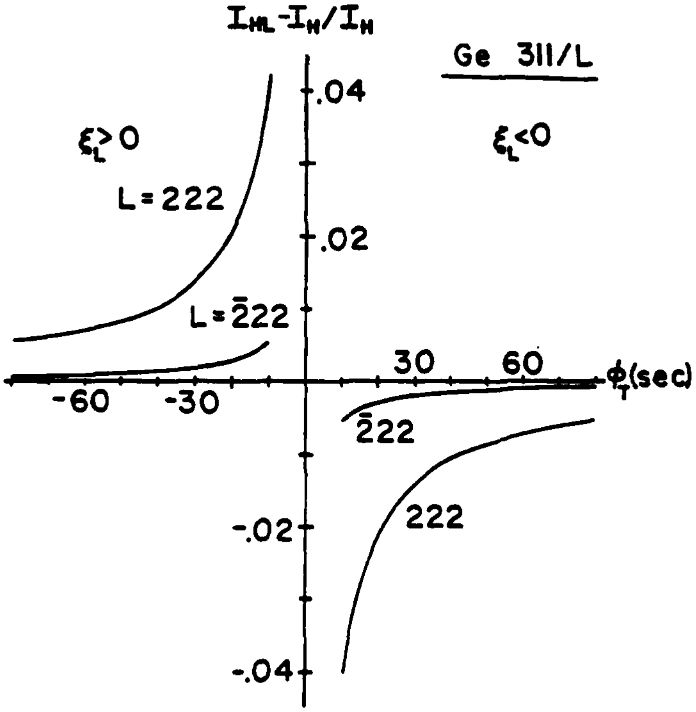

Fig. 5 Relative change of integrated intensity of the Ge 311/L interaction in a Renninger scan with azimuthal angle ϕ_T, for L = 222,$\bar{2}$22. λ = 1.541 Å. ξ_L measures the distance of L from the Ewald sphere. σ-polarization only.

SECTION II: SOLID STATE

B. MICROSTRUCTURE PHOTOPHYSICS

Professors S. Arnold and K.M. Leung

Unit SS5-2

1. OBJECTIVE(S)

Our objective is to develop a quantitative understanding of the detailed interaction of electromagnetic radiation with microstructures of dimensions (a) comparable to and much less than the wavelength (λ) of the incident radiation.

In some cases the broad features of this interaction, and especially the enormous resonant enhancements, may be understood qualitatively by using a classical model for the local electromagnetic field (e.g., surface enhanced Raman scattering).[1] In others this approach has not proven to be fruitful (enhanced photoemission from small Ag particles).[2] The lack of a cohesive framework must in part be due to the limitations of the current classical model in the face of the properties of real materials and structures. Unfortunately, careful attention has not been paid to these limitations. This neglect has usually been dictated by experimental bounds or by theoretical limitations. But, at this time, a fuller understanding of the limitations, and, by implication, a more systematic exploitation of their remarkable consequences, rests precisely on more attention to detail and on quantitative comparison of experiment and theory.

Here we propose such a study, relying on tight interplay between theory and experiment, that emphasizes both far field and near field features such as scattering, fluorescence and energy transfer, on single structures of fully characterized geometry, and extending into a limit $a/\lambda \ll 1$ where particle properties are expected to deviate from their macroscopic behavior.

In addition to linear processes, our experiments and our theoretical investigations will be extended into a regime in which the incident radiation can change the physical nature of the system. Along these lines, we have already demonstrated ultrasensitive infrared detection by using absorbed IR radiation to shift visible structure resonances.[3,4] Perhaps a more exciting possibility is our prediction of IR <u>optical bistability</u> of Raleigh-sized semiconducting particles.[5] Experiments on this and other effects make use of the unique single-particle levitation facility which we have improved substantially during the past three years, particularly in the direction of extending the range of particle sizes from 50μ to below 100Å in diameter.

2. SUMMARY OF RECENT PROGRESS

This section presents a brief summary of recent progress; more detailed descriptions are contained in the next section in conjunction with the state of the art so that the nature of the contributions can be understood more clearly.

SECTION II: SOLID STATE

The program in Microstructure Photophysics is composed of two interactive parts. Experiments are carried out at the Micro particle Photophysics Laboratory (MP^{3}L) under the direction of S. Arnold while theoretical work on associated phenomena is carried out by K.M. Leung. This past year has been particularly productive in three major areas.

A. Microstructure Enhanced Energy Transfer[6]

The discovery, based on observation of microstructure luminescence [using Microparticle Fluorimetry (MPF)[7]], that electronic energy transfer within a condensed matter phase can be enhanced by orders of magnitude if the material is contained within a microstructure.

B. Microparticle Optical Bistability (OB)[5]

Theoretical work indicates that the intensity dependent refractive index of semiconductors such as n-type InSb near the surface plasmon resonance should lead to Optical Bistability in both scattering and absorption. This exciting prospect will be tested during this coming year.

C. Photophysical Interactions with Ultramicrons

Over the past year we have constructed a new high vacuum levitator facility which will be used to investigate the validity of classical electrodynamics for particles with sizes down to 100Å in diameter.

A number of other research projects which are relevant to the above have been investigated during the year and have lead to additional publications. In all the publications already credited to JSEP for 1985 are:

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3. STATE OF THE ART AND PROGRESS DETAILS

The physics of micron and submicron structures is part of everyday reality. This is especially true in the area of microelectronics. And yet, the plethora of recent publications on the new physics of such structures indicates that our understanding is far from complete. In part, the existence of new microprobes and more sensitive instruments has made data in this area available. The new data have led to new surprises. Thus Raman scattering from molecules adsorbed on lithographed surfaces is found to be enhanced[8] by as much as 10^7, and light scattering from roughened metal surfaces contains an enhanced frequency doubled component.[9,10] A host of other photophysical enhancements has been reported; most notable from the standpoint of electronics is the hundred-fold enhancement in photoemission from silver spheres 50Å in diameter.[2]

Much is not yet understood, however, it is generally agreed that the most important physical influence in phenomena such as surface enhanced Raman scattering is the local field which develops in response to electromagnetic excitation. For a time, work on dispersions of 100Å sized particles could not be accounted for in this manner; now, however, the anomalous behavior is understood through particle clustering into dimers, trimers, etc.[17] The reason for the anomalous behavior in photoemission still lacks understanding, however, one certainly would draw a great deal of comfort from experiments on well defined particles.

In contrast to the work at other laboratories, the approach at the MP^{3}L is to do experiments on a <u>single</u> well defined particle. Our work is exemplified by the experiments and theory on photophoresis which have just been completed.[18,19] Here, we found that the radiometric force induced by a CO_2 laser[11] showed resonances and reversals with changing size which could only be accounted for using a self-consistent model for the local field.[12] In what follows we will show how this approach is being used to probe the phenomena outlined in the previous section.

A. <u>Microstructure Enhanced Energy Transfer</u>[6]

Our interest in energy transfer arose during the modeling of photophoresis. So long as theory was carried out on nonfluorescent particles we were able to say that the heat evolved at a given point was proportional to the square modulus of the local field as computed from the solution to the electrodynamic boundary value problem; i.e., Mie theory. The only exception was in our work on fluorescent particles.[13] Things do not quite fit in this case. It was clear that although the absorbed energy had been generated at a particular place a good deal of it became delocalized. At about this time a theoretical paper by Gersten and Nitzan[14] appeared in the literature which suggested that a microparticle could stimulate energy transfer between an external excited molecule (donor) and a diametrically opposed unexcited molecule (acceptor) due to a small particle surface plasmon resonance. Our particle was dielectric and contained no surface resonance in the region of interest, however, we decided to look more carefully at the fluorescence spectroscopy in the light of Ref. [13]. To answer this question the first Microparticle Fluorimeter (MPF) was constructed.[7] With this device we have been investigating the fluorescence of a microparticle in the presence of a small acceptor impurity. We discovered that a great deal of the energy which is originally absorbed by the donor molecules within the particle is received by the acceptors although the acceptor concentration is too low for conventional dipole-dipole transfer to be effective. This phenomenon is demonstrated in Fig. 1, in which the luminescence from a particle with a nominal radius of 10μ has been recorded. This dielectric particle contains two dyes, a donor (9AA) and an acceptor (R6G) in the indicated concentrations. In bulk essentially no acceptor luminescence is found in the spectrum [as indicated by the lower curve in the region of acceptor luminescence (approx. 570nm)]. As one can see, the luminescence in the particle shows a distinct contribution modulated by structure which is resolution limited. Since our report of this work,[6] theoretical groups at the Polytechnic, Harvard, and Northwestern have begun to search for an explanation for this new enhancement. A preliminary mechanism which has been evoked is that the originally excited molecule communicates with the acceptor through well-defined morphological resonances of the particle. The communication requires that the 10μ particle have resonances with a quality factor (Q) of 10^7. If so, our experiments provide the first evidence for such low loss modes in a microparticle.

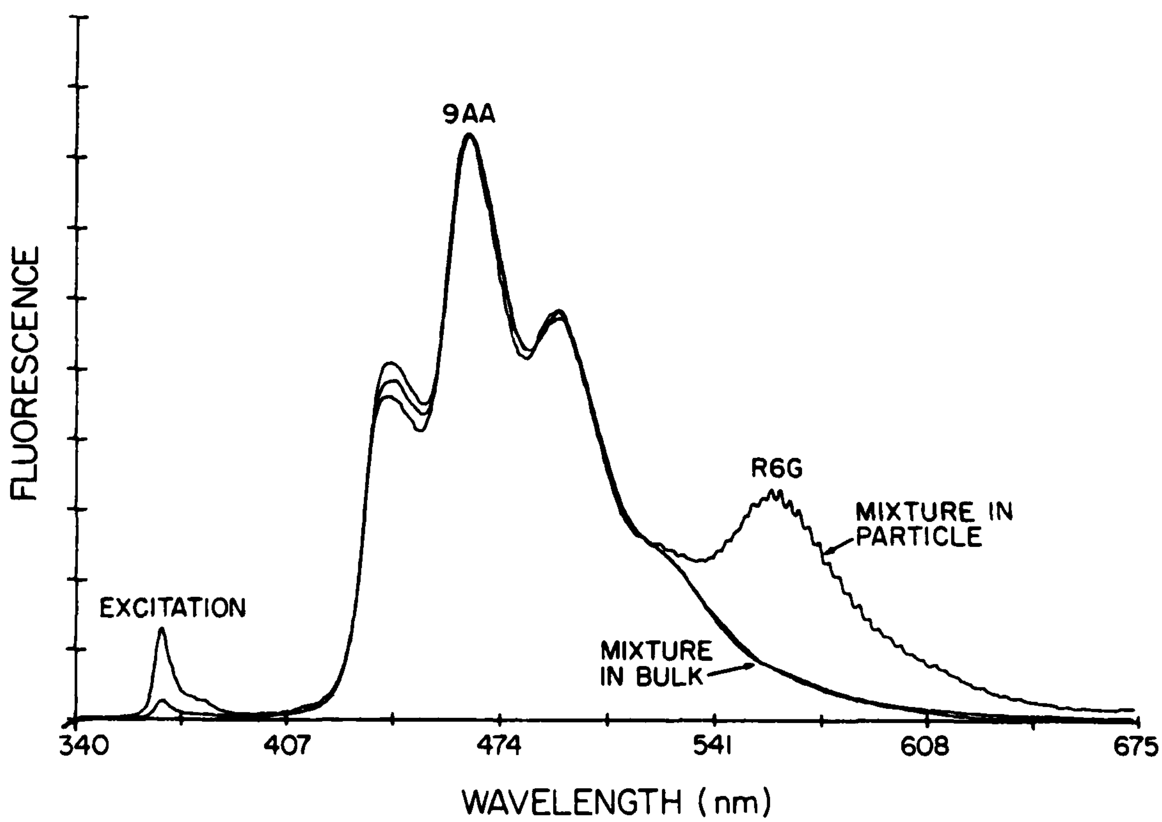

Fig. 1 Luminescence from a single dielectric microparticle about 10μ in size with donor and acceptor impurities.

B. Microparticle Optical Bistability (OB)[5]

Professor Leung has made an exploratory study of how submicron sized objects behave in the presence of intense electromagnetic radiation. Despite the importance of this topic for device application and for defense purposes, relatively little theoretical work has been reported, especially in the physics community. This is due to the fact that in the presence of an intense field materials respond nonlinearly, and the resulting Maxwell's equations form a set of coupled nonlinear differential equation whose solutions are notoriously difficult to find. The arsenal of mathematical techniques such as Green's functions, Fourier transforms and integral methods, which are so successful in dealing with linear problems, are quite incapable of treating intrinsically nonlinear problems. Consequently most theoretical works are numerical in nature, and, as such, only a relatively small physical parameter region can be explored even with today's most powerful supercomputers. Thus, important new insights and totally new physical effects may be lost. On the other hand, analytical studies are extremely rare. Except with planar geometries,[15] even the electrostatics involving simple objects with intrinsically nonlinear dielectric susceptibilities has not been studied. Our work represents an important step toward this direction.

We[5] find that as the intensity of infrared radiation impinging on a model n-type InSb sphere, of Rayleigh size and with a plasmon excitation wavelength of 10.6μ, is increased the internal energy vs. incident intensity follows a triple-valued curve, as shown in Fig. 2. It is well known that the points of infinite slope represent instabilities at which switching will occur, as shown by the rightmost dotted line. As the incident field is decreased, hysteresis appears. Therefore, in effect the microparticle is acting as an optical memory element; the model particle is optically bistable.

Presently, experiments are being conducted at the MP^3L for testing this model. As stated in Ref. 5, one may also expect similar behavior when ka>>1. Theoretical calculations[16] show that a part in 10^4 change in the refractive index due to optical nonlinearity for a CdS sphere of 0.64μ radius causes a shift in stimulated visible Van de Hulst resonances of 10 linewidths. Considering the sensitivity of such particles to refractive index one can expect low intensity switching and perhaps the same sort of OB properties as predicted for Raleigh particles.[5] It should be emphasized that the present theory is not yet in a position to predict an analytical form for the nonlinear behavior of an optically large particle. Although our present work for Rayleigh particles is at the cutting edge, this field is clearly in its infancy from the standpoint of both theory and experiment.

C. Photophysical Interactions with Ultramicrons (particles $\lesssim$ 100Å)

Over the past year we have assembled a high vacuum levitator for the purpose of carrying out scattering experiments on single particles 100Å and below. This levitator is nearly completed, and the exploding wire source of metallic ultramicrons is in the process of being designed. It is intended that the high vacuum levitator will be substituted for the atmospheric pressure levitator currently being used in the Microparticle Fluorimeter set-up. With luck, work on the scattering from individual ultramicrons could be started within this next year.

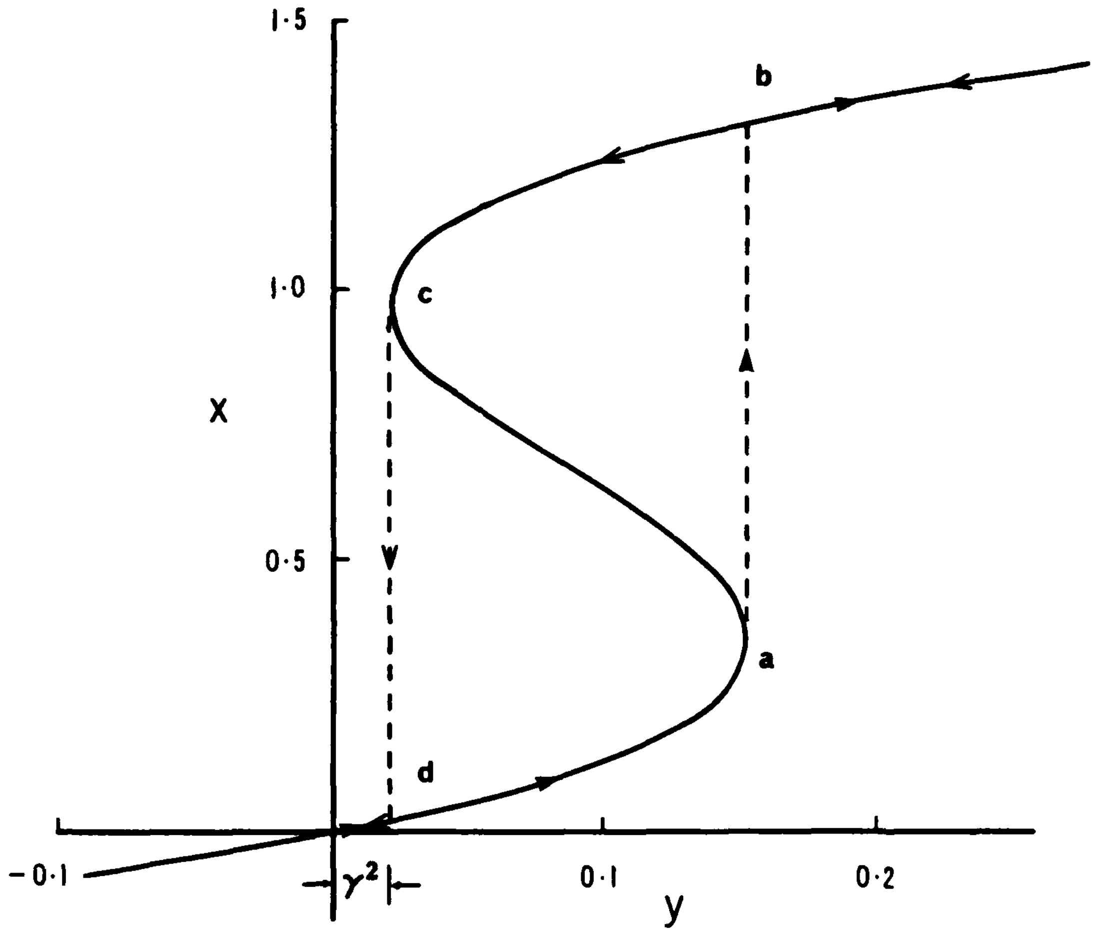

Fig. 2 Internal energy (x) vs. incident intensity (y) in a model n type InSb sphere of Rayleigh size at an excitation wavelength of 10.6μ. The theoretical calculation demonstrates the existence of optical bistability.

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C. DYNAMICAL AND NON-EQUILIBRIUM PROPERTIES OF SURFACE AND INTERFACES

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Unit SS5-3

1. OBJECTIVE(S)

To develop a theoretical and experimental understanding of some specific interactions of surfaces with electrons, photons, atoms, and with each other, that govern the dynamical properties of surfaces and interfaces - the emerging crucial "missing link" between current surface science studies and the practical behavior of surfaces. Since no unified framework exists to attach the myriad of problems of probable importance, we will study three situations, representative of the range of questions that must be answered, that offer the greatest hope for fruitful analysis and potential impact in this new area. The general theme of phonon interactions, from microscopic to macroscopic time and length scales, couples the three target problem areas within the field of dynamical and non-equilibrium phenomena.

Under this common theme, the specific theoretical problems chosen address the relaxation mechanisms of hot electrons in very small structures and the dynamics of surface reactions with incoming atoms or molecules. Accompanying experiments will concentrate on developing second harmonic light generation in interface regions as a tool for studying time-dependent strains in those regions.

The emphasis of most current surface studies on the gross aspects of surfaces, such as their electronic properties or their average structural relaxation, has been very successful in understanding many of the major new features seen or expected there. However, at the next stage of detailed quantitative descriptions of particular phenomena, evidences of new complexities are accumulating, that point to the need for re-examing critically the underlying theory in order to understand more fully the restrictions and new conditions, as well as the new degrees of freedom, imposed by the existence of a surface, and by its dynamical response. For example, electrons participating in current transport in a narrow surface region may encounter closely spaced barriers before being able to shed the excess energy gained in local regions of high field, and thus continue to remain 'hot.' Similarly, atoms colliding with a surface often do so in times so short that they do not allow for a full exchange of energy to reach thermalization. The common features of phenomena such as these are, first of all, that they deal with processes that start out far from, and may never reach, steady states close to thermal equilibrium; and, secondly, that because of the existence of the surface, or an interface, the importance of various relaxation mechanisms may differ markedly from their relative strengths in bulk material.

Within this broad context, we are proposing to examine a number of specific problem areas, selected primarily because of the project participants' wide background in the conventional treatments of these topics, and also because of the real opportunity they present for transcending the conventional treatment and to make concrete new contributions. The problem areas relevant to this proposal are:

SECTION II: SOLID STATE

A. The theory of electron-phonon scattering rates in small electronic devices is in an unsatisfactory state because there is serious disagreement between experiment and theoretical expectations.

B. Although many atom-surface interactions of current interest involve molecular beams, almost nothing is known on the theoretical forefront of the reaction dynamics of non-equilibrium transient species involved in surface reactions.

C. While the generation of optical second harmonic signals in the surface region of solids has been studied for more than a decade, and has received considerable theoretical attention, the separation of signals originating in various regions below the surface of real materials has not been given much study, nor, in particular the relation of these signals to the structure and the strain pattern in the surface region that are now emerging as having major importance.

2. SUMMARY OF RECENT PROGRESS

A. Electron-Phonon Scattering by Hot Electrons in Quantum Well Microstructures

The research has focused on the mechanisms whereby optically excited electrons in the immediate vicinity of an interface relax towards lower energy states. We have developed a formalism that is capable of describing the scattering of electrons by interface optical phonons. Unlike previous formulations[14,15] the dynamical properties of the materials on both sides of the interface play important roles in the scattering processes. The equilibration of optically excited electrons proceeds mainly by inter sub-band scattering, since this dominates the rate of energy loss. The rate of energy loss has been calculated in the second Born Approximation.

B. Non-Equilibrium Surface Reaction Dynamics

This section presents a brief summary of recent progress within this research unit. A more detailed description of this is given in the next section in conjunction with the state of the art. In short, we have concentrated on four related areas concerning non-equilibrium effects in surface reaction dynamics. Those are:

(i) We have developed a comprehensive theory for thermal desorption rates in presence of weak-to-moderate dissipation and non-Markovian, frequency-dependent friction. This generalization allows for the calculation of desorption rates of adparticles beyond the heavy ad-particle limit. We find that the rates are suppressed over those calculated within the heavy ad-particle approximation.

(ii) We have completed a literature search on the topic of "Escape From a Metastable State" and wrote a comprehensive review (to appear in J. Statistical Phys. 42, 105 (1986)) wherein we interpreted, reported and extended various theories of noise driven escape.

(iii) We have addressed the problem of surface kinetics at low temperatures where one expects to find a characteristic temperture at which a crossover from thermal hopping (Arrhenius behavior) to quantum tunneling occurs.

(iv) Finally, we have studied mean sojourn times (inverse of rate) in diffusive surface reactions which are of the Langmuir-Hinselwood type. For the first time, we obtained novel results for non-white, correlated random walkers that were inaccessible up to present time. We find that typical sojourn times before absorption (or reaction) are enhanced over the usual results based on Gaussian white noise.

C. Second Harmonic Generation Studies of Surface Structure

Our objective in these studies is to utilize second harmonic generation as a probe for the structure of surfaces. In so doing we will go beyond current descriptions which deal principally with electronic relaxation along the surface normal by including structural rearrangements that have recently been shown to exist in directions both parallel and normal to the surface.[1]

The program in second harmonic generation from surfaces has so far made progress in two areas:

(a) The construction of a unique instrument for examining second harmonic generation based on low light intensity excitation from a Ga-Al-As laser diode and detection by synchronous photon counting.

(b) The measurement of the dependence of second harmonic generation on the azimuthal angle between the single harmonic excitation and the surface crystal axes in Ag. A surprising preliminary result in this case is that the signal appears to show angular periodicity implying that a large part of the effect is due to atomic layers other than the first.

3. STATE OF THE ART AND RESEARCH DETAILS

A. Electron-Phonon Scattering by Hot Electrons in Quantum Well Microstructures

The size of electronic components has decreased rapidly over the last decade, to such an extent that many of the classical concepts developed for bulk materials have become completely inappropriate for their description. An important consequence of the reduction of the size of electronic devices is that the internal electric fields become very large. Fields of the order of 10^3 V/cm are quite common in present day integrated circuits, while fields strengths of the order of 10^5 V/cm can be found between the neighboring gates of charge coupled devices and in quantum well layered devices. At such large fields, the electrons are rapidly accelerated and acquire large kinetic energies. The net result is that the conducting electrons cannot be regarded as being in equilibrium with the rest of the microstructure, and the conduction process becomes extremely non-ohmic at room temperatures.[2] This regime is characterized by extremely non-equilibrium thermodynamics.

The manner in which the electron gas exchanges energy with the rest of the system becomes extremely important. As we shall outline later, there is considerable evidence that the dissipative process for these high energy electrons is completely different from the processes that usually occur for the electrons in thermal equilibrium. This is even more true for quantum well systems such as MOSFET's[3] or quantum well[4] heterojunctions in which the saturation velocities of 10^6 cm/sec are considerably lower than the bulk values of 10^7 cm/sec.[5] The presence of the interfaces may be of crucial importance in the description of the non-equilibrium effects.

At room temperature, it is generally believed that the mobility is governed and limited by phonon scattering, and that most of the excess energies are transferred to the lattice via optical phonons. But, as Ando et al[1] have pointed out in their recent review article, the theory of phonon scattering for the electronic mobility is quite unsatisfactory. The calculated mobility[6] is much larger than the experimental value. Even more distressing is that the one-phonon process leads to a mobility that is almost independent of the density of electrons in the inversion layer. The experiments show a $N_s^{1/3}$ dependence on the electron density.

At this time, therefore, a more general investigation of the processes through which an electron can emit or absorb phonons and equilibrate with the lattice is called for. In particular, it should take into account the specific nature of the phonon spectra near the interfaces, as well as the possibility that the energy exchange between the electrons and phonons may become a resonant process. This possibility is offered since the separations of the various subbands nearly match the bulk phonon energies in some systems.[7] In addition, the role of the effects of higher order phonon processes must be clarified. In bulk materials, such effects are usually neligible, as may be implied by Migdals theorem.[8] However, in quantum well systems the theorem no longer applies so the multiphonon processes could be of importance. The presence of these multiphonon events may strongly influence the hot electron relaxation rates, but may also be responsible for the discrepancy between the experimental data on mobilities in the ohmic regime and theoretical calculations that only consider single phonon scattering events.[1] Other authors[1] have speculated that these discrepancies may be due to the effects of electron correlations in the final states, but apparently no one has investigated the possibility of the multiphonon processes that we suggest.

The optical properties of inversion layers show related anomalies, presumably also associated with the electron phonon scattering mechanisms. Kneschaurek and Koch[9] have studied the temperature dependence of the inter-subband optical transitions. These and related experiments[10,11] show that the widths of the resonance lines present a problem at high temperatures, in that the widths do not increase concomitantly with the increase in the phonon-induced relaxation rate inferred from transport properties. This raises the question of how well the transport scattering rate is correlated with the corresponding optical rate in the presence of multiphonon events. There are two obvious differences that come to mind. One is the weight of the factor $(1-\cos\theta)$ that usually enters into the momentum scattering rate,[12] and the other is the frequency dependence of the scattering rate.[13] The presence of important multiphonon processes[17] may be such that these relaxation rates become completely different from each other.

The research focuses on the properties of an electron gas at the interface between a semiconductor and another material where band bending effects induced by the external field drive the conduction band below the fermi level, in the vicinity of the surface. The electronic motion normal to the surface is confined by the electrostatic potential. The confinement within this narrow potential well causes the electronic energy levels to be quantized. The electrons remain free to move parallel to the surface. Thus, we consider the sequence of subbands with energy levels $E(n,k_{||})$ given by

$$E(n,k_{||}) = \Delta_n + \frac{\hbar^2 k_{||}^2}{2m^*} \qquad (1)$$

where $k_{||}$ is a two-dimensional wave vector parallel to the surface, m^* is the electronic effective mass and Δ_n is the energy of the nth subband at $k_{||} = 0$.

We have explored the influence of electron-phonon interactions on the properties of the electrons in these inversion layers, in particular the multiphonon processes.

We have generalized the electron-phonon interaction formulated by Evans and Mills[14] to the case of an interface. We have considered the scattering from both the bulk and interface phonons, since it has been noted[15,16] that at interfaces with large dielectric mismatch the optical phonons may have large energies (670°K).

Thus, the two frequencies of the interface/optical phonons are given by the condition

$$\varepsilon_1(\omega_s) = -\varepsilon_2(\omega_s) \qquad (2)$$

in which $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ are the frequency dependent dielectric functions for the materials on either side of the interface. The frequencies of the interface phonons are generally intermediate between the LO and TO phonon frequencies of each medium. The electrostatic potential set up by such phonons satisfies Laplace's equation, if one neglects the effects of retardation. Hence, the potential for an interface phonon with a wavevector $q_{||}$ parallel to the surface has the spatial dependence of

$$\exp\,[i\,\vec{q}_{||} \cdot \vec{x}_{||} - q_{||}\,|z|] \qquad (3)$$

where z is the distance measured normal to the interface. Because of this z-dependence, we find that electrons trapped on one side of the interface should be appreciably scattered by the potential set up by both interface modes.

In contrast, the bulk phonons decrease rapidly in amplitude at the interface bounary, as can be seen by the following elementary argument. The bulk phonons of region 1 satisfy the condition $\nabla \cdot D = 0$, by virtue of $\varepsilon_1(\omega_{LO^1}) = 0$. In region 2, if $\varepsilon_2(\omega_{LO^1}) \neq 0$, we must have $\nabla^2 \phi^2 = 0$. Thus for $z < 0$, the potential is

$$\phi_2(z) = \phi^0{}_2 \exp [i \vec{q}_{||} \cdot \vec{x}_{||} + q_{||}z] \tag{4}$$

Continuity of ϕ at $z = 0$ requires $\phi_1{}^0 = \phi_2{}^0$. Continuity of D then gives $\phi_1(o) = \phi_2(0) = 0$, so that the potential ϕ_1 has the form

$$\phi_1(z) = \exp [i \vec{q}_{||} \cdot \vec{x}_{||}] \sin q\, z \tag{5}$$

which vanishes as z approaches zero. Thus, the potential due to the high frequency bulk LO phonons will not penetrate across the interface to where the electrons are located, while, as argued above, the interface phonons do.

The frequency of the interface optical phonons is given by ω_s where

$$\omega_s{}^2 = \frac{1}{2} [\frac{\varepsilon_1(0)+\varepsilon_2(\infty)}{\varepsilon_1(\infty)+\varepsilon_2(\infty)} \omega_1{}^2 + \frac{\varepsilon_2(0)+\varepsilon_1(\infty)}{\varepsilon_2(\infty)+\varepsilon_1(\infty)} \omega_2{}^2$$

$$\pm \sqrt{ \{(\frac{\varepsilon_1(0)+\varepsilon_2(\infty)}{\varepsilon_1(\infty)+\varepsilon_2(\infty)}) \omega_1{}^2 - (\frac{\varepsilon_2(0)+\varepsilon_1(\infty)}{\varepsilon_1(\infty)+\varepsilon_2(\infty)}) \omega_2{}^2\}^2$$

$$+ 4 \{\frac{\varepsilon_1(0)-\varepsilon_1(\infty)}{\varepsilon_1(\infty)+\varepsilon_2(\infty)}\}\{\frac{\varepsilon_2(0)-\varepsilon_2(\infty)}{\varepsilon_1(\infty)+\varepsilon_2(\infty)}\}]$$

in which ω_1 and ω_2 are the transverse optical frequencies of the materials on either side of the interface. Likewise, $\varepsilon_1(0)$, $\varepsilon_2(0)$ and $\varepsilon_1(\infty)$, $\varepsilon_2(\infty)$ are the zero frequency and high frequency limits of the dielectric constants. Thus, electrons in material 1 can scatter with interface phonons, and the energy transfer can involve large frequencies, of the order of ω_2. By contrast, the bulk phonon scattering rate may only involve energies of the order $\hbar\omega_1$, which could be significantly smaller.

We have calculated the energy loss rate from the second Born Approximation. We find that the rate $1/\tau$ for an electron in state $n,\vec{k}_{||}$ to lose energy is given by

$$\frac{1}{\tau} = \sum_{q_{||},} \hbar\omega_s \{P_{n,m} (\vec{q}_{||}) - P_{n,m} (-\vec{q}_{||})$$

$$= \sum_{q_{||}m} \hbar\omega_s \, M_{nm}(\vec{q}_{||}) \, M^*_{nm}(\vec{q}_{||})$$

$$[\{1+N(\omega_s) - f_m(\vec{k}_{||}-\vec{q}_{||})\} \, \delta(\varepsilon_n(\vec{k}_{||}) - \varepsilon_m(\vec{k}_{||}-\vec{q}_{||}) - \hbar\omega_s)$$

$$- \{N(\omega_s) + f_m(\vec{k}_{||}-\vec{q}_{||})\} \, \delta(\varepsilon_n(\vec{k}_{||}) - \varepsilon_m(\vec{k}_{||}-\vec{q}_{||}) + \hbar\omega_s)]$$

in which N(x) and f(x) are the Bose-Einstein and Fermi-Dirac distribution functons, respectively. The summation over $\vec{q}_{||}$ must be performed numerically. The results are tabulated in reference 18.

B. Non-Equilibrium Surface Reaction Dynamics

(1) General Background

This problem area deals with the interaction of atoms or molecules reacting with a surface. For processes such as molecular beam epitaxy, chemical vapor deposition, molecular beam scattering, laser assisted desorption, etc., the elementary process of absorbing or desorbing of particles on a surface presents the key element of the surface reaction dynamics. All these processes are rather complex. In particular, a particle that impinges on a surface cannot be viewed as a mere golf ball landing in a sand trap. There are a variety of entangled energy transfer processes, which determine the rate limiting steps. A detailed understanding of the relevant role of various competitive processes, such as thermal energy activation, loss of transverse kinetic energy, coupling to phonon-like and electronic degrees of freedom of the substrate-surface, etc., are all essential if one wants to assess the general scheme responsible for an enhancement or suppression of the surface kinetics.

(2) Thermal Description and Frequency-Dependent Dissipation

Since the initiation of this research unit on non-equilbrium surface reaction dynamics in April, 1985, we have begun research in the area of thermal desorption processes. In particular, we re-examined the literature of this extensively studied phenomenon[1] and isolated the areas containing short-comings, but which allow for substantial novel improvements. In most of the published literature,[1] standard transition state theory (TST) has been employed.[1] The important point, that such a standard approach is not suitable in many situations, has already been made in convincing form by Iche and Nozières in a tutorial paper dating back to 1976.[2] They demonstrate that an approach along the lines of Kramers[3] is superior. Following this line of reasoning, limiting forms of a Kramers-type approach have already been utilized recently in th literature by restricting oneself to the heavy-ad-atom limit: Considering only the interaction of the ad-atom with electronic degrees of freedom of the substrate, this problem has been tackled (in the heavy ad-atom limit, i.e., white Gaussian noise limit) by Suhl and co-workers.[4] A coupling to lattice vibrations has been considered in the white Gaussian noise limit (heavy ad-atom) by a French group.[5]

Our scheme for evaluating desorption rates is broken up into three steps:

(a) First, we express the equation of motion of the ad-particle in the form of a stochastic equation. With such an approach, the interaction with the residual degrees of freedom (surface phonons) manifests itself via a generally frequency-dependent friction and a random force.

(b) Then, we must explicitly determine the systematic binding force $F(x) = -\frac{\partial V(x)}{\partial x}$ of the ad-particle for the problem under investigation and evaluate the frictional force in terms of the coupling parameters to the residual degrees of freedom.

(c) Once the stochastic equation is completely specified, it must be solved for the desorption rate. Of particular interest is the calculation of the prefactor, (the exponential leading part is given by the Arrhenius factor) which otherwise is also known as "sticking-coefficient."

We have considered the motion of an ad-particle of mass M, trapped in a potential V(x) near a solid surface (Fig. 1).

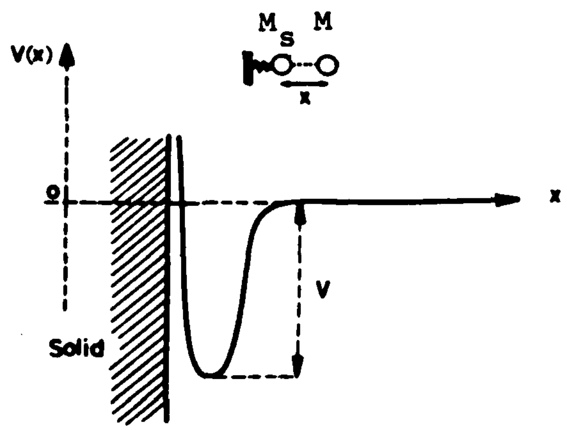

Fig. 1 Pictoral representation of a one-dimensional model of the ad-particle bound to the surface: x = X-Y, where X denotes the ad-particle (mass M) position and Y indicates the horizontal coordinate of the surface atom (M_s).

Following the outline of our original proposal we have completed steps (a) and (b) via transforming the dynamics in terms of center of mass and relative coordinates. We succeeded in deriving a generalized Langevin equation for the velocity $v = \dot{X} - \dot{Y}$

$$\dot{v} = -\frac{1}{\mu}\frac{\partial V(x)}{\partial x} - \int_0^t \bar{\gamma}(t-\tau)v(\tau)d\tau + f(t) \tag{1a}$$

The random force f(t) obeys the generalized fluctuation-dissipation theorem[6]

$$\langle f(t)f(t+\tau)\rangle = kT\,\bar{\gamma}(\tau) \tag{1b}$$

wherein $\bar{\gamma}(\tau)$ can be related to the dispersion of surface phonon modes $D(\omega)$.

From the physics point of view, the regime of weak-to-moderate friction strength is the physically relevant regime. The non-equilibrium dynamics can be modeled by a Fokker-Planck equation in the energy variable.[7] Following reference 7, the influence of memory-friction, $\bar{\gamma}(\tau)$, is taken into account via an effective energy diffusion D(E)[7] (J denotes the action)

$$D(E) = kT\, J(E) \int_0^\infty \bar{\gamma}(\tau)\, \frac{\langle v(\tau)v(o)\rangle}{\langle v^2\rangle}\, d\tau \qquad (2a)$$

$$\leq kT\, J(E) \int_0^\infty \bar{\gamma}(\tau) d\tau \equiv D(E)^{\text{heavy ad-atom}} \qquad (2b)$$

This then allows one to perform step (c); i.e., to perform an out-of-thermal-equilibrium calculation for the sticking coefficient P, beyond the standard transition state theory result for the rate, Γ_0, and beyond the heavy ad-particle limit; i.e., the corrected rate Γ reads

$$\Gamma = P\, \Gamma_0, \quad P < 1 \qquad (3)$$

Our main finding is that the <u>sticking probability P is characteristically suppressed</u> compared to the result in the heavy ad-particle limit ($M \gg M_s$).

Presently, we are preparing a publication of these novel and general results. In addition, we plan to apply our results to the problem of desorption from argon from tungsten and NO from Pt(111).[8] In the last case, we can also compare our theoretical predictions with experimental results for molecular beam studies[9 11] of the sojourn times τ, i.e.,

$$\tau \sim 1/\Gamma \qquad (4)$$

(3) <u>Escape From A Metastable State</u> (Review)

Over the last 8-12 months or so, we actively prepared a comprehensive review, in which we have reported, interpreted and extended the present state-of-the-art approach for the fundamental problem of noise-activated escape. This article has been accepted for publication in the Journal of Statistical Physics (Ref. 12), and it will appear shortly. This work also served as the motivation for an extensive literature search in this field. Clearly, this topic forms the key input for an accurate description of various non-equilibrium surface kinetics phenomena. It is hoped that this very article will serve as the key guide for future work in this and related fields, thereby assuming the role of a "land-mark" paper for the next decade or so. For the first time, this report also summarizes the recent developments of the quantum version of the Kramers approach. Thus, this provides the possibility to describe dissipative escape at all temperatures in a unified way. In this context, it is only fair to mention that two of the investigators in this research unit have been playing an active role at the forefront of these important novel developments.[13,14,15]

(4) <u>Surface Kinetics at Low Temperatures: Crossover from Thermal Hopping to Tunneling</u>

Presently, we are exploring the possibility of applying some aspects of those novel results to low temperature kinetics,[7,13-15] as they might be applicable to model the low temperature dynamics of dissociative chemisorption of CH_4 (and CD_4) on W(110).[16] The experimental findings indicate that the dissociation mechanism proceeds via tunneling through a one-dimensional parabolic barrier.[16] If true, our recent theory[14] would predict that the Arrhenius behavior should start to fail at sufficiently low temperatures around a characteristic temperature, the crossover temperature T_o

$$T_o = \frac{\hbar\tilde{\omega}_b}{2\pi k_b} = (1.22\cdot 10^{-12}\mathrm{secK})\ \tilde{\omega}_b \tag{5}$$

where $\tilde{\omega}_b$ denotes a dissipation and frequency renormalized barrier frequency $\tilde{\omega}_b \lesssim (\frac{1}{M} U''(x_b))^{1/2} \equiv \omega_b$. Below this temperature, the Arrhenius factor $(\exp -E_b/kT)$ ceases to describe the exponential part of the rate law. It would, indeed, be a crucial check for the proposed mechanism if on a variation of temperature one would observe experimentally for this reaction the crossover temperature in an Arrhenius plot.

(5) <u>Surface Reaction Dynamics: Sojourn Times and Diffusive Migration</u>

We also have started to investigate the problem of diffusion-controlled surface reactions. We concentrate on a reaction between species A-particles which are in a surface adsorbed precursor state s-A and a species B in a surface adsorbed precursor state s-B; i.e., we focus on a Langmuir-Hinselwood-type mechanism

$$\text{s-A} + \text{s-B} \rightarrow \text{g - AB} \tag{6}$$

where upon a collision we have a reaction into the gas phase (g-AB). Also we assume that species B is much more mobile compared to species A. The latter species A-particles are allowed to aggregate, i.e., there are "islands" of A-particles. The surface reaction can then be viewed as a diffusive stochastic process wherein the B-particles are regarded as "random walkers." With the assumption that the B-particles are unaffected by lateral interactions (no aggregation) the B-particles can be regarded as "free" random walkers until they eventually hit the boundary of an island of A-particles where immediate absorption (i.e., reaction into g-AB) occurs. Formally, we can write for the two-dimensional diffusive random walk of the B-particles

$$\dot{\underset{\sim}{x}}(t) = \underset{\sim}{\xi}(t) \tag{7}$$

where $\underset{\sim}{\xi}(t)$ denotes a random force. The surface reaction is then specified if we complement Eq. (17) with absorbing boundary conditions, distributed in 2-dimensional phase space at the location of A-islands, together with a characterization of the noise statistics for $\xi(t)$. In contrast to previous work,[17] where $\xi(t)$ is assumed to be standard white Gaussian noise, we allow for a finite lifetime for correlated jumps (no white noise assumption). Our interest is in the experimentally monitored observable, the mean sojourn time τ of species B before absorption occurs (note, that the reaction rate Γ is proportional to $1/\tau$). This very same problem is not only of interest in the present context of diffusive surface reactions, but also has far reaching applications in engineering sciences (switching times) and control theory (error rates).

In a recent piece of work (Ref. 18) we succeeded in obtaining new, exact results for the mean sojourn time for a one-dimensional walker driven by exponentially correlated random noise (non-markovian, memory-dependent random walk), that were previously totally inaccessible. In particular, we found that the mean sojourn times are always enhanced over the case with white Gaussian noise. Moreover, the mean sojourn times obey, in contrast to the white Gaussian noise case, jump conditions on the boundary of absorption; i.e., the residence times for a random walker, which starts out very close to an absorbing boundary does not approach zero with decreasing distance from the boundary, but exhibits a finite value determined by the parameter describing the mean life time of correlations.

Our recent work already has spurred great interest among other groups[19] modelling chemical reaction schemes.

Now, our goal is to generalize our findings to a two-dimensional random walk with randomly distributed A-islands. In particular, we hope that the findings of our new theory are able to explain the recent Monte-Carlo simulation results by Silverberg and Ben-Shaul[20] on the effects of adsorbate aggregation on the kinetics of surface reactions. Those authors convincingly demonstrated that the standard methods for calculating reaction rates[17] are inadequate for this situation.

C. Second Harmonic Generation Studies of Surface Structure

In principle, the generation of second harmonic light (SHG) provides a very sensitive probe of surface properties in all materials of centrosymmetric structures. Because of the nature of the major interactions giving rise to SHG, it is forbidden to first order in the bulk of such materials, and therefore arises primarily in those regions where this symmetry is broken,[2] and predominantly so in the surface region. The relaxation of atomic positions along the surface normal provides the most obvious mechanism of lowering the symmetry there.

Most theories of SHG take this into account by allowing for electronic relaxation along the surface normal[3] but without specific reference to any structural rearrangements. On the other hand, evidence is accumulating from other types of experiments that even the simplest and purest of metals may show rearrangements in their surface structure in both the normal and the parallel directions. Such rearrangements are of comparatively long range character along the surface, and therefore can usually be described by strain distributions. They must also contribute to SHG, although they have never been taken into account, nor searched for systematically. Just as most other structural changes, such as roughness,[4] lead to enhancements in the electromagnetic responses of the surface region, the signature of these signals would be given by increases in SHG intensities, but, more importantly, it is also governed by selection rules characteristic of the strain pattern. Selection rules have recently been applied successfully to identify another symmetry-breaking process that occurs in bulk under high levels of excitation.[5]

In fact, when SHG is used to identify surface strains, one also has to consider that bulk strains throughout the skin depth of the interaction may equally contribute to the SHG signal because of its symmetry lowering effects. This particular additional potential source of SHG has not been taken into account, either, in most discussions of SHG data. Some related results concerning the dependence of SHG on static electric fields applied to the surface, which show a quadratic variation with field,[6] strongly suggest that bulk strains do contribute to the observed signals, since field-induced strains obey the same quadratic variation,[7] but this connection has never been made explicitly, nor confirmed quantitatively.

Both the increasing interest in the detailed structural relaxations in metallic surfaces, and the possibility of using SHG as a weakly interacting but quantitative tool for characterizing some of the longer range correlations in these relaxations make a systematic investigation of the strain contributions to SHG very timely. Other probes, such as slow electrons (LEED), or x-rays, because of their small wavelengths, sense such long-range correlations only in line broadening. SHG, on the other hand, whose signal from an ideal surface should be largely π-polarized, ought to show an additional π-polarization component in the presence of these relaxations, and this would provide a much more clearcut signal of their existence. At the same time, the use of pulsed light in principle allows time-dependent studies of strain development and propagation, in the range of characteristic times encountered in other sections of this research unit.

Over the last 9 months we have assembled a <u>unique instrument</u> for examining the second harmonic (SH) generation by a silver surface. Our major interest was in limiting the intensity at the surface, so that there could be no possibility of a laser-induced change in the physical properties of the surface. For this purpose we are utilizing a single heterojunction Ga-Al-As laser diode (LD) as an excitation source. This laser is cooled to LN_2 temperature so as to improve its duty cycle to 3%. In this way the average power incident on the surface is only 60mW (peak power is ~18W) at a wavelength of 800nm. The use of such a large duty cycle enables us to operate at peak intensity levels below 10^6W/cm^2, while still obtaining measurable signals. However, the signals are small (<20 photon counts/sec), so that a synchronous photon counting approach is being used. A diagram of the apparatus is shown in Fig. 1. The SH output is represented by

$$S_{SH} = [N_{so} - D(1-D)^{-1}N_{so}]/I_p^2$$

where N_{so} is the count number during the laser diode (LD) pulse, D is the laser duty cycle, N_{so} is the count number during the LD off period, and I_p is the laser intensity during the pulse.

Our first interest was in looking at the dependence of the SH generation on the azimuthal angle relative to the surface crystal axes, for various combinations of polarization of the incident and reflected beams. For polarization in the reflection plane one expects that the first layer of surface atoms on an epitaxially grown thin film of Ag on

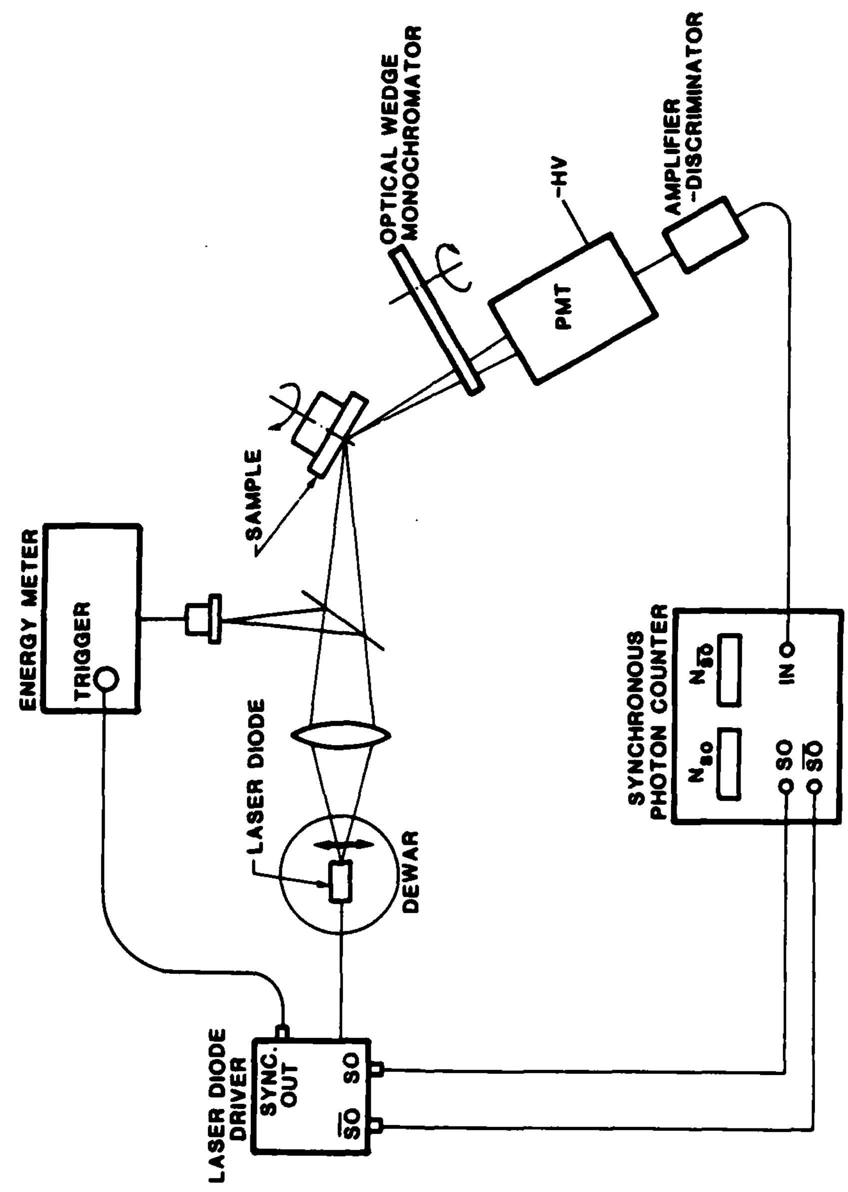

Fig. 1 Experimental set-up for low light intensity excitation of second-harmonic scattering from surfaces.

mica will have a six-fold axis of symmetry. Over the range studied, there clearly appears a 30 degree periodicity in the SH signal vs. azimuthal angle. This exciting preliminary result implies that the contribution from deeper layers is also being felt. In particular, the second layer of atoms has a six-fold axis of symmetry, but it is staggered with respect to the first by 30 degrees. In addition, our calculated count rate is two orders of magnitude less than what had been expected from previously reported nonlinear coefficients.[6] Apparently, some difference exists between the materials used. In our case the films are epitaxially grown. These films are virtually free of defects. In the previous experiments the films were nonepitaxially grown. It may well be that the nonlinear coefficients previously reported for Ag are nonintrinsic. Recently, it has been recognized that even small scale roughness can produce a considerable enhancement in the SH signal. All of this implies that one should look carefully at the effects that strain has on the scattered signal.

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D. INFRARED-LASER-INDUCED MOCVD

Professor D.M. Schleich

Unit SS5-4

1. OBJECTIVE(S)

The purpose of this work is to study the enhancement of chemical vapor deposition by I.R. laser irradiation of gas phase molecules. By this method we hope to prepare binary and ternary materials at substrate temperatures lower than those necessary in classical chemical vapor deposition (i.e., thermal excitation only). This low-temperature synthesis will allow for processing of temperature-sensitive devices, limit impurity diffusion, and perhaps allow for the preparation of materials exhibiting vapor pressure and phase problems. Our first objective will be the preparation of simple silicon compounds (SiO_2 and Si_xN_y) from SiH_4 and either N_2O or NH_3 in the presence of continuous I.R. irradiation (CO_2 laser). We will then determine the relationship between minimum substrate temperature and irradiation as well as the effect of I.R. absorbing species (i.e., SiH_4 or NH_3). Our second objective will be to determine if the deposition can be enhanced by adding an infrared absorber (SF_6) into the reaction chamber. Our third objective will be to carry out Metal Organic Chemical Vapor Deposition (MOCVD) of more sophisticated materials (III - V's and transition metal chalcogenides) using oganometallics with I.R. chromophores.

2. SUMMARY OF RECENT PROGRESS

In attempting to carry out the I.R. laser-assisted chemical vapor deposition of silane we observed two problems with our existing system:

1. The power available with our CO_2 laser (~10 W) was insufficient to cause adequate gas excitation without strong focusing. This in turn limits the deposition of silicon to very small wafer surfaces.

2. The deposition chamber, controlling system and vacuum system, were inadequate for several reasons. The lack of mass flow controller feedback to a vacuum throttle made the monitoring and regulating of more than one gas component very difficult. The seals on the deposition chamber were inadequate to prevent slight oxide formation when none was desired. The diffusion pump system resulted in long prepump times as well as oil contamination of surfaces. In order to overcome all of these difficulties, we are in the process of completely rebuilding the hardware for our experiments.

A high power CO_2 laser (100 W Advanced Kinetics) has recently been purchased with outside funds to allow adequate gas phase excitation. In cooperation with a commercial manufacturer of high vacuum systems (Vactronic), a new deposition systems has been designed and built (expected date of delivery, December 13, 1985). This system is designed to obtain rapid, clean, high vacuum (turbo-molecular pumping system) as well as the mass flow regulation of three gases. The system is also equipped with a quadrupole mass spectrometer and optical ports for simultaneous cross excitation to aid in identification of gas species.

3. STATE OF THE ART AND PROGRESS DETAILS

The preparation of quality thin films either as noncrystalline substrates or epitaxical single crystals is of vital importance to the fabrication of electronic devices and sensors. The approaches available for high quality thin films are basically two:

a. Moleculuar Beam Epitaxy (MBE)

b. Chemical Vapor Deposition (CVD)

Molecular-beam epitaxy is a process of epitaxial deposition using molecular or atomic beams in an ultrahigh vacuum ($\sim 10^{-10}$ Torr) system. This system appears to be most appropriate to the fabrication of very thin heteroepitaxial layers; however, the large investment costs, slow growth rates and difficult wafer throughput limit the applicability of this technique to special systems. Large scale production of materials by MBE is not generally observed in a manufactuing environment.

The basic principle behind CVD is rather simple. Particular chemical species in the vapor phase are decomposed to form a thin film onto a substrate. The major modifications of this technique are the types of chemicals used to introduce the species of interest, i.e., organo-metallic or inorganic substances, and the method used to excite the gas phase molecules and cause subsequent decomposition. The most common way to decompose the gas species is simple thermal heating of the substrate. However, this simple technique has problems associated with it when the temperature needed to cause the necessary gas decomposition is deterimental to the substrate itself or the film being formed. Alternative approaches have been explored to decompose the molecules in the gase phase without directly heating the substrate. The two most common approaches are plasma-enhanced CVD (PECVD) or laser-assisted CVD (LCVD). Some difficulties associated with PECVD include radiation damage, and release of contaminating species from reactor walls. The most common approach of LCVD is to photolyze the gas phase species with photon energy from a UV laser source. The energy transfer is usually a single photon process, although many of the detailed mechanisms of the deposition process are still poorly understood.[1]

We are exploring a modification of this process by using an IR laser to aid in the excitation of the gas phase species. This process was originally studied as a possible alternative to the plasma technique for the deposition of amorphous silicon.[2 7] The UV laser technique is not suitable for silane excitation since astrong absorption does not occur until very high energies (<150 nm);[8] however, silane readily absorbs the P(20) or P(36) CO_2 laser lines. In addition, very high laser power can be obtained at moderate costs for CO_2 lasers, unlike UV lasers. Very recent work has been carried out to further explore the use of CO_2 laser excitation for producing amorphous silicon.[9,10] It was observed that, unlike the results found for silane, no wavelength dependence for deposition was observed for disilane.[9] However, this particular experiment was performed in a perpendicular rather than parallel direction, and therefore the quartz substrate was probably being heated beyond the decomposition temperature of the unstable disilane. It might also be mentioned that the fundamental absorption bands of disilane are accessible to the 10.6μ band of CO_2 but not the 9.6μ band which also was used in this experiment.[11] It is of interest to verify that when disilane is heated in the gas phase by the 10.6μ laser lines homogeneous chemical reactions can indeed occur.

Additional research by Bilenchi and coworkers[10] has shown that boron and phosphorus can be incorporated into amorphous silicon prepared by CO_2 laser-assisted decomposition of silane. In these reactions, diborane and phosphene were added into reactor vessels. These gases are not directly heated by the CO_2 absorption; however, they may be excited by transfer of energy through collision with excited silane molecules, or they may actually form complexes wth the excited silane species in the gas phase. Since no analysis of the gases was performed in these experiments, additional work must be performed to determine the reaction mechanisms for these more complicated systems. This result however does seem to indicate that the proposed topic of depositing binary systems by CO_2 laser-assisted CVD should be feasible even when one of the gas species can not be directly excited.

These additional results also indicate that additional analyses of the gas phase reactions are necessary to better understand the processes occurring in CVD reactions. It is for this reason that a quadruple mass spectrometer was introduced into our new system as well as additional optical ports for Raman analysis and fluorescence measurements. Also in cooperation with Dr. N. Peterson (Polytechnic Institute of N.Y.) we will be performing computer modelling of our gas phase reactions. The combination of the laser excitation, mass spectra and optical analysis, together with computer modelling, should allow us to determine substantial information about the reaction mechanisms and kinetics of the CVD processes we are exploring, specifically:

$$SiH_4 \rightarrow Si + 2H_2$$

$$3SiH_4 + 4NH_3 \rightarrow Si_3N_4 + 12H_2$$

$$SiH_4 + 2N_2O \rightarrow SiO_2 + 2N_2$$

It is probably the lack of detailed mechanistic data which is the major shortcoming of the CVD process.

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SECTION III

INFORMATION ELECTRONICS

SECTION III: INFORMATION ELECTRONICS

A. ADAPTIVE FILTERING AND SPECTRAL ESTIMATION

Professor A. Papoulis

Unit IE5-1

1. OBJECTIVE(S)

Our objective is the investigation of various theoretical and applied aspects of spectral estimation as outlined in the proposal. Presently, we concentrate on adaptive echo cancellation with emphasis on the elimination of long, acoustically generated, echos and on the suppression of instabilities. The underlying analysis is based on an extension of Floquet theory to discrete-time systems with random perturbations. Work continues also on spectral estimation from non-consecutive data and on the reconstruction of random signals in terms of past samples.

We are now starting a new and, we believe, promising area of investigation: the study of polyspectra. This topic has extensive applications in many fields including the phase problem in systems identification, the detection of nonlinearities in scismic signals and ocean waves, in blind deconvolution in equalizer design, in the detection of phase coupling among harmonic components, and in nonlinear estimation.

The concept of polyspectra has been under investigation for over two decades. However, it is only recently that it is being used extensively. In our investigation, we plan to develop the underlying theory and to apply the results to a variety of problems. Preliminary considerations suggest a long list of problems involving various extensions to polyspectra of well known results from ordinary spectral analysis.

2. SUMMARY OF RECENT PROGRESS

We have developed a new algorithm for the determination of the maximum entropy spectrum S(w) of a discrete-time process x[n] in terms of the values of its autocorrelation R[m] for m in an arbitrary set D of integers (IEEE Trans. on Info Theory). Known results are limited to consecutive data.

We reexamined various aspects of filtering and estimation and we determined the analytical properties of the general class of extrapolating spectra under consecutive correlation constraints. The results are based on the four-terminal properties of lattice filters (SIAM Review, September, 1985, pp. 405-441).

We showed that a bandlimited stochastic process can be recovered in terms of its past samples only provided that the sampling rate exceed but can be arbitrarily close to the Nyquist rate (IEEE Proc., August, 1985, pp. 1332-1333). The results are applied to discrete-time processes (IEEE Trans. on Acoustics, Speech, and Signal Processing, August, 1985, pp. 933-938). In this paper, we also reexamine Wold's decomposition in the context of innovations.

We are investigating various aspects of spectral estimation involving contraints in the form of outputs of linear functional. The underlying theory is based on the concept of entropy rate in the context of linear operators (Proceedings of the Third Workshop on Maximum Entropy and Bayesian Methods, July, 1985).

3. STATE OF THE ART AND PROGRESS DETAILS

Work outlined in the proposal is in various stages of completion. We comment below, briefly, on the problem of long echoes (references 12 to 18) and we conclude with an outline of our new area of concentration: the study of polyspectra and their applications (references 19 to 26).

Adaptive Echo Cancelling and Data Reduction

A signal $x[n]$ is transmitted from point A to point R. The return signal is a sum

$$y[n] = s[n] + \varepsilon[n]$$

where $s[n]$ is the useful signal and $\varepsilon[n]$ is the echo due to the incoming signal $x[n]$. The echo is electrically generated as in telephone transmission (Fig. 1a) or acoustical, due to the feedback from the loudspeaker emitting $x[n]$, to a microphone (Fig. 1b). Our objective is to reduce the echo, to eliminate instabilities, and to do so with the minimum of computational complexities.

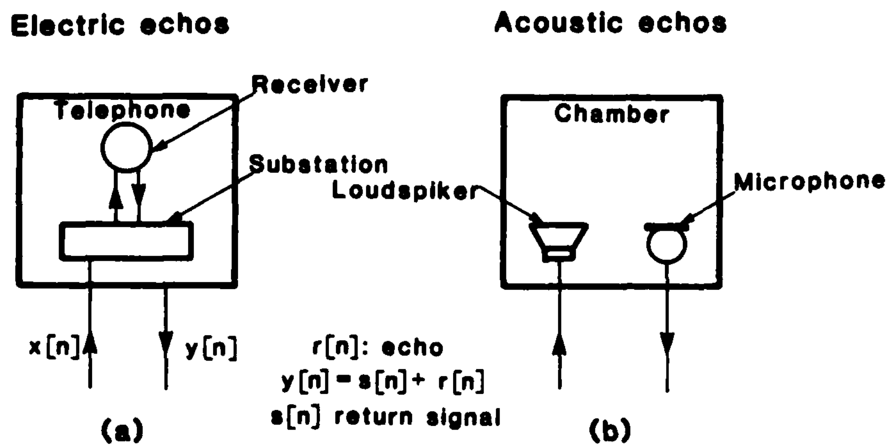

Fig. 1

The echo problem has been studied extensively, however, most papers deal with electrical echos. Acoustical echos present special problems because their duration is relatively long. If, therefore, we use an adaptive FIR filter to compensate for the echo (Fig. 2), the number N of weights required to simulate the impulse response of the electro-acoustical transducer is large. This leads to computational complexities and to low convergence rates and instabilities. We shall address these problems using as compensation a modified form of the adaptive filter of Fig. 2. The modification is based on the introduction of suitable data transformations reducing the number of adaptively controlled parameters to the number of degrees of freedom necessary to characterize approximately the electro-acoustical transducer of Fig. 1b.

We examine, in particular, a data transformation based on the concept of running FFT's. We outline below the Floquet theory approach to the resulting stability problem.

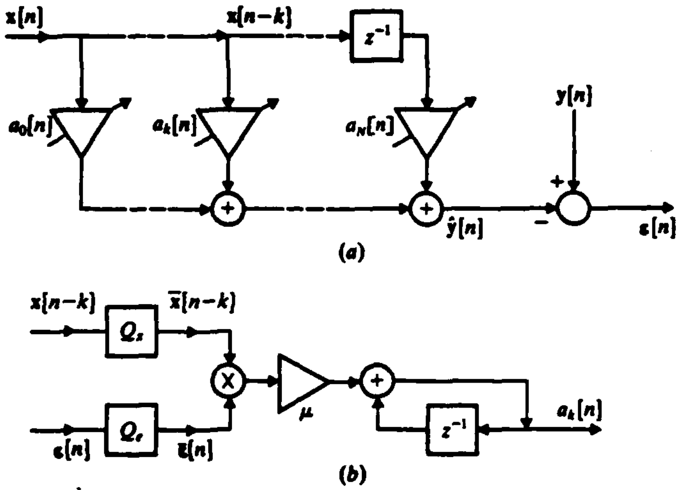

Fig. 2

The unknown stochastic process y[n] (Fig. 2) is estimated by the sum

$$\hat{y}[n] = \sum_{k=0}^{N-1} a_k[n]\ x[n-k] = X^T[n]\ A[n]$$

where X[n] is the incoming signal vector with components x[n-k] and A[n] is a vector with components $a_k[n]$. The adaptive algorithm is a first order recursion

$$A[n+1] = \Gamma\ \bar{e}[n]\ X[n]$$

where $\bar{e}[n]$ is a quantization of the error

$$e[n] = y[n] - \hat{y}[n]$$

To reduce the number of adaptively controlled parameters, we introduce the transformation matrix W, the modified data vector P[n] and the new weight vector B[n]

$$A[n] = W\ B[n] \qquad\qquad P[n] = W^T\ X[n]$$

This

$$\hat{y}[n] = P^T[n]\ B[n]$$

The selection of the matrix W is directed by the following considerations

1. The modified data covariance matrix

$$E\ \{P[n]\ \underline{P}^T[n]\}$$

must be nearly diagonal.

2. The resulting number of the adaptively controlled parameters must be small.

3. The spectral properties of the data must be utilized.

The resulting stability problem is stochastic and strongly nonlinear. However, as we show, a perturbation approach leads to a linear model with periodic coefficients.

Bispectra, Blind Deconvolution, and Phase Estimation

In the early stages of this investigation we shall apply the theory of bispectra to the phase problem in echo cancelling. We mention below, briefly, the underlying concepts. We wish to determine the system function

$$H(\omega) = |H(\omega)|\ e^{j\phi(\omega)} \tag{1}$$

of an unknown system. The input to the system is a stationary process v(t) and the output is the process x(t). We have no access to v(t). We know only that v(t) is white noise with power spectrum $S_{vv}(\omega) = N$. We observe x(t) and we measure its power spectrums $S(\omega)$. Since

$$S(\omega) = S_{vv}(\omega)\ |H(\omega)|^2$$

knowledge of $S(\omega)$ permits us, therefore, to determine the magnitude $|H(\omega)|$ of $H(\omega)$ but not its phase. If the system $H(\omega)$ is minimum-phase, then $\phi(\omega)$ can be computed from $|H(\omega)|$. Otherwise, $\phi(\omega)$ cannot be determined from $S(\omega)$. To find $\phi(\omega)$, we compute the bispectrum

$$F(u,v) = |F(u,v)|\ e^{j\psi(u,v)} \tag{2}$$

of x(t). This is the Fourier transform

$$F(u,v) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} R(\lambda,\mu)\ e^{-j(u\lambda+v\mu)}\ d\lambda d\mu$$

of the third order moment

$$R(\lambda,\mu) = E\ \{x(t+\lambda+\mu)\ x\ (t+\lambda)\ x(t)\}$$

of $x(t)$. The function $R(\lambda,\mu)$ can be expressed in terms of the given sample of $x(t)$ as an appropriate time-average (ergodicity). If $F_{vv}(u,v)$ is the bispectrum of the input $v(t)$ then the bispectrum $F(u,v)$ of the output $x(t)$ equals

$$F(u,v) = F_{vv}(u,v)\ H(u)\ H(v)\ H^*(u+v) \qquad (3)$$

This relationship can be used to determine the phase $\phi(\omega)$ of $H(\omega)$. Indeed,

$$F_{vv}(u,v) = B$$

because $v(t)$ is white noise. Hence

$$F(u,v) = B\ H(v)\ H(u)\ H^*(u+v) \qquad (4)$$

From (1), (2) and (4) it follows that

$$\phi(u) + \phi(v) - \phi(u+v) = \psi(u,v) \qquad (5)$$

This equation can be used to express recursively $\phi(\omega)$ in terms of the phase $\psi(u,v)$ of the bispectrum of $x(t)$. Integrating, we obtain

$$\phi(\omega) = \frac{1}{\omega}\ [2 \int_0^\omega \phi(y)\ dy - \int_0^\omega \psi(u,\ \omega-u)\ du] \qquad (6)$$

This integral equation can be solved recursively.

We start by investigating various numerical methods for maximum accuracy, utilizing the fact that (5) is overdetermined.

We continue with a systematic development of the general properties of bispectra and with an evaluation of the various estimation techniques. We cite below several illustrations of the topics under consideration:

Conditions for a function $F(u,v)$ to be a bispectrum.

Conditions for third order ergodicity.

Statistical properties of the time-average estimate of the third order moment $R(\lambda,\mu)$.

The truncation problem in the estimation of $F(u,v)$ from partially known $R(\lambda,\mu)$.

Properties of bandlimited bispectra.

Estimation of $B(u,v)$ based on autoregressive approximation of $x(t)$.

Can Levimon's algorithm be extended to bispectra?

Could the method of maximum entropy be applied?

Considerations for window selection.

Conditions for third order stationarity of line spectra.

Numerical methods for phase correlated lines.

Returning to the phase problem, we note that the redundancy in (4) can be used to reduce the two-dimensional spectrum $F(u,v)$ to a one-dimensional spectrum that, unlike $S(\omega)$, retains the phase information of $H(\omega)$. Indeed, from the inversion formula

$$R(\lambda,0) = \int_{-\infty}^{\infty} e^{i\lambda u} \int_{-\infty}^{\infty} F(u,v)\, dv\, du$$

it follows that the Fourier transform of the moment

$$R(\lambda,0) = E\,\{x^2\,(t+\lambda)\; x(t)\}$$

equals

$$\int_{-\infty}^{\infty} F(u,v)\, dv = B\, H(u) \int_{-\infty}^{\infty} H(v)\, H^*(u+v)\, dv$$

To determine the phase of $\phi(\omega)$ it suffices therefore, to estimate $R(\lambda,0)$. This simplifies the problem of estimation and it suggests that in various applications it might be sufficient to consider the transform

$$F(\omega) = \int_{-\infty}^{\infty} R(\lambda,0)\, e^{-j\lambda\omega}\, d\lambda$$

of the special third order moment $R(\lambda,0)$.

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B. ROBUST AND NONLINEAR FILTERING, DETECTION AND ESTIMATION IN TELECOMMUNICATIONS, RADAR AND SONAR PROBLEMS

Professor L. Kurz

Unit IE5-2

1. OBJECTIVE(S)

In recent years the general area of robust detection and estimation has received considerable attention. In tis context, "robustness" was meant to signify insensitivity to small deviations from the assumptions about the noise model. Frequently, a robust method was described as being a procedure with uniformly good behavior within a family of contaminated distributions.[1-9] However, the exact meaning of "uniformly good behavior" and "contaminated family," though defined in distinct mathematical terms for a given situation, becomes in effect ambiguous for the data processor to which the input is a stream of observables with unknown and/or slowly time-varying statistics.

To alleviate this vagueness, further research efforts were concentrated on the stability of various stochastic distances[10-15] to give these properties a qualitative as well as quantitative meaures. Nevertheless, the stability does not always imply good performance in terms of the expected value of a cost functional and, moreover, these stochastic distances are usually too abstract to be easily related to the system design.

To by-pass the problems associated with the differences generated between theoretical and practical conceptualizations of robustness, one of the major objectives of the present research effort is to introduce descriptors of robustness which lead naturally to the design of practical detectors and estimators.

It was recognized by Chadwick and Kurz[16] that in low signal-to-noise ratio (SNR) environments nonparametric detectors should operate in a sequential mode to insure an increase in the information rate while maintaining a constant error rate. Brownstein and Kurz[17] demonstrated that group rather than sample-by-sample updating of the data is necessary for efficient operation of detectors in a sequential mode. They have also demonstrated that stochastic approximation algorithms represent a useful tool for an efficient operation of adaptive detectors.[18,19-22] The natural objective of the ongoing research is to investigate the use of variable threshold sequential detectors as practical and efficient means of truncation of the decision process.

With the advent of satellite communications, the problem of data transmission through satellite channels become particularly important.[23-26] Some of the techniques used in robust detection lead naturally to procedures which suppress interference due to the nonlinear nature of satellite transpowders. In general, optimization and evaluation of various modulation schemes used in satellite data transmission are among the objectives of the present research effort. Various forms of nonlinear filtering and equalization are also investigated.

2. SUMMARY OF RECENT PROGRESS

In the last year, the research effort was concentrated on the study of sequential partition detectors. It was demonstrated that for all classes of partition detectors, the optimum scores are the same for fixed-sample and sequential operations. In the sequential mode of operation, the transmission rate is up to four times that of its fixed-sample size counterpart. The importance of truncated and variable threshold detectors was demonstrated. In addition, preliminary results were obtained for evaluation of performance of partition detectors in dependent noise. For satellite data transmission systems the advantages of nonlinear equalization were shown.

As part of the ongoing research effort, a new model for generating practical classes of robust estimators based on orthonormal polynomial approximation was introduced. The preliminary results for the new model are promising.

3. STATE OF THE ART AND PROGRESS DETAILS

(a) Sequential Partially Ordered Partition Detectors[27]

The problem of achieving efficient operation of sequential partition detectors in very small and large signal-to-noise ratio environments was approached using partially ordered detectors. The detectors were optimized using asymptotic measures of performance for small signal-to-noise ratios and then the approach was extended to the large signal-to-noise operation. The performance was compared to the exact and computer simulated results.

Some truncated and curved boundary decision rules in sequential operation were introduced. This leads naturally to an efficient operation of the detector even in extremely low signal-to-noise environments by eliminating the influence of occassionally unbounded sample sequences which are an integral part of sequential detectors operating in severe noise.

For severe noise environments variable boundary detectors are particularly useful. Two forms of variable boundaries were introduced for which the maximum sample size is guaranteed at the point the boundaries cross zero. How fast the terminating point is approached depends on certain preselected parameters which affect the derivative with respect to n in the neighborhood of zero. This approach yields parabolic and hyperbolic boundaries. For parabolic boundaries $\underline{a}$ and $\underline{b}$ are multiplied by $1/r^2N_T^2\ (n^2-2rN_Tn+r^2N_T^2)$, where $\underline{a}$ and $\underline{b}$ are the original thresholds, N_T is the final truncation point and the parameter r controls how fast N_T is reached as a function of the error rate. For hyperbolic boundaries the multiplier of the fixed bounaries is $(1-nr_1/N_T)/(1+nr_2/N_T)$, where the parameters r_1 and r_2 are positive numbers controlling the position of the asymptotes of the boundaries.

The maximum ASN is plotted in Figure 1 in terms of $\theta=\theta_c$ (critical value of the signal parameter) for the Lehmann alternative. In Figure 2 the error probabilities are plotted for $\theta_0=0$ and various values of θ_c for Lehmann and Gaussian alternatives. Figure 1 and 2 demonstrate that the ASN decreases significantly at the critical point $\theta=\theta_c$ while the

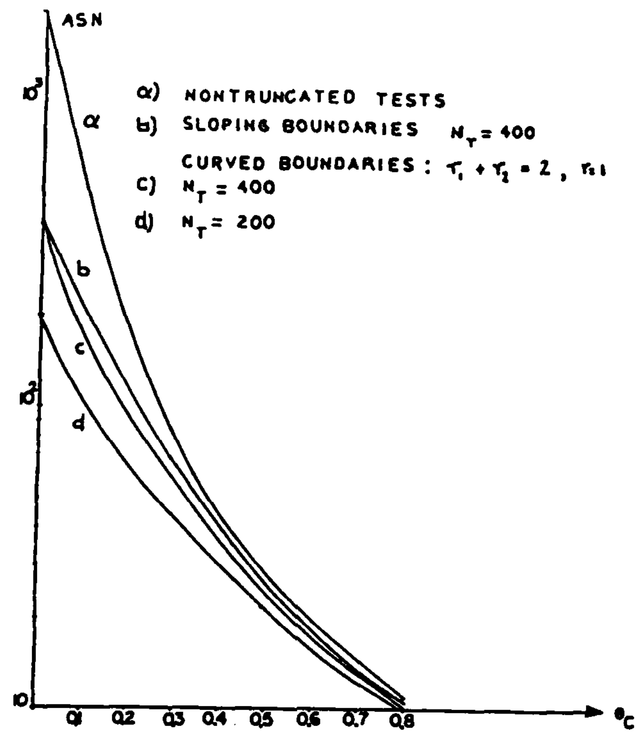

Fig. 1 ASN of Truncated ST_1D vs θ_C Lehamann Alternative, m = 3.

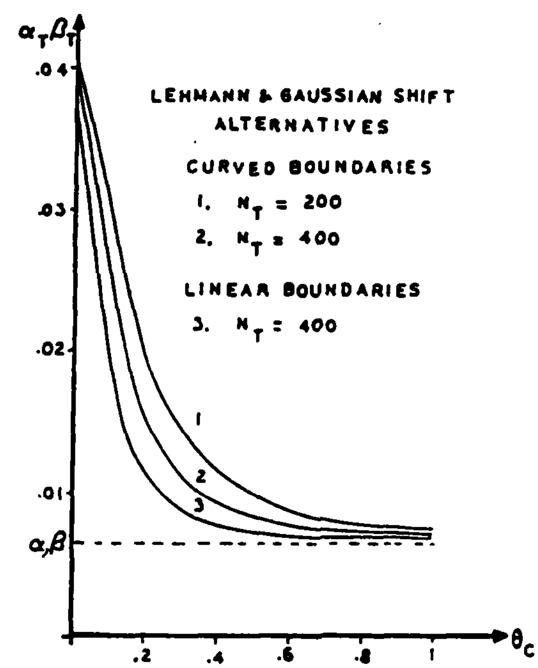

Fig. 2 Error Probabilities vs θ_C, $\theta = \theta_0$ and $\theta = \theta_1$

error rates increase only slightly. Though detectors with curved boundaries tend to have a slightly higher error rate for a fixed truncation point, they more than compensate for it by a reduced ASN.

(b) Robust Sequential m-Internal Polynomial Approximation (MIPA) Detectors with Dependent Sampling.[28]

The theory of sequential detectors based on MIPA principle was extended to include operation with dependent samples. Two forms of dependence were considered: bivariate and Markov. The detectors were designed to maintain near optimum performance for nominal noise envirnoments and robustness to changing noise conditions. Moreover, the efficiency of detection is improved, in some cases up to two times, if compared to sequential MIPA detectors with independent sampling at the expense of a slight increase in their structural complexity.

(c) Nonlinear Equalization in Satellite Data Transmissions Systems.[29,30]

The improvement of performance of a BPSK modulation procedure in satellite data transmission system by the use of linear recursive equalization was demonstrated by Elrefaie and Kurz in their conference paper.[23] Even further improvement of performance is possible if the linear equalizer is replaced by a nonlinear one which consists of a memoryless cubic nonlinearily followed by a linear filter. The reslts will appear in a forthcoming paper.[29]

Even further improvement in performance is possible if the nonlinear equalizer is replaced by a properly designed nonlinear Kalman filter.[30]

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