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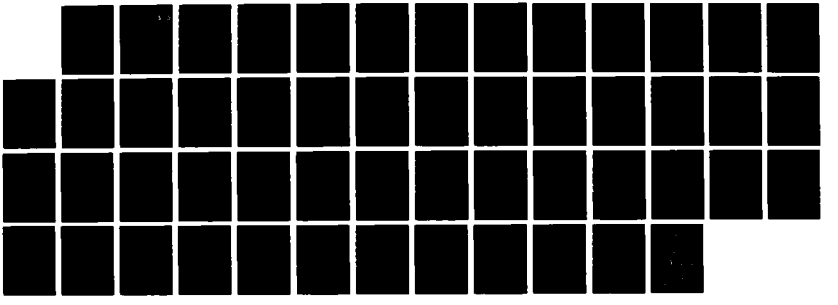

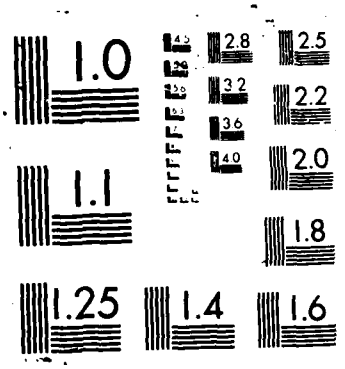
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19. ABSTRACT (Continue on reverse if necessary and identify by block number)

A summary of work undertaken under ONR Contract No. N00014-77-C-0397 is provided. The work covers the following subject areas;

(i) Electronic Structure of Superlattices; (ii) Electronic transport, magneto-transport, and magneto-optical properties of quasi two dimensionally (2D) confined single particle states and charge carriers; (iii) Collective properties of 2D electrons and holes; (iv) Point Defect Induced Deep levels in bulk compound semiconductors and superlattices; (v) The nature of Si/SiO_2 system and the role of interface disorder; (vi) Semiconductor/ Metal Systems, including the Si/Silicide interface; (vii) Spectroscopic Ellipsometry Studies; (viii) Nitridation Kinetics of SiO_2 on Si(100); (ix) Computer Simulations of molecular beam epitaxial growth of compound semiconductors and the atomistic nature of interfaces.

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18. (Cont'd) NITRIDATION OF SiO_2 ON Si(100), SPECTROSCOPIC ELLIPSOMETRY, MOLECULAR BEAM EPITAXIAL GROWTH OF III-V SEMICONDUCTORS, COMPUTER SIMULATIONS OF GROWTH MECHANISMS.

FINAL SCIENTIFIC REPORT

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"THEORETICAL STUDIES OF THE INTERFACE ELECTRONIC PROPERTIES OF TETRAHEDRALLY COORDINATED SEMICONDUCTORS"

SUBMITTED TO

THE OFFICE OF NAVAL RESEARCH

ELECTRONICS AND SOLID STATE SCIENCES

800 NORTH QUINCY STREET

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I. INTRODUCTION:

This "Final Scientific Report" on ONR Contract No. N00014-77-C-0397 summarizes the salient results, conclusions, inferences, etc. reached through a variety of theoretical investigations of the properties of III-V compound semiconductor interfaces and modulated structures such as heterojunctions, quantum wells and superlattices. Since these investigations were carried out over nearly 8 years, they cover a vast range of activities and manifest the evolving nature of not only the research conducted under this contract but also the field itself. To achieve therefore a sense of clarity, brevity and the inter-relationship of the evolution of issues addressed, in the following we have organized the report according to subject areas/issues investigated. These are,

1. **Electronic Structure of Superlattices**
2. **Electronic transport, magneto-transport, and magneto-optical properties of quasi two dimensionally (2D) confined single particle states and charge carriers**
3. **Collective properties of 2D electrons and holes**
4. **Point Defect Induced Deep levels in bulk compound semiconductors and superlattices**
5. **The nature of Si/SiO_2 system and the role of interface disorder**
6. **Semiconductor/Metal Systems, including the Si/Silicide interface**
7. **Spectroscopic Ellipsometry Studies**

8. **Nitridation Kinetics of SiO_2 on Si(100)**

9. **Computer Simulations of molecular beam epitaxial growth of compound semiconductors and the atomistic nature of interfaces.**

II. SUMMARY OF FINDINGS:

(II.1.) ELECTRONIC STRUCTURE OF SUPERLATTICES:

Much of the work relating to electronic states in superlattices was carried out during the period July 1977 through June 1981 and is summarized in an overview article written as part of an invited talk given at the AVS National Symposium held in Dec. 1981 at Anaheim, California (*publication No. 8 in the* attached "List of Publications". Hereafter all publication numbers quoted in this report shall correspond to this list). These investigations were some of the very first to address a variety of basic and important issues and took the approach of the EMPIRICAL TIGHT BINDING METHOD for calculating the nature of electronic energy levels, wave functions, etc. for heterojunctions and superlattices as a function of surface orientation, band edge discontinuity, the chemical nature of the constituent semiconducting materials, and the direct or indirect nature of the band gaps of the constituent materials. We briefly summarize here some of the more general findings. The details may be found in publications 1 through 7.

(II.1.1) THE TIGHT BINDING PARAMETERS:

The empirical tight binding (ETB) method relies upon determining the TB matrix elements through fitting to the energy-wave vector relationship (i.e. the band structure) as obtained for the individual bulk semiconductors from other methods, generally the empirical pseudopotential method. In 1977, the ETB method was just beginning to be exploited for superlattices but a major issue that was being overlooked by other researchers was the issue of reliability of the TB parameters obtained from (i) fitting only to the high symmetry eigenvalues of the bulk Brillouin zone (ii) ignoring reproducibility of effective masses, (iii) ignoring issues of self-consistent charge redistributions inevitably accompanying formation of interface chemical bonds, and (iv) the impact of even this short-ranged charge redistribution on the issue of what rule, if any, might one use as a guide for choosing the one basic parameter required to proceed on any calculation of the electronic structure of heterojunctions and superlattices - namely, the BAND EDGE DISCONTINUITY.

Given this state of affairs, the author's group was the first to impose severe constraints on the determination of ETB parameters by requiring that they reproduce not only high symmetry energies of the bulk Brillouin zone but also,

(i) reproduce all known bulk effective masses

(ii) each chemical element retain a single set of s and p state energies (i.e. the diagonal TB parameters), obtained in such a way that the same set would reproduce the band energies and effective masses of ALL bulk III-V semiconductors involving that element. For example, As diagonal energies are required to be the same in fitting to InAs, GaAs and AlAs.

(iii) The diagonal energies of both group III and V elements are further required to be such that they automatically reproduce the experimentally determined photothreshold of each III-V compound semiconductor.

The underlying physical motivation for imposing these severe constraints (not employed to this date in other TB calculations) was to (a) at least ensure that once a "rule", such as the photothrshold rule, was employed for choosing the band edge discontinuity, then no further arbitrariness was left in adjusting the parameters, and (b) account, at least in part, for the short ranged charge transfer effect at interface chemical bonds which would self-consistently change the diagonal TB parameters (i.e. the atomic energies) but which was not being taken into account by the usual method of fitting the TB parameters. Indeed, it is not clear that the general literature of such calculations of the time or even today has appreciated the significance of this very early attempt to partly account for many of the effects that several years later surfaced and led to a

second surge of calculations of the electronic structure of superlattices via such more powerful methods as the self-consistent pseudo-potential method.

(II.1.2) THE GaSb/InAs SYSTEM:

Although we calculated the electronic structure of GaAs/$Al_xGa_{1-x}As$(100) superlattices as our first attempt in summer 1977, we were more intrigued by the expected unusual band line-up of the GaSb/InAs(100) system and the experimental findings of Esaki and co-workers[1,2]. Consequently, we focussed on this conceptually and operationally more involved system and addressed the issue of *rectifying* versus *non-rectifying* junctions by performing two entirely different types of calculations;

A. TB calculation of GaSb/InAs(100) superlattices (SL) with varying individual layer thicknesses for different band edge discontinuities by direct diagonalisation of the SL Hamiltonian matrix. Such an approach is restricted to individual layer thicknesses of order 50 ML by the size of the matrix to be diagonalized. Through comparison of the calculated superlattice band gap variation with layer thickness (for different values of the band-edge discontinuity) with the optical absorption determined band gaps we not only confirmed the unusual nature of the band line up even for thin layers but also suggested the value to be near 0.06 eV

(rather than the 0.15 eV value suggested by the photothreshold rule and employed in the attempted fit[2] of a one dimensional Kronig-Penny approach taken by the experimenters themselves). We also predicted a semiconducting to semimetallic change in the nature of transport in the SL growth direction to occur at SL unit cell thickness near 120 A. To the best of our knowledge, this value is confirmed by the available experimental information. Later self-consistent pseudopotential calculations[3] of the SL band structure found the band edge discontinuity to be near 0.05 eV, remarkably close to the value suggested by our TB calculations. (*See publications* 1,2 and 4).

B. The empirical TB method was combined with the Green's function method to calculate the surface electronic structure of semi-infinite semiconductors. It was then combined with a generalization of the Koster-Slater method to calculate the electronic structure of the interface between semi-infinite GaSb and semi-infinite InAs. Through such calculations it was demonstrated that layer density of states (LDOS) in the band gap regions of the individual components becomes non-zero at and near the interfacial planes due to the unusual band edge discontinuity of the GaAs/InAs system. This also clarified the issue of rectifying versus non-

rectifying nature of such a heterojunction by explicitly bringing out the relationship between the depletion and accumulation regions in GaSb and InAs respectively and the thickness of the individual layers in a multilayered structure. For thicknesses larger than these intrinsic band bending regions the multilayered structure would behave as a semiconducting system in spite of a non-zero LDOS at and near the interface. (See publications 3 and 5).

(II.1.3) THE HOMOPOLAR-HETEROPOLAR COMBINATION:

Issues relating to the growth and expected electronic structure of homopolar-heteropolar combinations such as Si/GaP, Ge/GaAs and Si/GaAs were addressed early on. In particular, through elementary chemical considerations of bonding, valency saturation and charge transfer induced electrostatic fields we independently, though in parallel with Harrison et.al.[4], were amongst the first to advocate growth of such structures on surface orientations other than the polar (100) and (111) surfaces. In particular, orientations providing both cations and anions (i.e. group III and V respectively) in the same atomic plane and sufficient discrimination between sites for incorporation of these were argued to be suitable from the view point of growth kinetics in molecular beam epitaxial growth. The parallel experimental work[5] of Kroemer et.al. on the (110)

and (211) orientations was found to be consistent with these considerations.

The ETB method was employed to calculate the electronic structure of the lattice matched Si/GaP(110) system. It was concluded that the interfacial chemical bonds - Si-P and Si-Ga - were sufficiently distinct from the bulk Si-Si and Ga-P bonds that INTRINSIC interface states (i.e. interface states arising solely from chemical bonding effects in an otherwise atomically perfect interface) were most likely in homopolar-heteropolar systems. This finding was in contrast to the opposite conclusion reached through our work on heteropolar-heteropolar combination. (See publication 6).

(II.1.4) THE INDIRECT-INDIRECT GAP COMBINATION:

An intriguing issue is the possibility of realizing a direct gap superlattice through a combination of two indirect gap semiconductors. We investigated this issue via ETB calculations of the electronic structure of GaP/AlP(100) superlattices. It was shown that as a function of the individual layer thickness there is a regime in which direct band gap superlattices can be realized. To our knowledge this prediction has yet to be experimentally tested. (See Publication 7).

(II.2) THE 2D ELECTRON GAS---SINGLE PARTICLE PROPERTIES:

A wide variety of properties of the quasi 2-dimensionally confined carriers realized in Si/SiO_2 based metal-oxide-semiconductor (MOS) structures, and compound semiconductor based heterojunctions, quantum wells and superlattices were investigated during the course of this research contract. Perhaps the most outstanding feature of our work is the early recognition of the significance of electron-phonon (acoustic and optic) interaction in these systems. As early as 1977 (see publication 9) we had argued that a significant part of the cyclotron resonance data and Shubnikov-deHaas data on Si-MOSFET's must contain significant effect of electron-acoustic phonon interaction even though the thinking, explanations and theories of the time were being advanced solely in terms of the electron-electron and electron-impurity interactions[6]. We were motivated to consider the electron-phonon effects as likely to be important by the realization that the very low Fermi energies in these systems (of order a few to a few tens of meV) spanned the relevant range of acoustic and optical phonon energies. Consequently, given the similar time scale of electron and lattice motion (unlike normal 3D electron gases which have Fermi energies about two orders of magnitude higher than the phonon energies) significant influence on each other's properties is likely. In the following we summarize some of our significant findings for the behavior of the single particle properties. Most of the work described in this section was also supported by

a contract with the AFOSR.

(II.2.1) THE ELECTRON-PHONON VERTEX CORRECTION:

We showed that the leading order vertex correction for the electron-phonon interaction in a 2D e^- gas goes like,

$$\Gamma^{(1)} \propto \lambda \cdot (\Omega_o/E_F)^{1/2}$$

where λ is the dimensionless coupling strength, Ω_o the relevant characteristic phonon energy and E_F the Fermi energy. For d.c. transport Ω_o is $\Omega_{ac.}(2k_f)$, whereas for coupling with optical phonons it is the zone center optical phonon energy. We thus showed that since $(\Omega_o/E_F)^{1/2}$ is of order unity (unlike 3D systems for which $(\Omega_o/E_F) \sim 10^{-3}$), the vertex corrections in the quasi 2D systems can be assumed to be small (as was common practice at the time) only if it could be demonstrated that itself was much smaller than unity. Indeed, all mobility data on Si MOSFET's in 1977 indicated that this may not be the case, thus pointing to strong electron-phonon effects. (See publication 9).

(II.2.2) CYCLOTRON RESONANCE BEHAVIOR:

The data on cyclotron resonance measurements on Si MOS structures in 1977 was being interpreted in terms of the e-e and e-impurity scattering mechanisms. The observed position of the resonance line (ω_{CR}) was identified with,

$$\omega_{CR} = eB/m^*c$$

from which an effective mass (m^*) was deduced for different electron densities knowing the magnetic field B. The difference

of the m^* so deduced from the bulk mass was attributed to the e-e interaction. The cyclotron resonance line width (Γ_{CR}) was experimentally found to go like,

$$\Gamma_{CR} \propto B^{1/2}$$

and a theory[7] based upon short ranged e-impurity interaction which gave the same dependence was hailed as correctly explaining the observation. However, another experimental observation that

$$\Gamma_{CR} \propto T$$

(where T is the temperature) up to $T \sim 25^{\circ}K$ was ignored, even though it could not be explained by the e-impurity interaction alone contained in the above noted theory.

We undertook development of a theory of cyclotron resonance which accounted for both e-impurity and e-phonon (acoustic) interactions. The two most salient features of our theory are,

(i) $\Gamma_{CR} \propto T$ and $\Gamma_{CR} \propto B^{1/2}$

(ii)
$$\left(\frac{m^*_{cr}}{m^*_b}\right) = \left\{1 + \lambda\left[1 - (2\nu+1)\,\frac{f(\nu)[1-f(\nu)]}{\nu + f(\nu)} + \frac{2T}{\omega_c} \times \left(1 - \tfrac{1}{2}\,\frac{f(0)}{\nu + f(\nu)}\right)\right]\right\}$$

The former explained both, the temperature and magnetic field dependence. The observed $B^{1/2}$ field dependence was shown to arise from a cancellation of a factor of B in the numerator arising from the electron-phonon interaction and a factor of $B^{1/2}$

in the denominator arising from the electron-impurity interaction. The proportionality of Γ_{CR} to $B^{1/2}$ in the earlier theory[7] was thus shown to be a fortuitous consequence of Γ_{CR} being proportional to impurity induced broadening only in this earlier theory.

A major significance of result (ii) above which appears to have largely gone unheeded in subsequent work is that, to the best of our knowledge, it was the first piece of work to demonstrate that the behavior of the 2D electron gas in the presence of a magnetic field depends on the Landau level FILLING FACTOR, ν , rather than individually on either the electron density (n_s) or the magnetic field (B). It was customary at the time to plot data as a function of n_s or B not recognizing that ν is the fundamental quantity.

The oscillatory nature of the m^* (extracted from $\omega_{CR} = eB/m^*c$) as a function of ν found in our result (ii) above has largely gone unchecked, although some recent measurements tend to suggest such a behavior. (See publication 10 and 13).

(II.2.3) THE ELECTRON-PHONON COUPLING IN CONFINED SYSTEMS:

A comprehensive investigation of the coupling between quasi 2D confined electrons/holes and phonons (acoustic and optical) revealed an enhancement (over the bulk coupling strengths) arising from such effects as loss of certain momentum selection rules in finite structures (quantum wells) made of ultra thin layers, or zone folding effects in superlattices

(particularly for acoustic phonons). This may provide part of the explanation for the enhanced electron-phonon effects inferred from such measurements as the temperature dependent mobility[6].

(II.2.4) RESONANT COUPLING BETWEEN CONFINED e^-/h AND OPTICAL PHONONS:

To gain information on the nature and strength of the coupling between charge carriers and optical phonons (bulk-like, confined, interface), we proposed the idea of tailoring the confined e^-/h energy levels in quantum well structures in such a way as to achieve RESONANCE CONDITION between separation of two electronic levels (say E_1 and E_2) and an optical phonon frequency (say $\hbar\Omega_o$). In such a situation we showed through development of a theory, that a sharp resonant splitting of the degenerate $(E_1 + \hbar\Omega_o)$ and E_2 levels results, the magnitude of the splitting being proportional to the electron-phonon coupling strength. While the phenomenon occurs even in the absence of a magnetic field, appropriate usage of such a field can enhance the oscillator strengths by further reducing the two dimensional freedom and creating sharp peaks in the density of states. The predicted effect, though shown to be best realized in undoped quantum well, has been observed in its dc counterpart experiments on the GaAs/$Al_xGa_{1-x}As$ heterostructures as the magneto-phonon effect[8] and indications have been found in cyclotron resonance measurements in InAs/GaSb and GaAs/$Al_xGa_{1-x}As$ heterojunctions[9,10]. Such measurements have, however, suffered from

ambiguities arising from the free carriers present and the attendant issues relating to screening and effective mass renormalization. Recently, we ourselves have grown appropriate $GaAs/Al_xGa_{1-x}As$ (100) single quantum well structures and shown for the first time the existence of the resonant mixing phenomena through photoluminescence excitation spectra studies[11]. (See publications 14, 15 and 16).

(II.2.5) MAGNETO-TRANSPORT:

Much of the activity and excitement regarding quasi 2D electron systems in the Physics community began in the early 1970's with the report of observation of the electron effective mass enhancement as a function of the electron density, extracted from Shubnikov-deHaas (SdH) oscillations observed in the Si-inversion layer[12]. Much controversy followed in the experimental literature itself but it did not deter development of a wide variety of theories explaining the mass enhancement in terms of the e^--e^- interaction effects alone[6]. The simple SdH oscillation expression employed in the analysis of the data however was one provided by Titieca in 1932 and refined by Peierls, but limited to an electron gas with only e^--impurity interaction. We consequently undertook development of an appropriate theory which accounted for all three types of interaction effects which may be expected to play important role in such systems, namely,

(i) e^--impurity

(ii) electron-phonon, and

(iii) e^--e^- interaction.

Through a combination of the Memory function and diagrammatic techniques and relying upon the applicability of the Fermi-liquid theory, we provided a complete expression for the trans magneto-conductivity, σ_{xx}. This expression for the first time showed the presence of two different effective masses and scattering times with varying degree of contributions from the above noted interactions. It thus demonstrated that the effective mass appearing in the amplitude of the SdH oscillations has contributions from both e-phonon and e^--e^- interactions. Consequently, the mass enhancement extracted from measurements cannot be identified solely with the e^--e^- interaction as has been the case in the literature. (See publications 17 and 18).

(II.2.6) MOBILITY IN SINGLE QUANTUM WELL STRUCTURES OF COMPOUND SEMICONDUCTORS;

Theoretical investigations of the contribution of

(i) remote ion scattering,

(ii) interface roughness scattering, and

(iii) alloy disorder scattering

to the electron mobility in single quantum structures were undertaken. The low temperature mobility (where phonons are not the dominant scattering mechanism) was calculated employing the Memory function approach to compare with the behavior found for the usually studied single heterojunction (such as the high electron mobility transistor). Results were obtained for both,

uniformly doped and modulation doped structures as a function of (a) well width, (b) carrier density, (c) spacer layer thickness, and (d) barrier height. The alloy disorder scattering, arising from the penetration of the confined electron wave function into the alloy barriers in systems such as GaAs/$Al_xGa_{1-x}As$(100), or the alloy nature of the well material itself in systems such as $In_{0.53}Ga_{0.47}As$/InP(100), was investigated for the first time in these studies. Screening in the electron gas was accounted for through an improved dielectric function which took account of the thickness of the well.

The notion of "interface roughness" was carefully examined for the first time. We showed that depending upon the lateral length scale of fluctuations in the alloy composition, at least two physically distinct consequences vis a vis fluctuations in the interfacial potential are experienced by the electrons. These are (a) fluctuations in the width of the well, and (b) fluctuations in the barrier height (i.e. the depth of the well). The latter is a consequence of fluctuations in the local band edge discontinuity attendant to fluctuations in the local alloy composition on the length scale of the size of the scattering particle. It was argued that for most of the growth conditions commonly employed the nature of the quantum well potential is likely to be dominated by the band edge discontinuity fluctuations. (See publications 19 and 20).

(II.3) COLLECTIVE PROPERTIES OF THE 2D e^-/h GAS:

(II.3.1.) THE ANOMALOUS ACOUSTIC PLASMON:

Investigations of the nature of collective (plasmon) modes of a two-component, two-dimensional plasma, such as may be created in double quantum well structures of GaAs/$Al_xGa_{1-x}As$ or even a single heterojunction of InAs/GaSb involving spatially separated electron and hole gases, were carried out for the first time. We showed that in such systems there exists a critical spatial separation (given other characteristics, such as charge density) beyond which the in-phase oscillations of the two components acquires frequencies which lie out of the range of single particle excitation spectrum. Consequently, this mode of oscillation, called the acoustic plasmon since its energy is proportional to the wave vector for small wave vectors, becomes observable due to lack of Landau damping. (See publications 21 and 22).

This predicted anomalous acoustic plasmon was subsequently observed in light scattering experiments conducted by Olego et.al.[13] Our initial work has led to many subsequent theoretical and experimental investigations[6] of the collective mode properties of multiple quantum wells and superlattices, including the behavior of magneto-plasmon modes in spatially separated plasmas.

(II.3.2) QUANTUM WIGNER CRYSTAL:

The freezing of an electron gas into a solid at low densities and ultra low temperatures was predicted by Wigner in 1932. In a two dimensional electron (or hole) gas with an appropriately applied magnetic field the spatial motion of the particles is completely quantised and the possibility of realizing the quantum Wigner solid is greatly enhanced at sufficiently low densities, high magnetic field, and ultra low temperatures. Considerable theoretical work has been done on investigating this liquid-solid transition. We, however, addressed a different and pragmatic issue: what is the signature of the occurrence of the quantum Wigner solid in a particular non-destructive experiment which is also feasible given the particular configuration of the sample? We chose magneto-absorption as one possible experiment and performed calculations of this property as a function of (i) electron density, (ii) magnetic field, and (iii) temperature, assuming that the solid exists. The existence of the Wigner solid entered the calculations through a lattice expansion of the density-density correlation function in terms of the normal modes. These modes are the magneto-plasmon and acoustic phonon modes of the Wigner solid. Coupling of the acoustic phonon modes of the substrate material (i.e. the material containing the electron gas) which acts as the heat bath was included, thus allowing for the influence of the bath temperature on the

"softening" of the Wigner lattice.

We calculated the Wigner lattice absorption characteristics for single phonon absorption as well as multiphonon processes. The predicted temperature dependence for both these processes was found to be $\exp(-T/T_o)$ where T_o is a characteristic temperature through different for the two processes. This temperature dependence is distinctly different from the linear dependence of the free electron gas. Similarly, the electron density and magnetic field dependencies, though somewhat complicated, are distinctly different from those of the free electron gas. (See publication 23).

(II.4) THE Si/SiO_2 SYSTEM:

(II.4.1) ATOMISTIC NATURE OF THE INTERFACE:

Our theoretical studies of the properties of the electron gas in Si/SiO_2 inversion layers, as well as the general body of experimental literature, led us to the early recognition that reliable physical models could be developed only if a deeper understanding of the true atomistic and chemical nature of the Si/SiO_2 interface were available. Fortunately, our interests coincided well with the efforts underway at the Jet Propulsion Laboratory of Caltech under the direction of Dr. F. J. Grunthaner and Dr. J. Maserjian. We thus joined forces with this group and started participating in the high resolution X-ray photoemission

(XPS) studies of the Si/SiO_2 system. In particular, we carried out calculations of the band structure of α-Quartz and, through introduced structural changes in the SiO_2 unit cell, calculated the dependence of the Si to Oxygen charge transfer and redistribution as a function of the Si-O-Si bridging bond angle. Through the introduction of this **structure-induced-change-transfer (SICT) model**, we estimated the degree of chemical shift in the Si 2p core level as a function of the bridging bond angle over a range expected to occur at and near the Si/SiO_2 interface. These calculations were then used in conjunction with the XPS data to identify the presence of various size rings in the amorphous SiO_2 and their shift towards smaller ring sizes as one approaches the interface - a consequence of the lattice and structural mismatch induced strain. The presence of sub-oxide states involving Si^{+1}, Si^{+2}, and Si^{+3} states was also identified within an essentially one monolayer transition region from Si to SiO_2 through this SiO_x layer. This was the first time that an atomistic picture of the true nature of the Si/SiO_2 interface was provided. The basic picture has held pretty well under the extensive work and scrutiny that followed[14]. (See publications 24-27).

(II.4.2) THE U-SHAPED BAND GAP DENSITY OF STATES:

It has been known for some time that in systems such as Si/SiO_2, InP/SiO_2, etc., the band gap region of the

semiconductor exhibits a U-shaped background density of states with additional structure riding on top which is specific to the material combination involved. A variety of propositions have been advanced in the literature to explain this U-shaped background but none of them are consistent with all the known facts. We proposed that this background has a universal origin in the presence of disorder in the semiconductor within a couple of atomic layers at the interface. The disorder/strain arises from the non-lattice matched nature of these systems. To demonstrate the consequence of our proposition we calculated the energy dependence of disorder induced band tail states and showed, for the first time, that it varies nearly exponentially with energy as one moves away from the valence and conduction band edges. Not only was this calculation, based upon extending Lifshitz's consideration[15] of an alloy, the first to successfully calculate the band tail states over the whole range of band gap energies in a disordered semiconductor, but also explained the U-shaped background density of states in interfacial systems. Spectroscopic ellipsometry studies[16] of the Si/SiO_2 system provided experimental evidence for our proposed presence of disorder in the Si over two atomic layers near the interface. (See publications 28-31).

(II.5) DEEP LEVEL DEFECTS IN BULK III-V SEMICONDUCTORS AND SUPERLATTICES:

We began some studies of the deep levels induced by ideal point defects, such as vacancy and antisite defects, in 1979. The subject was just beginning at the time with particular emphasis on the usage of the empirical tight binding approach. Given our experience with this method in the context of the electronic band structure of bulk semiconductors as well as superlattices (see sec. II.1), we were also quite familiar with the limitations and pitfalls of this approach. Consequently, we undertook investigations of the deep levels in a systematic approach comprised of,

(i) Testing the sensitivity of the ideal point defect induced deep levels in bulk semiconductors to the choice of the ETB parameters.

(ii) Calculation of surface point defect levels.

(iii) Calculations of point defect levels in superlattices as a function of superlattice unit cell thickness and spatial location of the defect.

(iv) Development of a technique for calculating neutral deep levels associated with NON-IDEAL point defects, but of short range such as in point defect complexes, the situation encountered in real systems.

The reliability and meaningfulness of the ETB method was examined through study of the ideal vacancy induced deep levels in bulk III-V compounds using the Koster-Slater Green function

method. Results were obtained using fitted ETB parameters obtained by other groups as well as our own. While each of these sets of parameters give equally good fit to the bulk band energies, they were nevertheless shown to give significantly varying deep level energies. We identified this problem as arising from the sensitivity of the deep levels to the bulk wave functions (i.e. charge distribution) as well, a feature most uncertain in ETB approaches. The study nevertheless showed that the vacancy levels scale with the ionicity of the semiconductor contained in the choice of the ETB parameters. Consequently, the established correlation between the ionicity and the photothreshold of the III-V semiconductors was exploited in our studies and imposed as a condition which ensured that our ETB parameters produce the correct trend in bulk ionicity and consequently the vacancy induced levels.

Next we investigated the ideal vacancy and antisite induced deep levels at (110) surfaces and in (110) as well as (100) superlattices. Results were obtained for the GaAs/AlAs(100) InAs/GaSb(100) and, as a model system, the InAs/GaSb(110) system. The deep levels were shown to be sensitive to (a) the location of the defect with respect to the interface (b) the band edge discontinuity, and (c) the presence of alloy disorder inherent at the interfaces of superlattices. While these studies of deep levels in superlattices remained the only studies until a few years ago, our basic conclusion as to the range of uncertainty in calculated values being too large to be of value for interpreting

experiments (when these themselves become sufficiently unambiguous and reliable) we believe holds even at present. (See publications 32 and 33).

Realistic point defects in fact have a finite size arising from such things as relaxation of atoms in the neighborhood and/or presence of two or more point defects within proximity of their range of associated potentials. To tackle such problems within the standard Slater-Koster type of approach quickly leads to dealing with enormously large matrices requiring unreasonably long computational time. We consequently undertook development of a new method of dealing with this realistic class of problems and one which can be used with any underlying choice of description of the ideal crystal band structure such as tight binding, or pseudopotential method, or any other. The new method exploits the transfer-matrix technique to provide a new way of solving the Dyson equation, requiring as input only a few Green's functions of the perfect crystal. These Green's functions are matrices whose size is determined by the number of localized orbitals per atom in the chosen representation for the bulk band structure calculation. The method enables determination of the deep level energies without directly seeking zeros of the commonly employed determinantal condition. We applied this method to the calculation of the deep levels associated with oxygen substitutional impurity in the alloy $GaAs_xP_{1-x}$ and for the As antisite defect in GaAs, employing the commonly used sp^3 basis set. Breathing mode lattice distortions around the oxygen atom

were examined. The results were found to be in good agreement with the experimental findings of the time.
(See publications 34 and 35).

(II.6) METAL-SEMICONDUCTOR INTERFACES:

We investigated a model semiconductor-metal system to examine some basic aspects of interfacial bonding, presence of true intrinsic interface states, and the self-consistent adjustment of the Fermi energy in the semiconductor band gap. The calculations were based on a tight binding model of a semiconductor and a metal, combined with the Green function method and solution of the appropriate Dyson's equation for the coupled system. Results were obtained for (i) dispersion curves of the truly localized states in the semiconductor band gap, (ii) the density of states of the interface states, (iii) the charge on the metal and semiconductor atoms at the interface, (iv) the charge in the chemical bond between the metal and semiconductor atoms, and (v) the dependence of the density of interface states on the strength of the metal-semiconductor bond. We also introduced, for the first time, a self-consistency in the charge distribution (and thus associated interfacial dipole) through usage of the Friedel sum rule for phase shifts, thus ensuring overall charge neutrality. Many of these same results have been rederived in recent times in an attempt to provide explanations for the Schottky barrier problem. (See publication 36).

We also participated in some experimental studies of the

formation of Ni, Pd and Pt silicides on Si undertaken by Dr. Paula Grunthaner of Jet Propulsion Laboratory (Caltech) during 1979-81. The studies were carried out via vacuum deposition of thin metal films ($\backsim$100 A) and subsequent thermal treatment to form various silicide (mono, di, etc.) phases. The Si/Silicide interfaces were examined via high resolution XPS. Two significant findings of this work are (a) the Si/silicide barrier height was shown to be linearly correlated to the chemical shift of the interfacial Si 2p core level, and (b) the barrier height is predominantly controlled by the intrinsic chemical bonding effects at the interface. (See publications 37-40).

(II.7) <u>SPECTROSCOPIC ELLIPSOMETRY STUDIES</u>:

Starting in 1980, with the help of some supplementary funds, efforts were begun to establish an experimental facility for variable wave length (spectroscopic) ellipsometry measurements on quantum well samples. During 1981-82 we thus set-up such a facility covering the energy range 1.6 eV to 5.7 eV. The ellipsometer is a fully automated system run by a LSI 11/23 computer. A brief description of the instrument is provided in sec. III.

As a way of testing and calibrating our instrument we began ellipsometric studies with the Si/SiO_2 system --- a system well studied by Aspenes and co-workers who were also the first to design and use this type of ellipsometry system. A variety of systematic studies and the corrective actions suggested by them

were carried out over a period of a year, including development of sophisticated computer programs for analysis and display of the data. Programs were written for the different levels of models and resulting theories for the behavior of inhomogenous and/or multilayered systems. These included the standard ideal multi-layer model which describes the dielectric function of a lyered composite structure in terms of the bulk dielectric functions of the individual layers and disregards any changes arising from the interfacial chemical bondings, confinement of electronic states, etc., as well as the effective medium models and theories for such inhomogenous systems as alloys. Programs for modelling within the Bruggeman effective medium approach for multicomponent systems were generated and tested.

Spectroscopic ellipsometry studies were begun with a study of some GaAs/$In_xGa_{1-x}As$(100) multiple quantum well (MQW) structures and single layer alloy films grown via molecular beam epitaxy (MBE) at the Jet Propulsion Laboratory under a separate joint ONR contract. These MQW structures, however, did not turn out to contain well defined layered structure (as revealed in parallel electron microscopy studies) and thus tended to give spectra similar to alloys. The difficulties were traced to control and calibration of the group III (i.e. Ga and In) fluxes and associated transients in the MBE machine, as well as the growth conditions employed. While awaiting availability of higher quality GaAs/$In_xGa_{1-x}As$ MQW structures, we decided to undertake a study of Si implanted with Si samples.

(II.7.1) IMPLANTED Si:

The motivation for examining this system arose from the rather intriguing possibility suggested in the infra-red reflectivity measurements for these samples by our colleagues, W.G. Spitzer and Co-workers, that upon annealing of the as-implanted disordered (or amorphous) Si, it first undergoes change to a NEW, but STILL AMORPHOUS, METASTABLE STATE, before transforming into the crystalline phase via epitaxial regrowth[17]. If correct, this would have been a remarkable observation with implications for a wide variety of materials as well as the existing understanding of the formation of amorphous phase and its subsequent transformation. Attempts to examine the suggestion of Spitzer et.al. by Donovan et.al.[18] via calorimetric measurements gave no positive results, indicating that the free energy differences between the two amorphous states may be below the detection limits of these calorimetric measurements. We consequently undertook to examine this issue via spectroscopic ellipsometry which is capable of providing information on such physical aspects as changes in densification (i.e. void fraction in the film). We particularly felt that such physical information, if complimented with chemical information such as may be extracted from high resolution X-ray photoemission studies of the core and valence levels, should be able to shed light on whether the new state found in the IR reflectivity

measurements is a truly new state involving changes in bond polarisability arising from chemical effects, or whether it may be only a manifestation of physical effects.

Our spectroscopic ellipsometry studies, combined with XPS studies led us to conclude that the changes observed in the visible to ultra-violet (UV) dielectric functions of the as-implanted and anneal-stabilized a-Si states could be accounted only partially due to differences in density, recrystallization during preparation of the anneal-stabilized state, or differences in the surface conditions of the samples. Thus, intrinsic changes in the bond polarisability are indicated by the ellipsometric measurements and are confirmed by the valence charge redistribution indicated by the XPS measurements.
(See publication 41).

(II.7.2) $GaAs/Al_xGa_{1-x}As$ QUANTUM WELL SYSTEM:

Towards the end of this research contract we acquired access to our own molecular beam epitaxy machine and grew some $GaAs/Al_xGa_{1-x}As$ (100) quantum well structures as well as alloy layers. We thus examined the behavior of the dielectric function ($\epsilon(\omega)$) of three single quantum well structures, all grown under identical, reflection-high-energy-electron-diffraction (RHEED) determined growth conditions with only the GaAs well width varying. The three samples had well widths 14.1 A (5 ML), 28.3 A (10 ML) and

59.4 A (21 ML) and the $Al_xGa_{1-x}As$ alloy composition of 0.31 $\pm$ 0.01% Al. The measured $\epsilon(\omega)$ of all three samples was found to be distinct from that calculated from the classic multilayer model noted in the preceding, thus indicating the presence of electronic confinement effects AT ENERGIES AWAY FROM THE ZONE CENTER. The L-point transitions, E_1 and $(E_1 + \Delta_1)$, were observed to be shifted to higher energies with *decreasing well thickness, indicating presence of* confinement effects at the L-point of GaAs. A systematic analysis of the data via fairly sophisticated deconvolution procedures allowed determination of the shifts in the critical point energies with an accuracy of $\pm$ 7 meV. *Modelling of these shifts on the basis of a simple square* well model of the L-point band-offsets and appropriate effective masses was found to give results consistent with the observations. (See publication 42).

(II.8) NITRIDATION KINETICS OF Si/SiO_2:

During the course of our investigations of the structural and chemical nature of the Si/SiO_2 interface (see sec. II.4) we were confronted with various issues relating to the nature and mechanism of the Si thermal oxidation process itself and the consistency of our findings with what was known on this issue at the time. As noted in sec. (II.4), a major finding in our work was the identifiation of the role of built in strain on the chemical nature of the interface via the introduction of the

structure-induced-charge-transfer (SICT) model. Thus starting around 1983 and early 1984 when some initial experimental results on the thermal nitridation of this SiO_2 films in NH_3 began to appear, one of the observations was that the nitrogen distribution initially peaks at the Si/SiO_xN_y interface but then moves 20-25 A away from the interface with increasing nitridation time. It thus occured to us that the strain present in the starting Si/SiO_2 system and its subsequent modification by the nitridation process must itself influence the kinetics of the nitridation process. Given the significant experience we had already developed in computer modelling of interfacial kinetic processes and their consequences for the resulting films in molecular beam expitaxial growth (see sec. II.9), we felt ideally positioned to examine the nitridation behavior. Thus began a systematic study of this problem primarily under separate sponsorship, but also benefitting from the ONR research contract under discussion here.

We carried out computer modelling of the kinetic processes involved in nitridation and revealed a mechanism in which diffusing species, initially consisting primarily of nitrogen, react with the Si substrate followed by formation of the oxygen-rich oxynitride due to reaction of the diffusing oxygen liberated by the slower nitridation of the SiO_2. The key physical effect, essential for obtaining agreement with the experimental findings (via XPS), we showed was the presence of the interfacial strain which reverses its sign in going from SiO_2

to Si, and its influence on the nitridation and oxidation kinetics.

In an attempt to check the chemical behavior against electrical properties we uncovered a direct correlation between the nitridation condition dependent nitrogen distribution and the magnitude of the flat band voltage shift in the Si/SiO_xN_y structures. We explained this correlation by proposing that a strain-dependent kinetics of defect formation near the interface operates in parallel with the strain-dependent nitridation kinetics itself, these defects being responsible for the change in the flat band voltage. A variety of predictions of our model and the computer modelling for such things as the temperature and time dependence of nitridation were subsequently investigated experimentally and were found to be correct. To the best of our knowledge, these ideas and modelling results remain the only systematic and consistent explanation of the behavior of the Si/SiO_xN_y system to date. (See publications 43-47).

(II.9) COMPUTER SIMULATIONS OF MBE GROWTH:

A major change in thrust of the research undertaken under the present contract began in 1981 with considerations of the atomistic nature of far-from-equilibrium vapour phase growth, such as is the case with molecular beam epitaxial (MBE) growth of III-V compound semiconductors, and its relationship to the resulting structural and chemical nature of the interfaces in heterojunctions and quantum wells. During 1981 and 1982 we

outlined a conceptual model of the MBE growth process, deriving heavily from the few experimental studies relating to surface kinetic processes in MBE of GaAs and from general literature on surface kinetic process. Thus the meaning and relevance of often used concepts such as sticking coefficient, surface diffusion, evaporation, etc. was examined, emphasising the role of surface molecular reactions in crystal growth. With these ideas and concepts in place in a starting model for the MBE growth process, we undertook computer simulations employing the Monte-Carlo method to represent probabilistic events according to assigned rates for individual kinetic processes. These early attempts were necessarily limited in their scope as well as the methodology of simulation. Nevertheless, they set the zeroth order framework from which more realistic and sophisticated simulation could be evolved. A summary overview of these early attempts is provided in publications (49) and (51).

Starting in 1983, with the arrival of a dedicated VAX 11/750 computer system acquired under a separate ONR contract, we began efforts at more realistic simulations. These efforts culminated with the proposition of the **Configuration-Dependent-Reactive-Incorporation (CDRI) model** of the MBE growth process reported at the 2nd International MBE Conference (San Francisco) in August 1984 (publication 52). As summarized in publications (52) and (54), the role of the As_4 dissociative reaction kinetics in competition with the Ga surface migration kinetics for a given Ga arrival rate (and hence for the usual MBE growth rate) was

shown to be at the heart of the atomistic nature of MBE growth and the resulting dynamics of the surface morphology (i.e. step density and terrace width distributions). In particular, two limiting regimes of the CDRI growth process were identified and systematically examined - (i) **Reaction Limited Incorporation** (RLI) regime, and (ii) **Configuration Limited Reactive Incorporation** (CLRI) regime. The former was shown to occur at low group V pressures and the latter at high group V pressures. In either case, damped oscillatory behavior of the time dependent growth rate was shown to occur due to the Ga configuration dependent arsenic incorporation kinetics. The growth mechanism under the usual GaAs MBE conditions was however shown not to be the conventional nucleation and growth mechanism as had always been assumed and asserted. Unfortunately, such unexamined assertions continue to be made even today.

A most significant finding of these simulations, and one of considerable pragmatic value as well, was the explanation of the **origin of the damped oscillatory behavior** of reflection-high-energy-electron-diffraction **(RHEED) intensity** during MBE growth. This phenomenon[19,20] was brought to the forefront in late 1982 and early 1983, about the same time as our independent computer simulations were providing the dynamics of the growth front morphology. Unfortunately, the very first of the experimental papers to discuss RHEED intensity oscillations erroneously identified[20] its origin to oscillations in the crystal growth rate that accompany the nucleation and growth

mechanism. Our work identified the RHEED intensity oscillations as arising from the time dependent change in the surface step density and terrace width distribution, explicitly demonstrating the presence of these RHEED oscillations even under growth conditions for which no oscillations in the crystal growth rate occur. (See publications 52 and 54).

We also examined the influence of the MBE growth parameters, such as the group V pressure and substrate temperature at a given growth rate, on the behavior of the time dependent surface morphology and the associated behavior of the RHEED intensity dynamics. A specific behavior of the RHEED specular beam intensity dynamics was predicted in which the existence of an optimum group V pressure was demonstrated. This prediction was confirmed in the experimental studies of GaAs RHEED intensity dynamics carried out in our own laboratory (under separate sponsorship) as well as at other laboratories[21]. (See publication 53).

The Monte-Carlo computer simulations of MBE growth have since continued in our group and have made significant contributions to a better understanding of the formation of $GaAs/Al_xGa_{1-x}As(100)$ interfaces. Within the past few years several groups around the World have initiated computer simulations of MBE growth and it appears that the subject is beginning to evolve into a major area of research.

III. SPECTROSCOPIC ELLIPSOMETER LABORATORY FACILITY:

The spectroscopic ellipsometer facility comprises a laboratory containing an optical table, the ellipsometer optics and electronics, an array-processor based computer for real time on-line data analysis, reduction and interpretation, several terminals with associated high resolution monitors for data entry, experimental control and theoretical modeling studies, and a sample preparation area. The ellipsometer has been designed initially with several goals in mind, following the pioneering and detailed investigations of Aspnes: broad wavelength region of data collection capability, high speed data collection and essentially real time data reduction and analysis, and associated interactive theoretical modeling and fitting. To this end, the initial design parameters for the ellipsometric system have included: a wavelength range of 8000 to 2000 A (1.6 eV to 6.2 eV) divided into 1500 steps of 4 A each, automatic integration of ellipsometric amplitude and phase measurement cycles for improved signal to noise ratio, real time Fast Fourier Transforms of the measured ac signal for rapid data accumulation and manipulation, and optimized overall accuracy in measurement of the dielectric function to 1 part in 10^3 with a relative precision of 1 part in 10^5.

The optical design is best described with reference to Fig. 1. A xenon arc lamp (150 W with F/1 UV grade collimating optics) acts as the light source, and is incident on the mounted sample at an incidence angle of 70^o after passage through appropriate

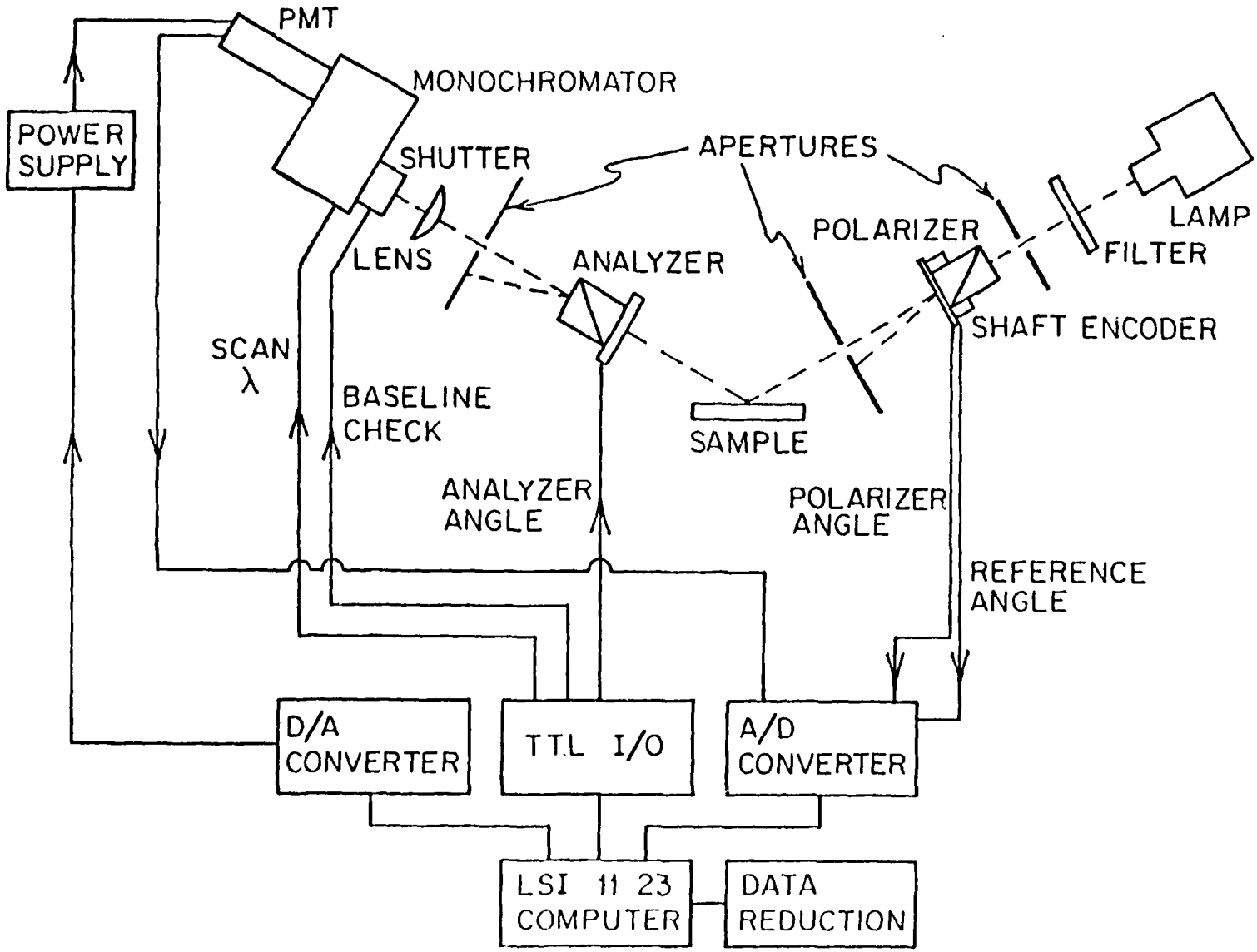

Fig. 1 Schematic diagram of USC computer-controlled spectroscopic ellipsometry facility.

filters (to eliminate unwanted infrared irradiation on the polarizer and sample) and a synchronously rotating Rochon prism polarizer. An aperture is employed to separate the ordinary ray from the unwanted extraordinary ray. The reflected beam is passed through a programmable angle Rochon prism analyzer, and is subsequently focused onto the entrance slit of a double pass monochromator with holographically ruled gratings. The signal beam emergent from the monochromator is detected with a high quantum efficiency photomultiplier, the output of which is current-to-voltage converted, digitized, and entered in the computer. The PMT power supply has provision for digital input so that the gain can be controlled to keep the PMT in its most linear regime regardless of the wavelength variation in light intensity from the source and variations in sample reflectance/absorbance. The rotating polarizer is optically shaft encoded to allow digitization of its rotation angle (in 256 increments) and consequent absolute phasing. A programmable shutter has been incorporated to provide automatic baseline compensation (dark current normalization) at each wavelength step, if desired. The sample is mounted on a flexible six degree of freedom sample holder that allows high orientational precision in alignment of the optical train.

Control of the apparatus, data collection, data reduction and error analysis, and theoretical modeling are implemented by means of an LSI 11/23 mainframe with associated array processor, disk drive, input/output terminals, high resolution

plotter/monitor, and a line printer/point plotter. The array processor allows a 256 point discrete Fourier transform to be performed in 50 msec., following data collection and signal averaging each wavelength.

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IV. PERSONNEL:

During the course of this research contract, several graduate students and post-doctoral visitors participated in the work. The following provides a list of those who had long association with the research.

(IV.A) GRADUATE STUDENTS:

1.	RICHARD P. VASQUEZ	(Ph.D. 1986)
2.	JOO-YOUNG KIM	(Ph.D. 1986)
3.	JOSE DELGADO	(M.S. 1980)

(IV.B) POST-DOCTORAL ASSOCIATES:

1.	ROGER NUCHO	(1977-78)
2.	B.HOROWITZ	(1978-79)
3.	N.V. DANDEKAR	(1978-79)
4.	S. DAS SARMA	(1979-80)
5.	M. GRABOWSKI	(1980-81)
6.	J. SINGH	(1980-83)
7.	S.V. GHAISAS	(1983-84)

IV. LIST OF PUBLICATIONS (SUPPORTED FULLY OR PARTIALLY BY THIS RESEARCH CONTRACT)

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