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REAL TIME SELF-DIRECTED MBE FLUX CONTROL
INCORPORATING IN SITU ELLIPSOMETRY: PHASE I

DR. DAVID PALAITH
MR. JEFFREY J HEYOB

TECHNOLOGY ASSESSMENT AND TRANSFER, INC.
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NOVEMBER 1992

FINAL REPORT FOR 05/27/92-11/27/92

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This report is releasable to the National Technical Information Service (NTIS). At NITS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

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EXECUTIVE SUMMARY

The overall objective of this program was to achieve real-time control of thin film properties during deposition by the molecular beam epitaxy (MBE) method. An integrated sensor-control scheme involving three major elements devised. These three functions included: 1) control over the stability of the MBE machine beam fluxes and substrate temperature (Beta Control), 2) control over the alloy composition and thickness of the film being deposited (Alpha Control) and, 3) control over the deposition boundaries such as temperature and flux limits (Qualitative Process Automation, QPA). The major function of the Beta Control Loop is to stabilize the molecular beam fluxes, especially during transients induced by effusion cell shutter openings and closings.

Considerable progress was made during this Phase I effort in the development of a software module that virtually eliminates these beam flux irregularities. The next step is to develop a means of anticipating (feedforward) these flux transients under all growth conditions so that the Beta Control Loop becomes autonomous, directed only by the film growth recipe. Similarly, considerable progress was made in incorporating ellipsometric control over the properties of the growing film. An ellipsometer is an optical instrument that is used to determine the composition and thickness of the growing film in real-time. The ellipsometric characteristics of low temperature GaAs and InGaAs were assessed during in situ growth. It was shown that film thickness, crystal quality, and substrate temperature could be determined with considerable sensitivity in real-time. It remains to use this type of information to close the Alpha Control Loop so that film development follows the instructions of the film recipe. Closure of both loops and their coordinated functioning will be major thrusts of a Phase II effort. In addition, a supra-supervisor will be developed (QPA) that tracks all the functions of the MBE system. It will have the responsibility for maintaining these growth conditions within bounds, at all times, by determining the most effective action when these bounds are exceeded.

During this Phase I effort, practical film recipes were acquired from Sandia National Laboratory and from the Electronics Laboratory at WP. Furthermore, both have indicated a keen interest in adopting the control technology for their device development efforts. Their participation in Phase II will expedite rapid refinement and transition of this technology.

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1.0   PROGRAM OVERVIEW

> The objective of this program was to achieve real-time control of thin film properties during deposition by the molecular beam epitaxy (MBE) method. Satisfying this objective required development of techniques that would permit rapid and accurate control of the beam fluxes of the chemical constituents of the growing film. This objective of precise flux control was to be achieved by: 1) using self-directed temperature and shutter control, and 2) employing ellipsometry for direct monitoring and feedback over alloy composition and film thickness.

The final completion of this program will facilitate the rapid development of new devices and enhance the yield for a broad spectrum of DoD and commercial electronic and electrooptic applications. In addition, the control methods developed will be directly applicable to other thin film deposition techniques such as MOCVD.

1.1   Potential DoD Applications

Many of the performance driven demands of future Air Force weapon systems are dependent on the availability of advanced solid state devices and components fabricated from new semiconducting materials and processes.

- active electronically-scanned arrays (AESA), like those being developed for the Air Force's Smart Skins program, which rely on wafer-scale integrated T/R modules consisting of an amplifier, attenuator and a phase shifter capable of shifting phase in less than 50 nanoseconds;

- radars capable of operating above 10^{12} Hz;

- opto-electronics modules for ultra-high-speed fiber optic communications and photo-detectors for high-speed thermal imaging in the F-16's low altitude navigation and targeting infrared for night (LANTIRN) system;

- millimeter-wave monolithic integrated circuits (MIMIC), currently an integral part of the planned upgrade to the AN/ALQ-136 jammer for the AH-1 Cobra and AH-64 Apache (the Longbow radar/missile system) attack helicopters, and to the AN/ALQ-165 airborne self-protection jammer (ASPJ).

1.2   Potential Commercial Applications

The impact of this process control technology on the commercial sector will be significant.

- The proposed control technology offers design engineers and fabricators the prospect of significant reductions in the design-to-fabrication cycle time. The impact of this reduction on U.S. technology competitiveness could be substantial. Currently, new device fabrication proceeds on the basis of experience gained during previous manufacturing trials. Once a usable process recipe is discovered, the protocols are fixed and, often, a furnace, zone refiner or MBE machine becomes dedicated to single device production. Understandably, there is considerable reluctance to alter the protocol or to use the dedicated facility for alternative device development. As a result, long lead times between the conceptualization, fabrication and marketing stages is common.

- Current GaAs devices are fabricated from single crystal GaAs produced from the melt. Devices are fabricated by cutting wafers from the boule then compositional films of AlGaAs (or other dopants) are grown/masked/etched/metallized/ and wire bonded depending on the particular device. But the wafers are so brittle that both device engineers and packagers find fabrication difficult. Rejection rates high and so, therefore, are costs. If GaAs could be reliably grown with repeatable properties on a more durable substrate, production rates would be increased and costs reduced.

- The next major breakthrough in computer technology probably will come from wide spread use of Multi-Chip Modules (MCM) on Wafer Scale Integration (WSI). The result will be the Cube Computer. In working toward this goal, two problems face developers today: 1) designing inter-connects in three dimensions; 2) thermal management, i.e. heat removal from the interior of very high density electronic packages. It is this latter problem that the proposed MBE process control system might address. One heat removal solution is forced fluid cooling between the wafers. The super computer company Cray is attempting this approach by applying its inter-board cooling system to these small modules. That is not an attractive approach if the Cube Computer ever is to reach a wide consumer base.

An alternative solution is to fabricate the individual wafers from diamond. The advantage is that diamond is simultaneously an excellent dielectric and possesses the highest thermal conductivity of any known material – including all metals. The problem is that individual dies must be thermally bonded to the diamond and that requires considerable polishing of the diamond surface – a process that is costly and time consuming. Due to these difficulties, GaAs dies are not even being considered for this application. If GaAs were deposited directly onto the diamond masks could be used to replicate such advantages of the dies concept as inter-die isolation and the ability to incorporate large numbers of functions on a single wafer. The

proposed process control system would be critical in exploring this approach and, therefore, in advancing Cube Computer technology.

1.3 MBE Process Control Requirements

For both DoD and commercial applications, the basic device materials are the group (III-V) semiconductors, especially those based on aluminum-gallium-arsenide (AlGaAs) and indium-gallium-arsenide (InGaAs) using gallium-arsenide (GaAs) and indium-phosphide (InP) substrates, respectively. Although molecular beam epitaxy (MBE) is well-established as the preferable method for producing these solid state devices, the relatively low production yield that results from sensitivity to deposition parameters has kept costs high, and reproducibility and productivity low. In fact, process automation and control has been identified as one of the major challenges to MBE materials processing, and remains the major obstacle to low-cost commercialization.

The major challenge to realizing repeatable processing with high wafer throughput is the achievement of effective control over the MBE deposition process. Specifically, the characterization and control of molecular beam flux is essential for the control of alloy composition and film thickness -- the two film characteristics sufficient for prediction of the materials properties.

Beam flux control begins with careful characterization of effusion (Knudsen) cell performance to form the basis for a tight control loop that stabilizes machine performance. When complimented by real-time feedback from ellipsometric film properties' sensors, reliable materials processing by the MBE technique will become a reality. With such control achieved, the processing advantages will be substantial. They will include:

- improved device performance through tight control of deposition parameters and concomitantly close tolerances in materials properties;

- increased production throughput because:

  1) wafers will contain fewer processing defects,

  2) when fatal defects do occur, it will be possible to abort the deposition before additional manufacturing resources are expended;

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- real-time process control system that will serve as a valuable development tool for engineering new semiconducting materials, and minimizing product development cycles and research expenditures.

SUMMARY

The most important MBE process parameter, the one that determines film thickness and alloy composition is beam flux. Of all the methods currently applicable to molecular beam flux control in MBE systems, the two most promising and most fully developed techniques for real time monolayer process control are:
- self-directed control with feedforward temperature and shutter position compensation:
- ellipsometry.

These comprise two of the three components of a fully automated MBE thin film deposition system. Specifically, they are:

- Self-directed Flux Control implemented through the Beta Control Loop and consisting of real-time feedforward temperature compensation and shutter control system;

- Materials Properties Control implemented through the Alpha Control Loop and consisting of real-time ellipsometric sensing of the growing film.

The third component is post-deposition evaluation and database acquisition implemented through the *Ex Situ* Loop.

1.4   Summary Of Phase I Achievements

During this Phase I effort, major advances were made in achieving full MBE process control. These are discussed in detail beginning in Section 3. The most significant are summarized below:

- A means for selecting the optimum process conditions for the proportional/integral/derivative (PID) controllers was developed, and appropriate control modules were installed on the two MBE machines in the Air Force Materials Laboratory.

- Bench testing of a potential Process Discovery Autotuner was successfully completed ahead of schedule. These positive results on a software module, required to automate the PID optimization process, virtually ensure successful Phase II implementation.

- A Shutter Opening Transient Compensator was tested as a concept design version. Bench testing resulted in a preliminary compensation function, thereby demonstrating the viability of this approach to MBE control.

- An ellipsometer was installed on the Vacuum Generators MBE and *in situ* measurements were made on growing Low Temperature-GaAs and InGaAs including a demonstration of potential film thickness control.

- Modular design of the overall MBE control system was completed.

- Potential customers for MBE process control were identified. A national laboratory expressed a strong interest in the technology being developed at WLML, and is prepared not only to fabricate a major semiconducting device from wafers grown with WLML's MBE deposition technology, but to adopt that technology for its own film development programs.

2.0 TECHNICAL BACKGROUND

Control of the MBE deposition process will be achieved by integrating the operation of three separate control loops: 1) an inner process control loop, the Beta Loop, which stabilizes beam equivalent pressure (BEP); 2) a materials sensor feedback loop, the Alpha Loop, which is used to modify thickness and alloy composition in real time; and 3) a product processes control loop, the *Ex Situ* Loop, which controls the product quality through post-deposition measurements. These loops are identified in Figure 1.

The Beta Loop, also called the "Process Control Loop" or the "Inner Loop", is designed specifically to stabilize the beam equivalent pressure (BEP). Since the BEP and the beam flux are proportional to one another, this loop also controls the flux. However, the beam flux cannot be directly monitored during film growth because the substrate must intercept the molecular beam. The substrate manipulator must therefore be removed so that measurements can be made to correlate the BEP and cell temperature. Thus, the Beta Control Loop directly stabilizes cell temperature which indirectly stabilizes the beam flux..

The Alpha Loop, also called the "Self-directed Control Loop" or the "Outer Loop", is designed specifically to stabilize and control the properties of the material being deposited. This is accomplished by varying the deposition parameters in real-time during growth using an ellipsometer as the sensor. The ellipsometer measures changes in the polarization of monochromatic light reflected from the surface of the growing material. Since these changes depend upon both the thickness and composition of the film, these measurements can be used to modify the growth conditions.

The *Ex Situ* Loop, also called the "Product Control Loop", is used to evaluate the post-growth product and compare it with the process recipe. Unlike the Beta and Alpha Loops, which operate in real-time, the *Ex Situ* Loop uses post growth measurements to adjust the recipe for subsequent growths. It does not control the deposition process in real time. As such, this loop need not be an integral part of the MBE machine; measurements can be performed using any available ellipsometer.
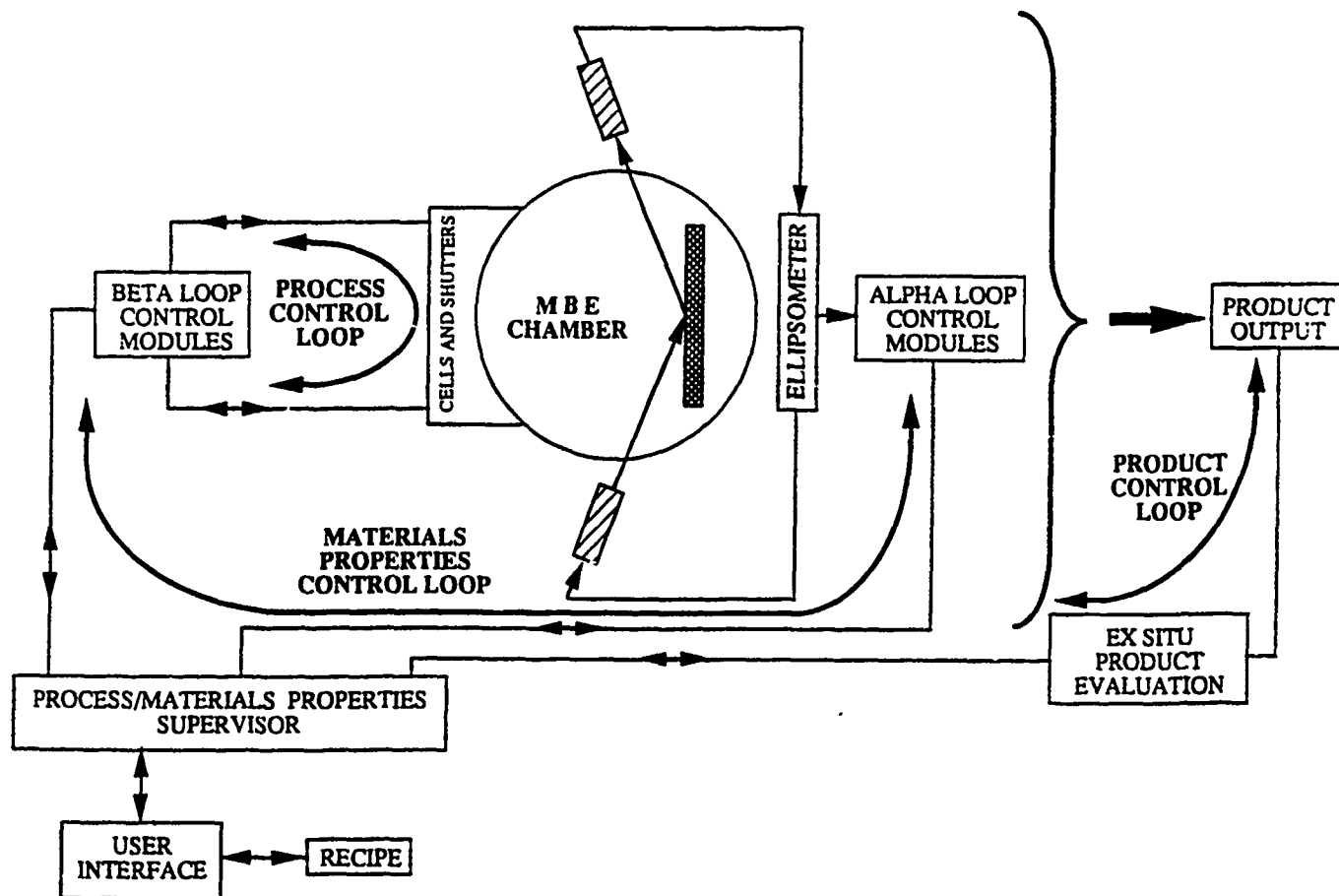
FIGURE 1   THE MBE CONTROL LOOPS

2.1   Beta Control Loop

Essential elements of the Beta Control Loop are shown in Figure 2. This loop is designed to produce time dependent beam fluxes as directed by the film growth recipe. These fluxes are not directly measurable, but they are proportional to the corresponding beam equivalent pressures (BEP). During film growth, however, even a BEP is not directly measurable. BEP is determined by the surface temperature of the material in the corresponding Knudsen cell. All Beta Control Loop functions are designed, therefore, to control effusion cell temperatures. The relationship between cell temperature and BEP is established by a calibration procedure; and the relationship between BEP and beam flux is confirmed by real-time film growth measurements. Both relationships are used by the Beta Control Loop to control effusion cell temperature. Subsequent closure of the Alpha Control Loop will, in part, mitigate the need for developing this relationship since the Alpha Control Loop will establish real-time control over the materials properties – particularly over film thickness and composition.

The User Interface and Supervisor/Sequencer of the Beta Control Loop are represented in Figure 2. The partly hashed lines show that these modules may incorporate additional control sensors such as a RHEED or laser fluorescence spectrometry. The Supervisor and Sequencer are first treated as separate modules to aid in isolating their individual roles. In the final implementation of the Beta Control Loop, these functions will be merged and replaced by a single Supervisor. This section describes current thinking on process parameters controlled solely in the Beta Control Loop.

The thermocouple that monitors the effusion cell temperature is located near the bottom of the cell. Thus, it is related to the surface temperature by the thermal conductivity of the material; the distance between the thermocouple and the surface; and the thermal properties of the cell itself. In addition, when a PID effusion cell controller supplies power to a cell, the temperature and the time response at any location within the cell depends on the heat capacity and mass of material. The relationships between power supplied to a cell, the material surface temperature, and its time rate of change are not straightforward.

The Process Discovery Autotuner-Controller (PDA-Controller) is designed to measure the parameters needed to establish a relationship between the power delivered to a cell and the temperature of the thermocouple. Two sets of data are required to accomplish this. First, a relationship between the static power input to a cell's heater and the temperature recorded by the thermocouple must be established. Second, the response time of the cell temperature to step

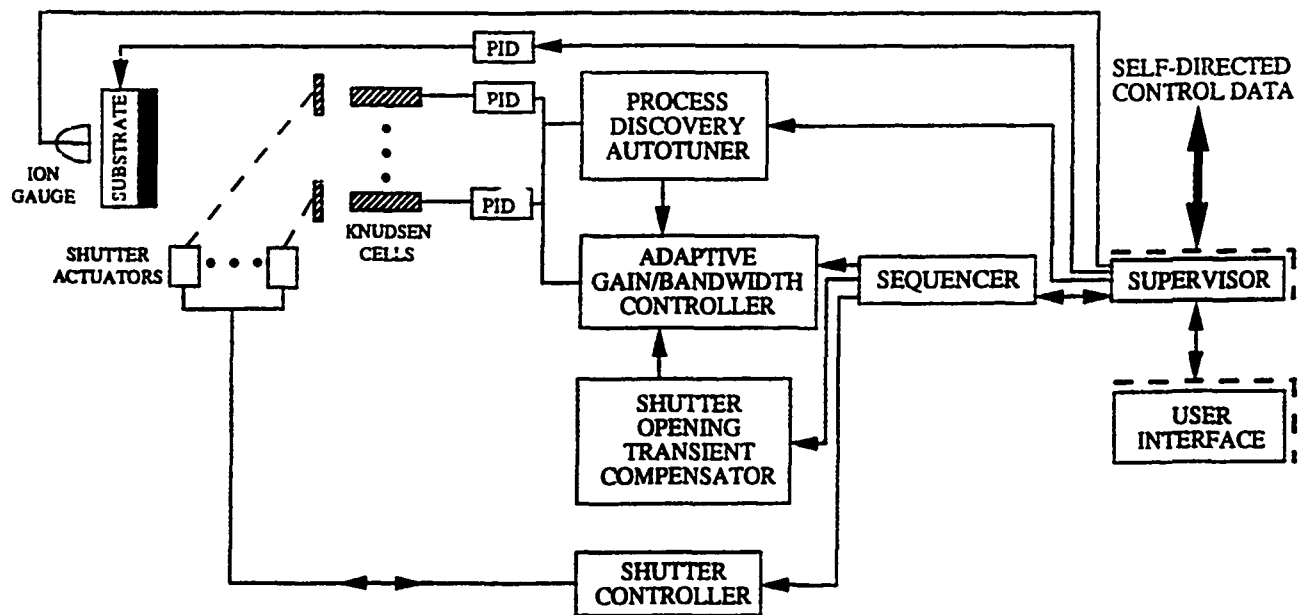changes in the power input must be recorded. In both cases, temperature changes are initiated by changing the

FIGURE 2.   THE BETA (PROCESS CONTROL) LOOP

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PID temperature set point rather than by changing the heater power directly. A typical PID response to a set point step change is shown in Figure 3.
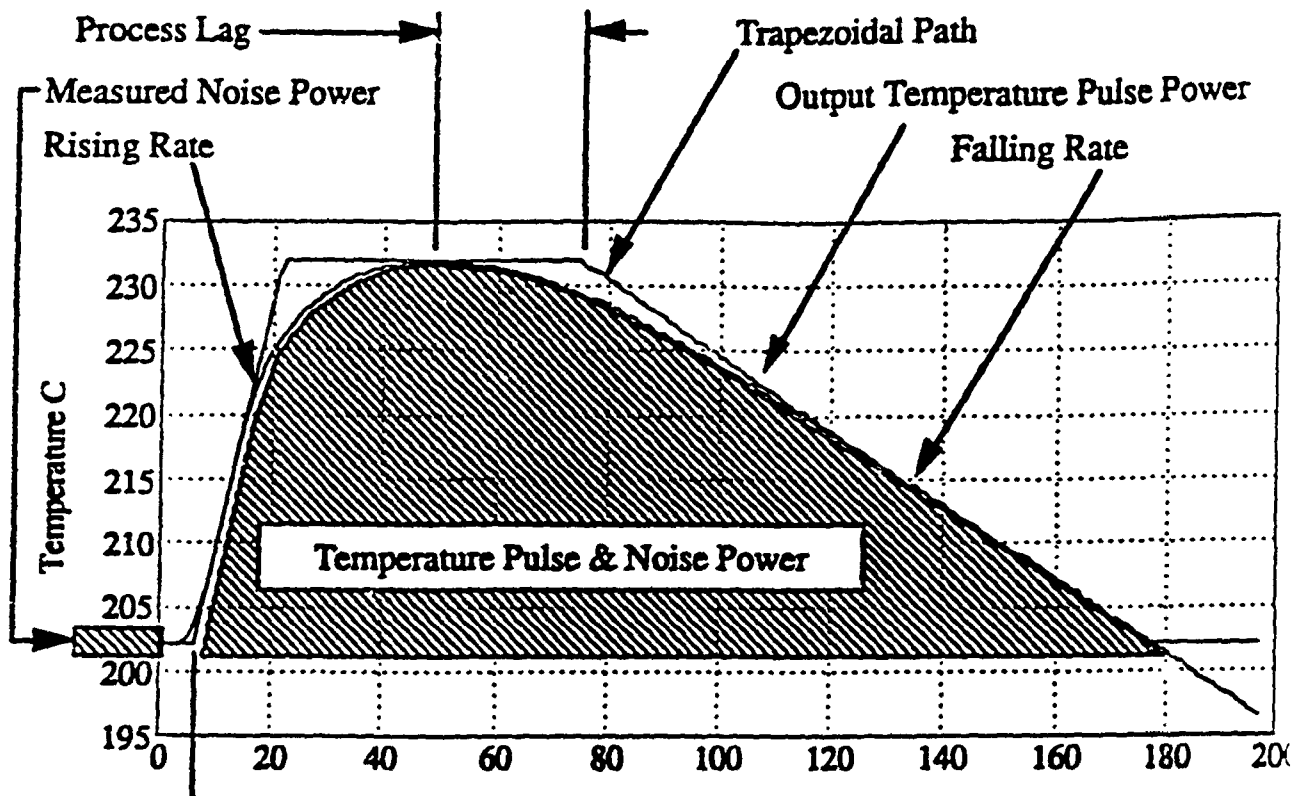

FIGURE 3   PID RESPONSE TO STEP SET POINT CHANGE

In the current implementation of the Beta Control Loop, these types of data are used during a calibration procedure to construct a look-up table that can be used by the PID-controller. During calibration, the Supervisor module opens the shutters and directs the Process Discovery Autotuner to build this table through a series of controlled set point step changes and temperature response measurements. The table consists of the slope and intercept of the three line segments simulating the response function as shown in the figure.

These lookup tables then will be used by the PDA-Controller. A demand for a static cell temperature will be communicated to the appropriate PID through the PDA-Controller. Those P, I and D parameters that optimize temperature stability will be extracted from the Process Discovery Autotuner lookup table and used to set the PID controller. For example, without proportionality and/or integration, (a Type-0 servo), a zero temperature offset error can be achieved only with infinite loop gain. But then, unity loop gain is assured of occurring at some frequency within the controller bandwidth at which point the loop will become unstable. Only for a Type-1 servo system, a servo system with at least one integrator, can oscillations be avoided while simultaneously achieving zero offset error. The objective of the PDA-Controller can now be restated as **"maximizing the gain-bandwidth product while maintaining stability."** Step changes, or other time-dependent variations, in the set point also will be implemented by using the lookup table to determine what P, I and D settings will affect this change as rapidly as possible. Accordingly, the bandwidth must be increased in proportion to the size of the step. Thus, the integration time constant must be increased, lowering the frequency of this effective low pass filter, to avoid oscillations. All of these adjustments will be performed automatically, in real-time, by the PDA-Controller in response to a temperature demand from the Supervisor/Sequencer.

The remaining data required to close the Beta Control Loop is the steady-state temperature-to-BEP transfer function, and the shutter opening-induced beam pressure transient. Both can be obtained from a single series of measurements on each cell. Both types of data require that the substrate manipulator be removed and replaced by an ion gauge. The transient response of a cell temperature and of the BEP/flux to shutter opening will be recorded. The long-term steady state temperature and beam pressure will also be tabulated.

With a constant power input to a cell, the surface temperature of the material will be higher with the shutter closed than with it open. This radiative loss from the surface of the reactant material, which lowers its temperature, cannot occur when the shutter is closed. The saturation vapor density in the space between the reactant material surface and the inside surface of the shutter will also be higher than it would be for the same PID power input to the cell if the shutter were open. When the shutter does open, the beam flux rises rapidly overshooting the steady state flux. This appears at the ion gauges as an overshoot in beam pressure followed by an asymptotic return to the steady state. At the same time, the reactant temperature cools rapidly to its steady state value. The temperature recorded by the thermocouple also falls, but more slowly since its response is delayed by thermal diffusion from the cell surface to the thermocouple. Similar considerations apply upon shutter closure, except that the change in beam equivalent pressure as measured by the ion gauge is abrupt. A qualitative representation of these processes is shown in Figure 4.
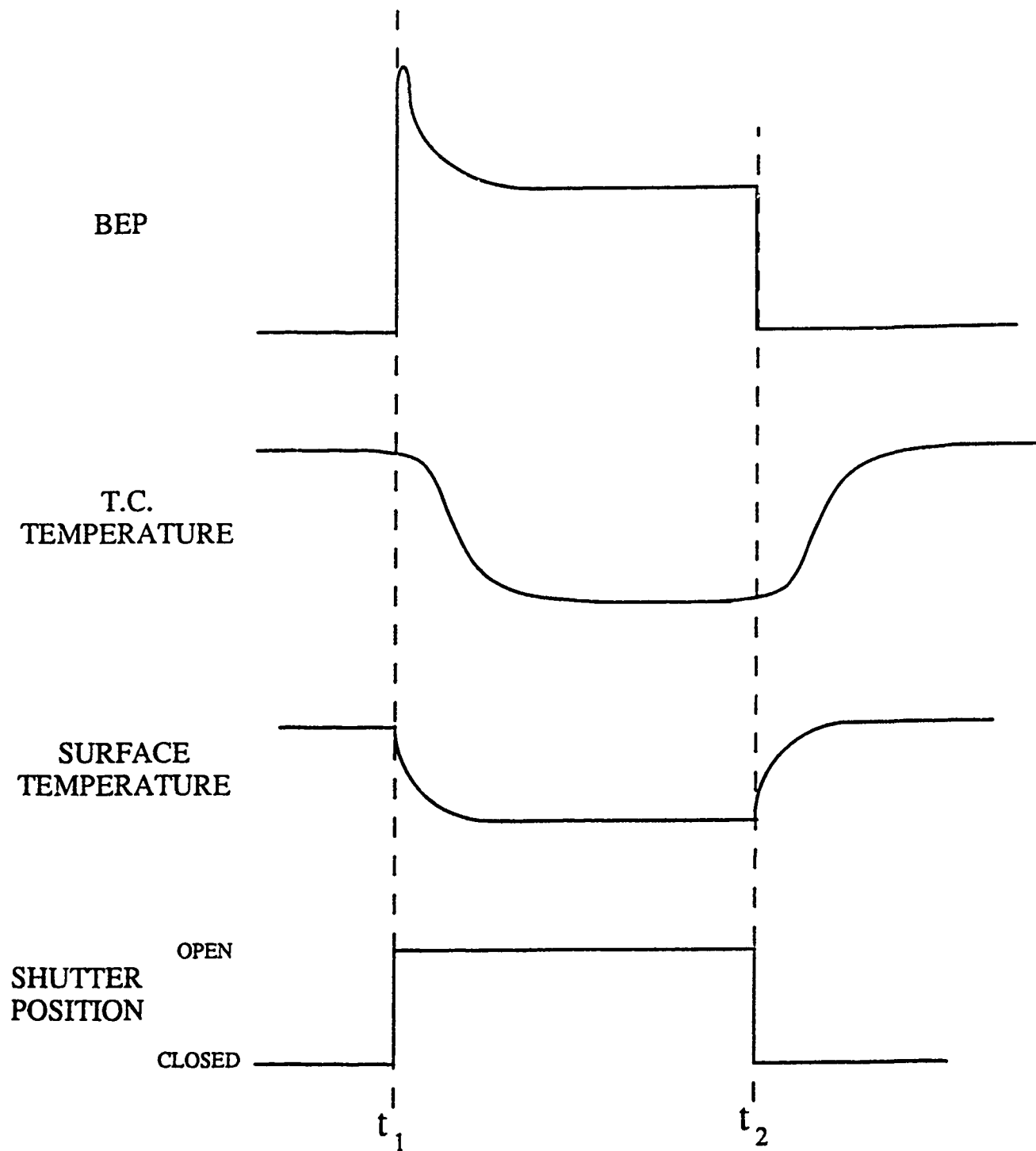
BEP

T.C.
TEMPERATURE

SURFACE
TEMPERATURE

SHUTTER
POSITION

OPEN

CLOSED

t_1

t_2

FIGURE 4   RESPONSE TO SHUTTER OPENING

The steady-state temperature-to-BEP transfer function can be obtained from this data if the shutter is open long enough for both the beam pressure and thermocouple temperature to reach steady state. Note that the thermocouple temperature approaches a steady state more slowly than does the beam pressure, and that the rate of change is zero near both t_1 and t_2. This beam pressure versus thermocouple temperature data would be stored as either a lookup table or linear function in a BEP database.

The beam pressure overshoot, and corresponding beam flux overshoot, could result in a non-uniform growth rate especially if accompanied by frequent shutter cycling. Therefore, in addition to static data, dynamical data describing this beam pressure overshoot are necessary. These dynamical data would be used to reduce the overshoot by adjusting the PID set point by an appropriate amount in advance of a shutter opening. The raw data needed for this correction would consist of the magnitude and rate of change of the BEP at a shutter opening and to a step change in the PID set point; this information could be stored in the Shutter Opening Transient Compensator. A function incorporating these data will be developed to describe the PID set point changes needed to minimize the beam pressure overshoot. It would also be stored in the compensator module. The lead time required to activate the PID compensation could be returned to the Supervisor/Sequencer module and linked to the shutter controller file. Alternatively, the function parameters could be stored in the Supervisor/Sequencer and, prior to shutter opening, could be sent to the Shutter Opening Transient Compensator, where they would be used to build the compensation function in real time and activate the appropriate PID set point change. Establishing the optimal choice for this control protocol function of the feed forward compensation will be incorporated in a Phase II effort.

As seen by comparing Figures 1 and 2, the Supervisor/Sequencer would be located outside of the Beta Control Loop. It would consist of one data file for each cell, and each file would consist of a sequence of PID set point, shutter transient compensation (feed forward) and shutter control commands. Command echoes and ac uator sensor outputs would be returned to the Sequencer sub-module both to confirm the communications, and to provide system monitoring to the Supervisor sub-module. This Supervisor sub-module would serve several functions. First, it would serve as a Virtual Instrument that could provide direct PID control for manual PID settings, temperature ramping and steady state growth conditions. Independent and uncompensated shutter control along with cell and substrate temperature monitoring would also be available. Second, the supervisor would permit the user to set up and run calibrations, acquire and display data, and store them in the appropriate files. Third, the growth sequence would be introduced through the Supervisor sub-module. The user would prepare a target materials-BEP-time sequence for new growth experiments based on *ex situ* materials properties measurements, having already

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established the relationships between materials composition/thickness and BEP-time sequences. Closure of the calibrated Beta Control Loop would, at a minimum, ensure process repeatability. Finally, the Supervisor sub-module would permit real-time monitoring of all system parameters including such MBE chamber parameters as the cryoshroud level and state of the vacuum.

In addition, a hierarchy of system interrupts would be bundled with the Supervisor/Sequencer module. This would permit operator intervention for a prescribed period of time following an unscheduled system change or upset depending on the seriousness of the system or growth sequence failure. Subsequently, a hierarchy of control interventions would be initiated that still could be superseded by operator intervention. Details of these controls would be developed during a Phase II effort.

Upon closure of the work on the Beta Control Loop, the user will be able to schedule reproducible sequences of beam equivalent pressures versus time. Since the relationship between beam flux and beam pressure is both linear and easily estimated, this amounts to user control over beam flux versus time and, therefore, to full process control. Control over the material product requires an additional feedback loop employing sensors that monitor the product and provide this information to the Supervisor/Sequencer. This Self-directed Control Loop, the Alpha Control Loop, is discussed next.

2.2 Alpha Control Loop

The objective of the Alpha Control Loop is to provide real time control over the composition and thickness of the growing film. The sensor for this self-directed MBE flux control system is an ellipsometer. The ellipsometer is an instrument that makes measurements of the polarization state of light reflected from the surface of a material. When applied to a thin film, this information can be used to determine the composition and thickness of that film. Because it is an optical technique, ellipsometry has a distinct advantage: it can be applied in adverse environments. By combining high speed data processing methods, ellipsometry can be used as a real time control method.

2.2.1 Ellipsometry – Instrumentation Overview   The hardware elements of an ellipsometer consist of a light source, a polarizer, a sample holder, an analyzer, and a detector. The polarizer is used to generate linearly polarized light. The analyzer is used to examine changes in the polarization when that light is reflected from a surface. Ellipsometry can be applied at a single wavelength or over a spectrum of wavelengths. Single wavelength, real-time ellipsometry can use either a laser as the light source, or white light with a spectrometer. For spectroscopic ellipsometry, the spectrometer is scanned. It is important to select a source wavelength at which changes in polarization (optical properties) are especially sensitive to materials properties. For

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example, a photon energy of 2.6 eV is usually chosen for the study of $Al_xGa_{1-x}As$ because variations in the dielectric properties with compositional changes are large at this wavelength. Static spectroscopic measurements made before and after film growth can be used both to assess the accuracy of the angle of incidence, and to provide comparative film structure data.

2.2.2 Ellipsometry – Sensor Response   Of the various types of automated ellipsometers that have been developed, those with rotating elements exhibit relative achromaticity and simplicity . Accordingly, they have been used most extensively. Entirely controlled by computer, the system generally consists of: alight source; fixed (rotating) polarizer; sample, rotating (fixed) analyzer; and detector.

In this configuration, the fixed polarizer is used to generate a linearly polarized light with its electric field oscillating in a direction denoted by the angle θ_p with respect to the plane of incidence. This is shown in Figure 5. It is convenient to treat this linearly polarized electric field, E, as being composed of two orthogonal, linearly polarized components oscillating in phase. These two components are usually designated as E_p, oscillating in the plane of incidence, and E_s oscillating perpendicular to the plane of incidence.

This wave propagates at an angle of incidence θ_o with respect to the unit normal at the material surface when this wave is reflected by θ_o from the ambient-material interface, the electromagnetic boundary conditions governing the reflection and transmission properties at this interface are different for the two components. Therefore, the amplitude and phase of the reflection coefficients for E_s and E_p generally are not the same; so, the reflected electric field is elliptically polarized.

This elliptically polarized reflected wave then passes through an analyzer to a detector. If the polarization axis of the analyzer makes an angle θ_a with respect to the plane of incidence, the amplitude of the wave incident on the detector is

$$E = E_o \{ |r_s| \sin\theta_p \sin\theta_a\, e^{i\delta_s} + |r_p| \cos\theta_p \cos\theta_a\, e^{i\delta_p} \} \tag{1}$$

where $|r_p| e^{i\delta_p}$ and $|r_s| e^{i\delta_s}$ are the complex reflection coefficients of the E_p and E_s components. The detector output is proportional to the square magnitude of these components and, after some algebra, can be written as

$$I(t) = I_o[1 + \alpha\cos(2\theta_a) + \beta\sin(2\theta_a)] \tag{2}$$

where
$$\alpha = [\tan^2\psi - \tan^2\theta_p]/[\tan^2\psi + \tan^2\theta_p] \tag{3a}$$

and
$$\beta = [2 \tan\psi \, \tan\theta_p \, \cos\Delta]/[\tan^2\psi + \tan^2\theta_p] \tag{3b}$$

in which two angles, ψ and Δ called the "ellipsometry angles", have been defined by

$\psi = \tan^{-1}(|r_p|/|r_s|)$ and $\Delta = \delta_s - \delta_p$. These can be solved for α and β with the result that

$$\tan\psi = [(1 + \alpha)/(1-\alpha)]^{1/2} \tan\theta_p \tag{4a}$$

and
$$\cos\Delta = \beta/(1 - \alpha^2)^{1/2} \tag{4b}$$

In order to extract α and β, and thus ψ and Δ, from I, the angle θ_a can be rotated about the axis of propagation and the detector output compared with (2). By this process, the constant intensity is eliminated. In practice, this rotation is accomplished by rotating the analyzer at a constant angular frequency Ω so that $\theta_a = \Omega t$, as is shown in Figure 5, produces a time-periodic detector output. This signal then can be either Fourier analyzed or fitted by regression to a sinusoidal function to provide α and β.

2.2.3 Ellipsometry – Pseudo Dielectric Function   When there is a single interface between ambient and bulk material, the relative dielectric function of the material can be easily obtained from the ellipsometry parameters (Δ, ψ) and the angle of incidence θ_o by using the relationship

$$\varepsilon = \varepsilon_1 + i\varepsilon_2 = ((1+\rho)/(1-\rho))^2 \sin^2\theta_o \, \tan^2\theta_o + \sin^2\theta_o \tag{5}$$

where $\rho = r_p/r_s = \tan\psi e^{i\Delta}$. In the case of one or more overlayers on a substrate material, ε is replaced by $<\varepsilon>$, the pseudo-dielectric function of the multilayer system. This function depends upon the angle of incidence, the film thicknesses and dielectric functions of the individual layers.

2.2.4 Ellipsometry – Materials Properties Control   The form of the ellipsometer output can be understood by considering a simple ambient/film/substrate structure, in which the film starts growing from zero thickness. Initially, the incident light beam is reflected only by the ambient/substrate interface. The measured parameters, ($<\varepsilon_1(t_o)>$, $<\varepsilon_2(t_o)>$), are those of the substrate, $(\varepsilon_1, \varepsilon_2)_{sub}$. As the film grows, the measured pseudo-dielectric function ($<\varepsilon_1(t)>$, $<\varepsilon_2(t)>$), traces a spiral in the ($<\varepsilon_1>$, $<\varepsilon_2>$) plane. Ultimately, no light reaches the substrate and the spiral converges to a single point, $(\varepsilon_1, \varepsilon_2)_{film}$, indicative of the bulk. Beyond this bulk equivalent film thickness, the substrate no longer affects the reflected beam, and ellipsometry no longer is sensitive to film thickness. The pseudo-dielectric function of the composite film-substrate structure then remains $(\varepsilon_1, \varepsilon_2)_{film}$. The length of the spiral is a measure of the penetration depth of the probing light in the film. Therefore, the thickness of the film can be determined by the position $<\varepsilon_1(t)>$ and $<\varepsilon_2(t)>$ on the spiral.
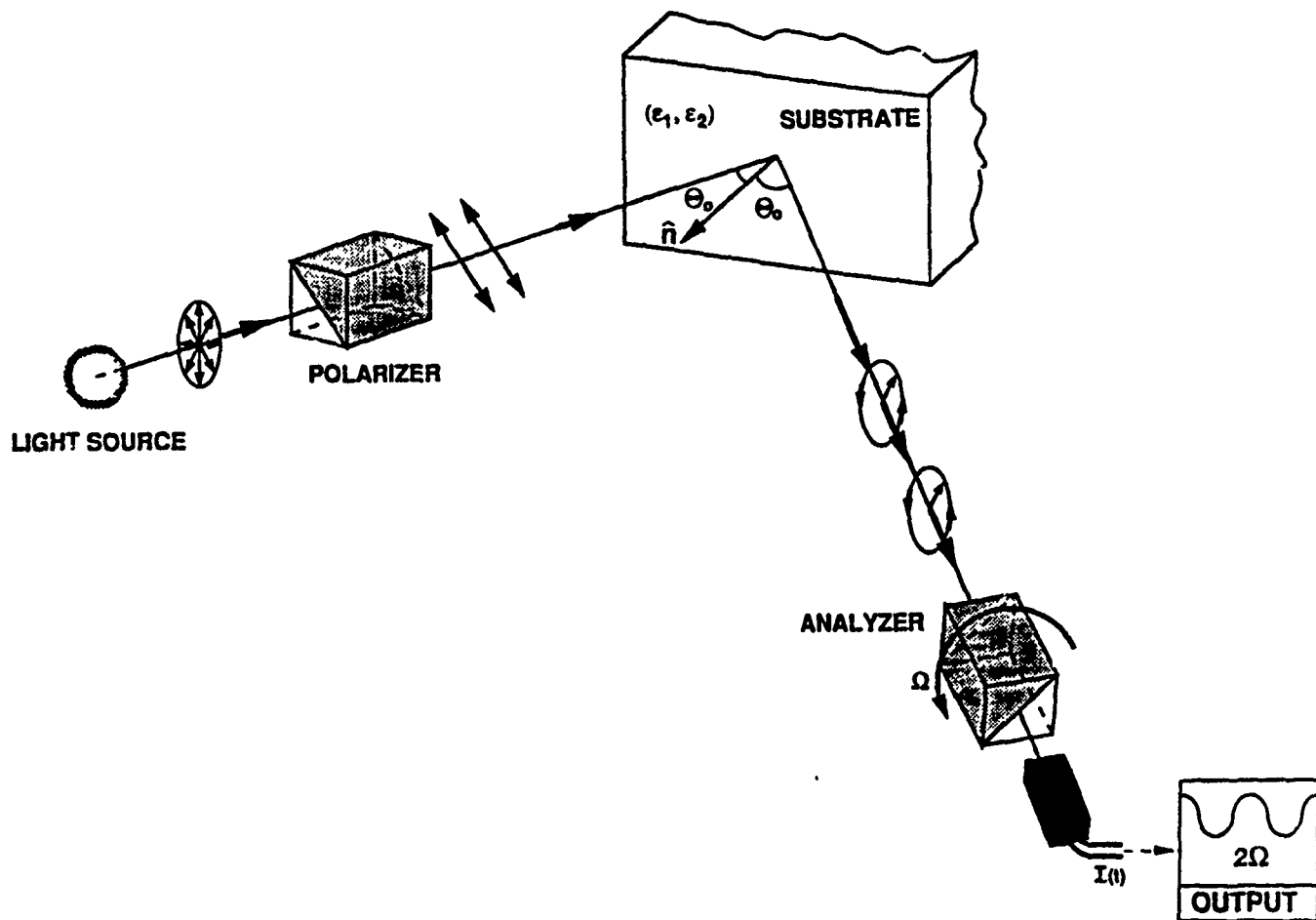
FIGURE 5. DETAILS OF ELLIPSOMETER COMPONENTS

Measurements of this type also can be used to obtain the instantaneous film thickness. Since the measurement space is two-dimensional, (α,β) or (ψ,Δ), and since the materials properties space is three-dimensional, $<\varepsilon_1,\varepsilon_2>$ and thickness, the mapping is not homeomorphic. In other words, additional data are needed to obtain $<\varepsilon_1,\varepsilon_2>$ and thickness unambiguously. These additional data are acquired through a series of *ex situ* measurements and stored in a database for subsequent use in the data analysis.

The means by which this data can be combined with real-time ellipsometry measurements to extract a real-time film thickness can be understood through example. For a three-layered medium consisting of a substrate, a film and the ambient environment, the reflection ratio r at the ambient-material interface takes the usual form:

$$\rho = \tan\psi \exp(i\Delta)$$

$$= \{[r_{01p} + r_{12p}\exp(-2i\beta)]/[1 + r_{01p}r_{12p}\exp(-2i\beta)]\}/\{[r_{01s} + r_{12s}\exp(-2i\beta)]/[1 + r_{01s}r_{12s}\exp(-2i\beta)]\}$$

$$(6)$$

where the r's are the Fresnel complex reflection coefficients at the interface between two semi-infinite media, and the subscripts 0, 1 and 2 refer to the ambient, film and substrate respectively. These can be expressed in terms of the index of refraction of each medium and the internal angle of incidence by the following:

$$r_{01p} = (N_1\cos\theta_0 - N_0\cos\theta_1)/(N_1\cos\theta_0 + N_0\cos\theta_1) \qquad (7a)$$

$$r_{01s} = (N_0\cos\theta_0 - N_1\cos\theta_1)/(N_0\cos\theta_0 + N_1\cos\theta_1) \qquad (7b)$$

$$r_{12p} = (N_2\cos\theta_1 - N_1\cos\theta_2)/(N_2\cos\theta_1 + N_1\cos\theta_2) \qquad (7c)$$

$$r_{12s} = (N_1\cos\theta_1 - N_2\cos\theta_2)/(N_1\cos\theta_1 + N_2\cos\theta_2) \qquad (7d)$$

where the N's are the indexes of refraction and θ_0 is the angle of incidence. The film thickness enters through the propagation factor which is given by $\beta = 2\pi(d/\lambda)N_1\cos\theta_1$. After some algebra, equations 6 and 7 can be used to express the thickness d in terms of the complex refractive indexes of the constituent materials. These refractive indexes then are extracted from the materials properties database and used to compute a value for d. Other procedures can be developed to extract materials properties from ellipsometry measurements. But all single wavelength procedures must encounter underdetermined data sets and must, therefore, resort to devices similar to the one described above.

3.0   RESULTS AND DISCUSSION

During the current phase of this effort, considerable progress was made in the development of Beta and Alpha control loops. The more significant achievements were identified in Section 1.4. In this section, a more complete description of these accomplishments is presented along with supporting data. As with any complex technical program, considerable experimentation was necessary and prolific quantities of data generated to reach the current stage of success. In the following discussion, only those data are presented that exemplify the most important advancements.

3.1   Alpha Control Loop

During this effort, considerable progress was made in developing ellipsometry as the real-time materials' properties sensor. The ellipsometry results can be conveniently divided into the following 4 areas of discussion:

- oxygen desorption from substrates;

- substrate temperature monitoring;

- crystal structure monitoring;

- film thickness control.

<u>3.1.1   Ellipsometry Monitoring Of Oxygen Desorption From GaAs</u>   The production of device-quality films will require ultra-clean substrates free of native oxygen. In one series of experiments, ellipsometry was used to monitor oxide desorption from GaAs substrates. The ellipsometry parameters (Δ, ψ) versus substrate temperature as measured by the substrate thermocouple are shown in Figure 6. At 700°C, ψ starts to decrease. Model simulations suggest that this decrease could be due to increased surface roughness, which could be the result of oxygen desorption. Above 740°C both Δ and ψ start to increase. Again, model simulations suggest that this could be due to removal of the oxygen overlayer and a smoothing of the overall surface. The importance of this interpretation became unexpectedly apparent in the course of this experiment. At one point the RHEED analysis, which was being used to compliment the ellipsometry data, ceased functioning. Oxygen desorption monitoring successfully continued, however, using only ellipsometry. Figure 7 shows a Double crystal X-Ray Diffraction (DXRD) measurement of a low temperature (LT) GaAs film on a GaAs substrate. The poorly defined film peak suggests low crystal quality of the LT-GaAs film. One explanation is incomplete oxide layer removal. In comparison, Figure 8 shows a DXRD measurement of a high quality LT-GaAs growth with the

presence of Pendellosung fringes. In this case, real time ellipsometry was used to ensure complete oxide layer removal. On the basis of these experiments, real time ellipsometry has since been used as a routine technique for monitoring oxide removal. As a result, repeatable growth of LT-GaAs films of high crystalline quality are now readily achieveable.

3.1.2 Ellipsometric Monitoring Of Growth Conditions

Low temperature GaAs films are of considerable importance due to their applications as high resistivity and optically dead buffer layers in GaAs devices. However, the properties of such films are extremely sensitive to growth conditions -- arsenic overpressure, substrate temperature and growth rate. Excess As atoms can either enter substitutionally at a Ga site, or be deposited between sites. The ability of the lattice to incorporate As atoms is proportional to the As over-pressure and inversely proportional to the substrate temperature. In either case, the lattice constant of the resulting film increases as more As atoms are incorporated. The substrate temperature of MBE is usually measured by a thermocouple attached to a molybdenum block sample holder on which samples are mounted with indium solder. The difference between surface and thermocouple temperature varies from one substrate to another due primarily to variations in the thermal contact provided by the indium sample mounting method. In order to deposit films with reproducible properties, it is absolutely necessary to have reproducible growth conditions. In this experiment, the temperature of a GaAs substrate was varied under controlled arsenic overpressure. Real-time ellipsometry was used to monitor the GaAs surface. A significant As film did not develop until the substrate temperature was below 100°C, while As desorption occurred at a substrate temperature above 350°C. These considerations establish a temperature window for the growth of LT-GaAs.

As mentioned above, the thermocouple is not a reliable indication of substrate temperature. But changes in the lattice constant due to surface modification of the GaAs film by excess As should be a good indication of the growth conditions.

Oxide Desorption GaAs#19(
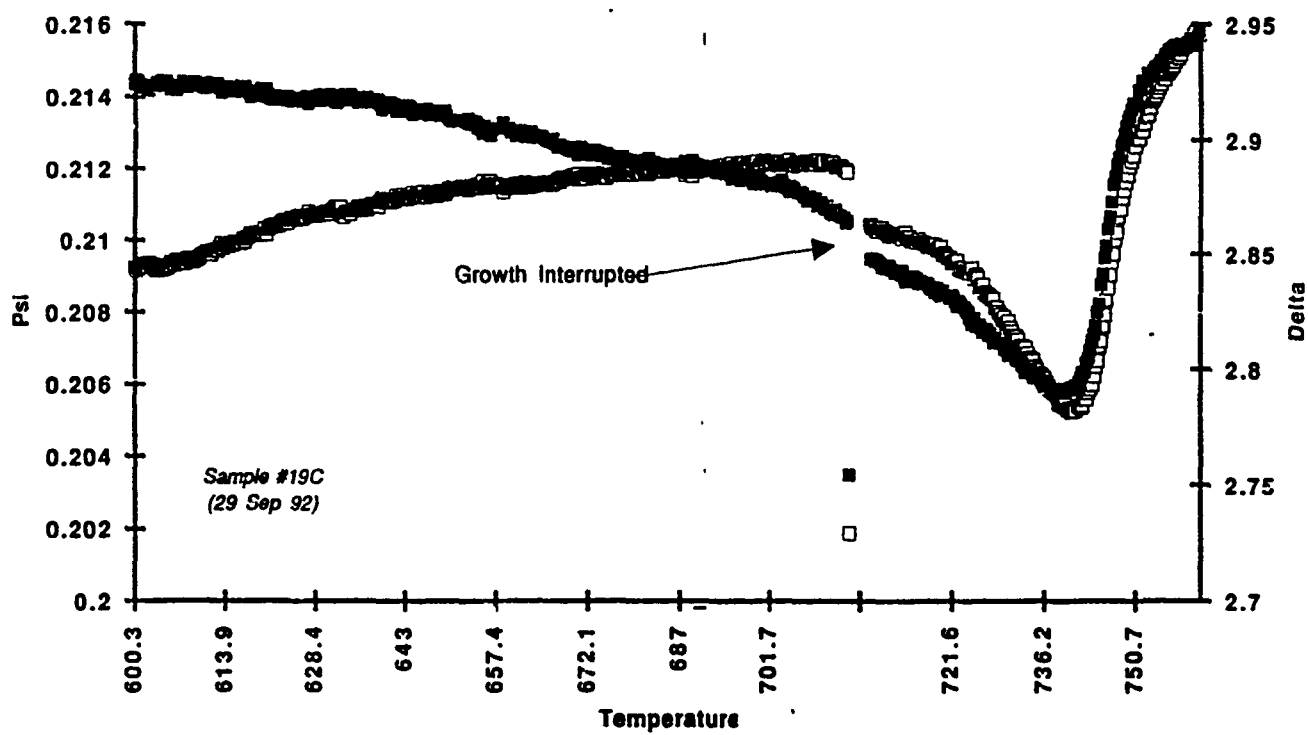
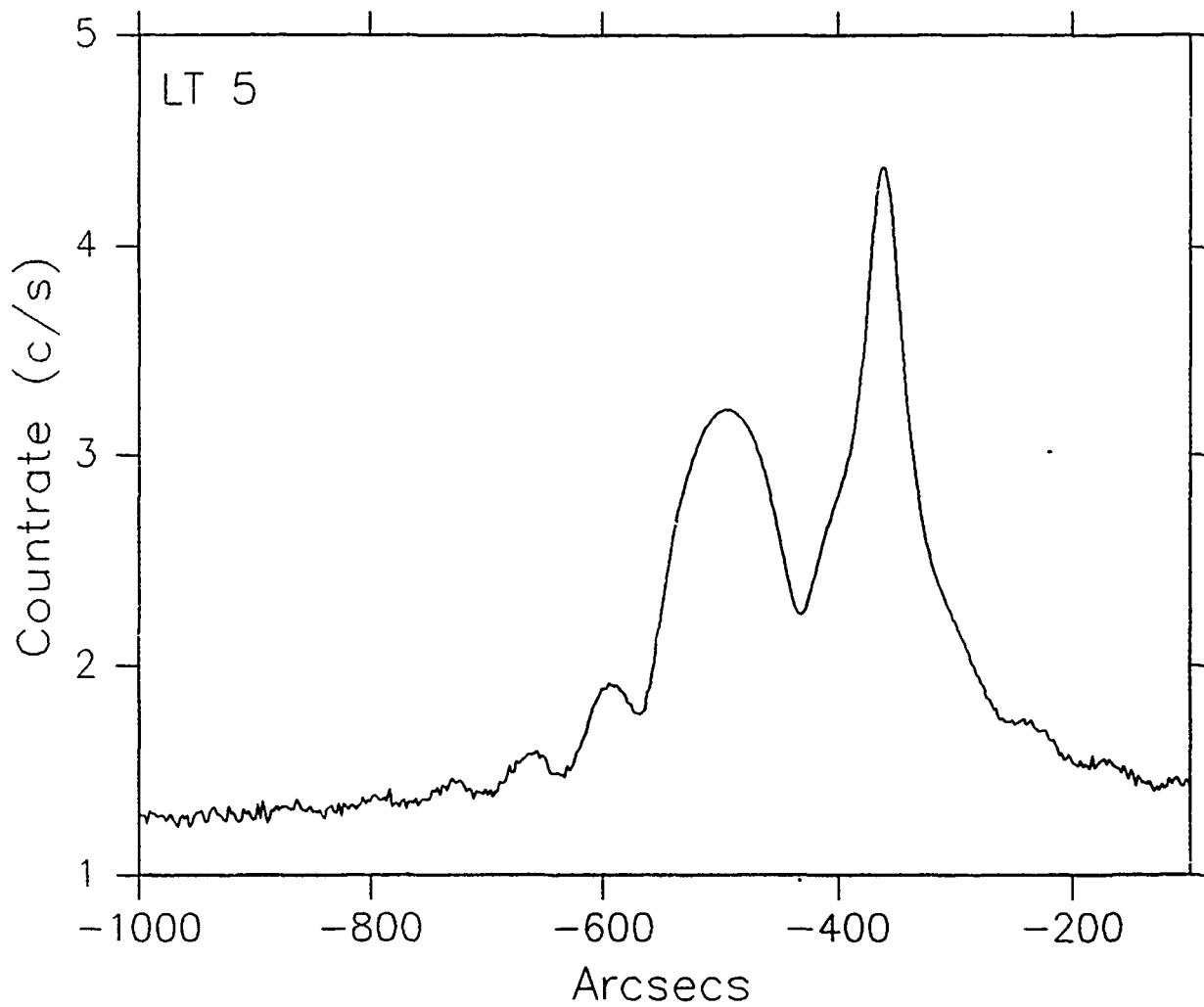FIGURE 6   ELLIPSOMETRY PARAMETERS VERSUS GaAs
SUBSTRATE THERMOCOUPLE TEMPERATURE
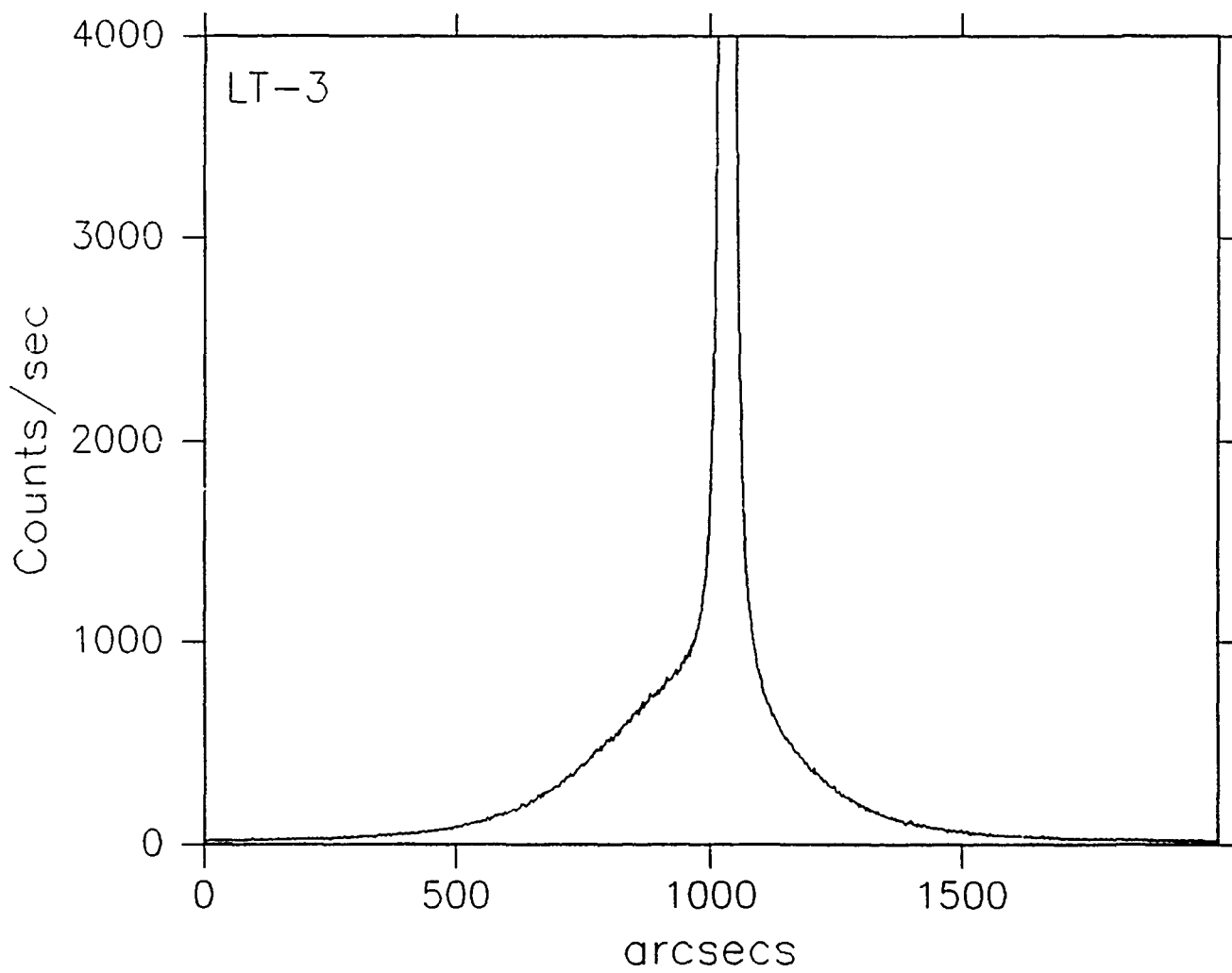
**FIGURE 7   DOUBLE X-RAY DIFFRACTION OF LT-GaAs
(incomplete oxide removal)**

FIGURE 8 **DOUBLE X-RAY DIFFRACTION OF LT-GaAs**
(complete oxide removal)

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Figure 9 shows an ellipsometry signature as a function of substrate temperature as measured by the thermocouple for a LT-GaAs film. The rapid decrease in ψ near 285°C is believed to have been caused by a GaAs surface modification brought about by excess arsenic. If so, it should occur at the same substrate temperature under specific arsenic overpressure. This possibility was explored by depositing two LT-GaAs films at the temperature corresponding to the minimum in ψ while using identical arsenic overpressures. The same ellipsometry signature was obtained in both cases. Although substrate temperatures at the minimum ψ as measured by the thermocouple were very different, in each case the dielectric properties and epitaxial layer thickness of the two LT-GaAs films were very similar. This strongly suggests that both were, in fact, grown at the same, true substrate temperature. Consequently, the ellipsometry signature is an excellent temperature indicator for reporducible LT-GaAs growth. The real-time control capabilities for LT-GaAs are obvious.

3.1.3   Ellipsometric Monitoring Of Crystal Structure   During this work it also was shown that ellipsometry could be used in real time to distinguish among possible crystal structures. Again, LT-GaAs was used as the demonstration film. It was found to consist of three regions with different crystal structures as shown in the ellipsometric data plotted in Figure 10. The first region, directly above the substrate, grow homogeneously with uniform dielectric properties. The properties, as well as film thickness, were dependent on the growth conditions. DXRD measurements indicated that this region corresponded to epitaxial single crystal LT-GaAs with low surface and interface roughness. Subsequently an amorphous layer nucleated on the epitaxial layer. Analysis of the real time ellipsometry data revealed that the nucleation of the amorphous layer was interfused with single crystal LT-GaAs. Continued growth produced an increasing amorphous volume thus forming a region with constantly varying dielectric properties. Thin film X-ray measurements, shown in Figure 11, confirmed these conclusions by demonstrating that no polycrystalline peaks were detected. As shown in Figure 12, thin film X-ray measurements of the final region revealed peaks corresponding to various crystal orientations indicating this region to be polycrystalline. The growth temperature for this film was chosen to correspond to the minimum value of ψ, as in the discussion above. Under the same arsenic overpressure, films also were deposited at high and lower substrate temperatures. It was found that the thickness of the epitaxial layer decreased and film absorption increased with decreasing temperature. The high contrast of dielectric properties and the more rapid breakdown of crystallinity appeared to be caused by the high arsenic incorporation in the film at lower growth temperature.
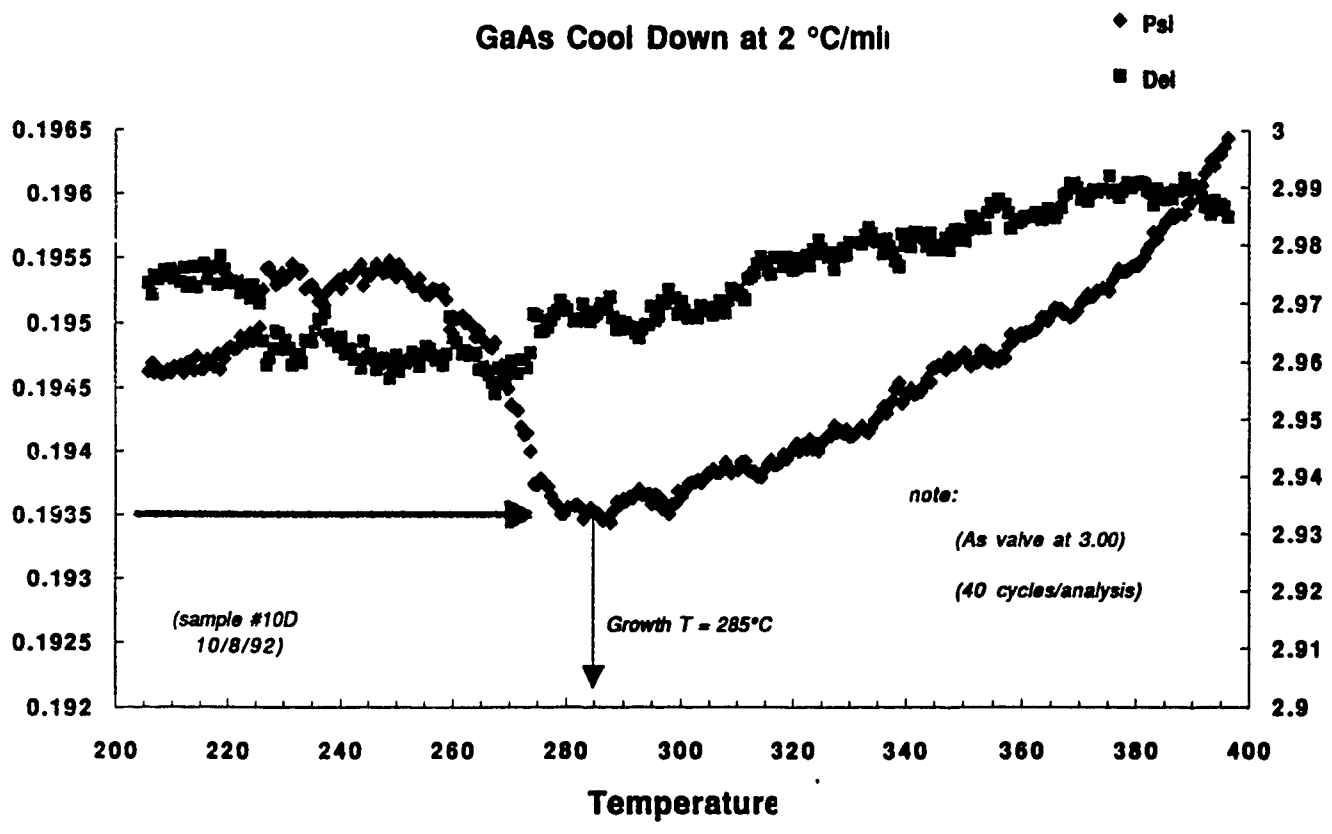
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GaAs Cool Down at 2 °C/min

◆ Psi
■ Del

note:

(As valve at 3.00)

(40 cycles/analysis)

(sample #10D
10/8/92)

Growth T = 285°C

FIGURE 9   EFFECT OF As ADSORPTION/DESORPTION

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Low Temperature GaAs Growth
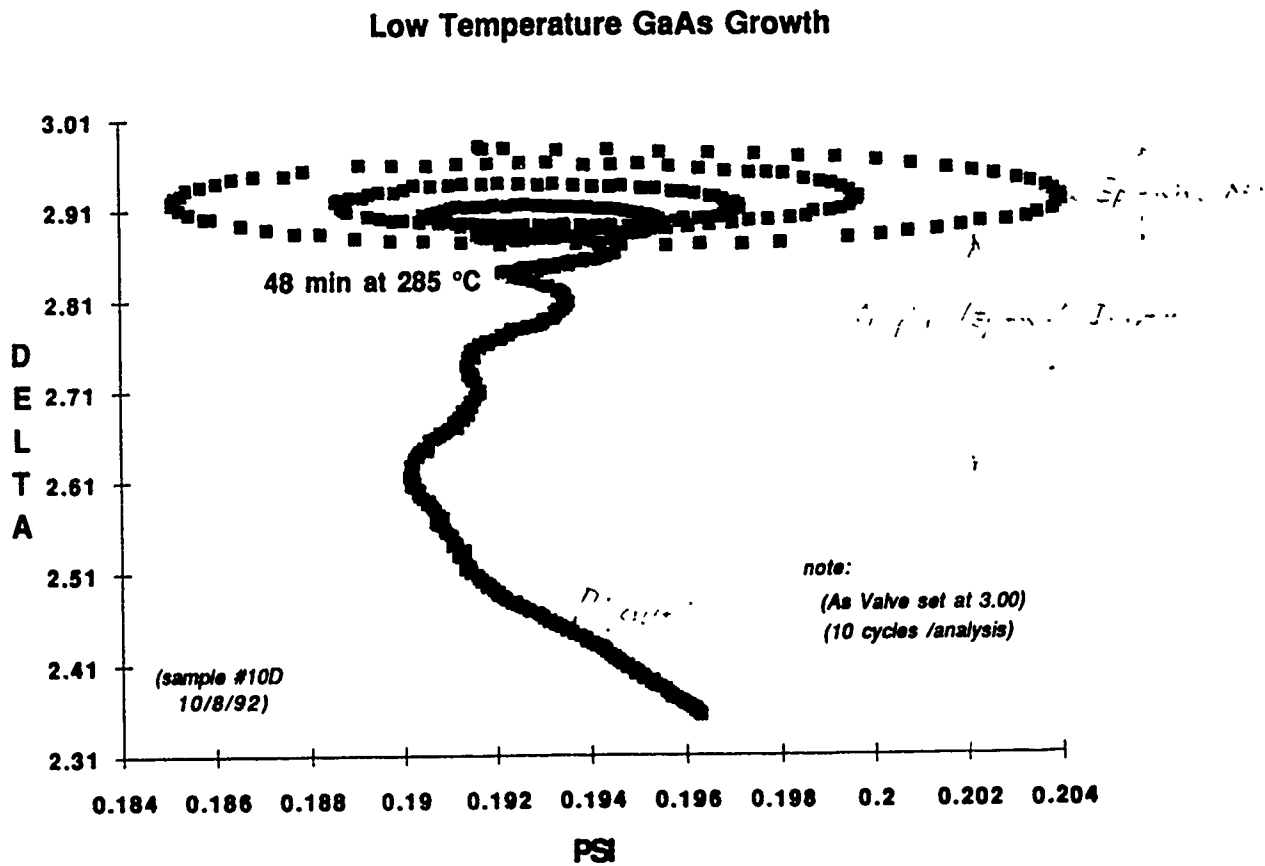
FIGURE 10   FILM STRUCTURE DURING LT-GaAs GROWTH MONITORED BY REAL-TIME ELLIPSOMETRY

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Z00191.RAW   # 19D

KGE LT-7
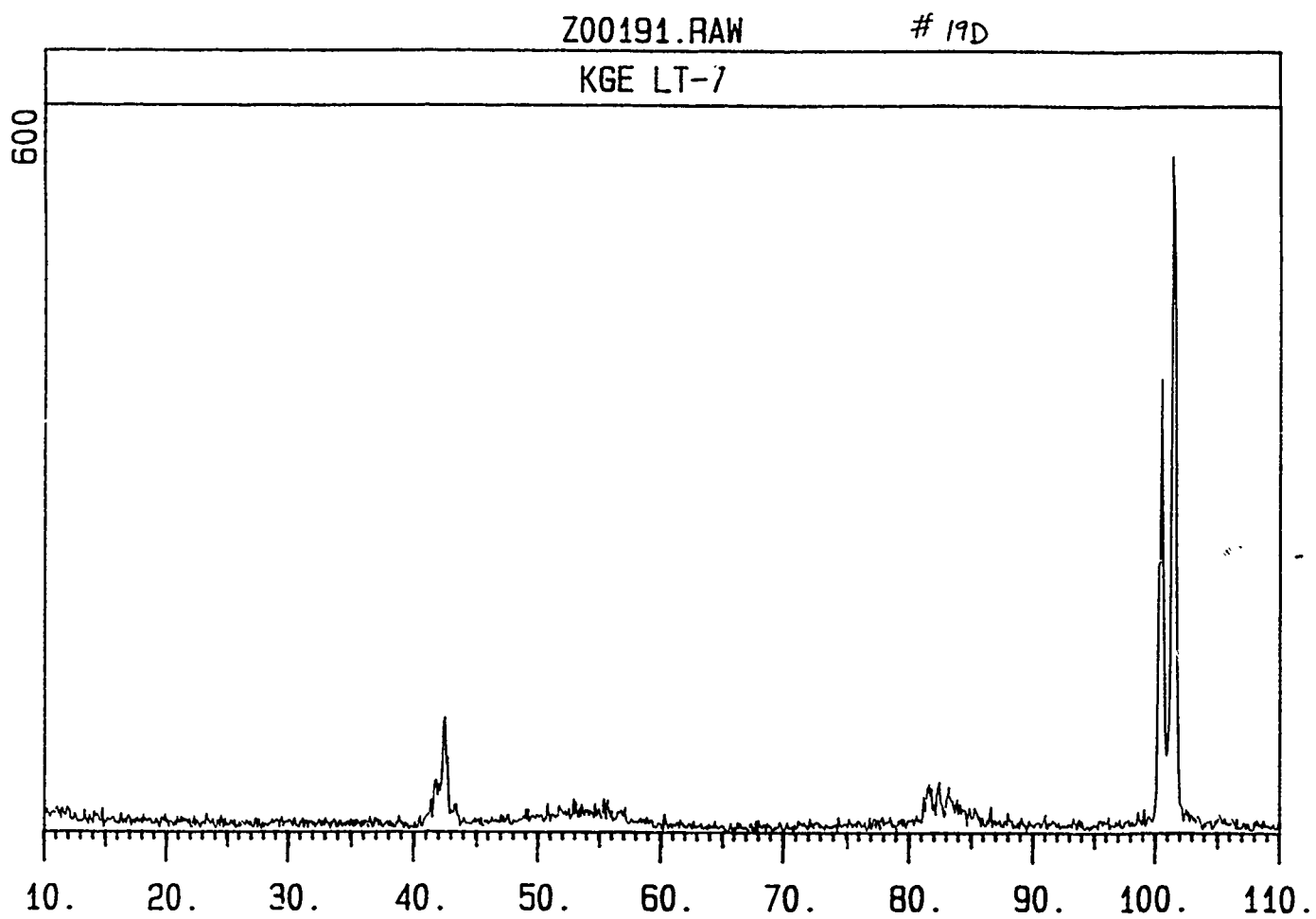
FIGURE 11   THIN FILM X-RAY MEASUREMENTS OF AMORPHOUS REGION SHOWN IN FIGURE 10

27   *MBE Flux Control - Final Report*
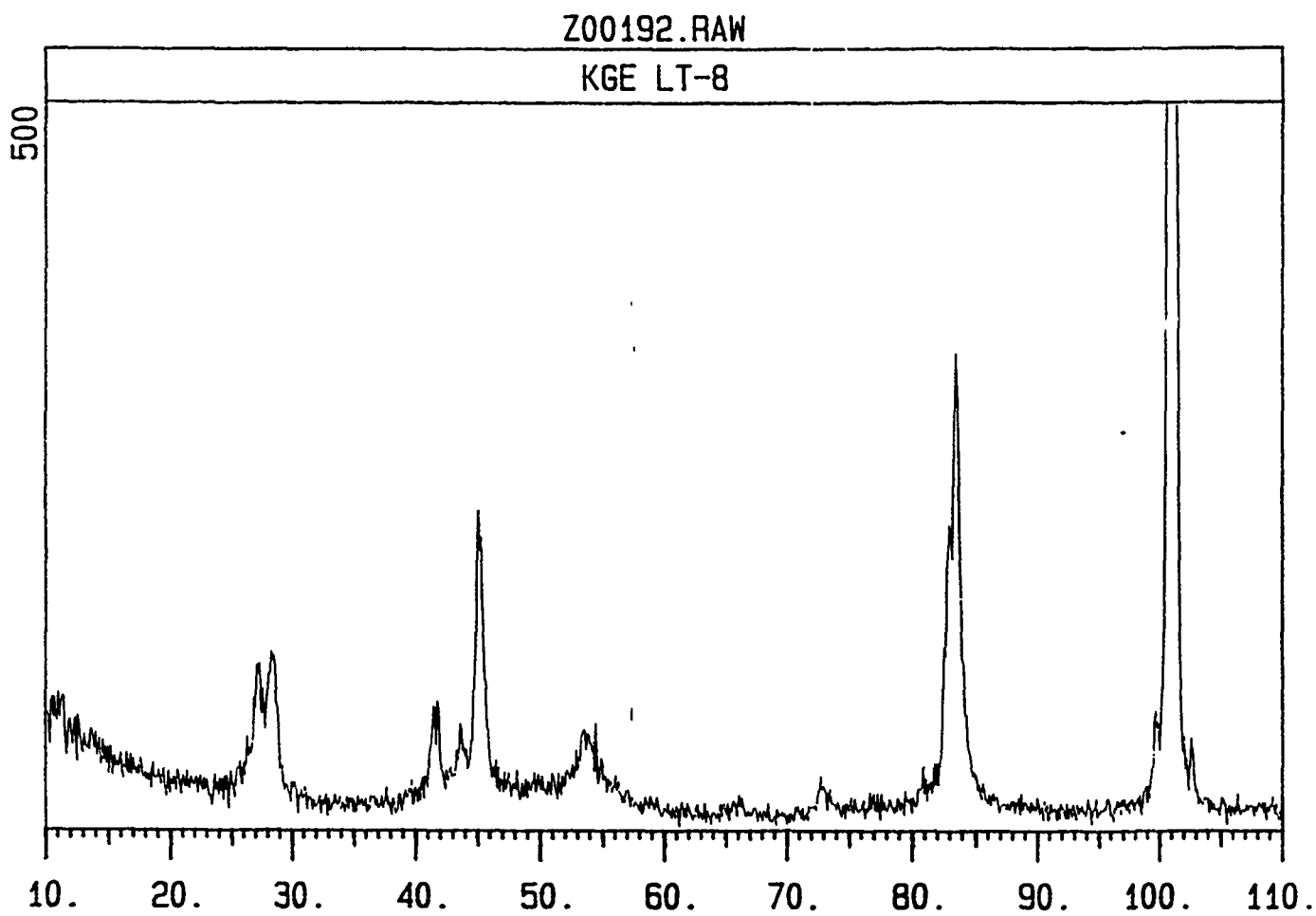
FIGURE 12   THIN FILM X-RAY MEASUREMENTS OF
             POLYCRYSTALLINE REGION SHOWN IN
             FIGURE 10

A second study of crystal structure utilized InGaAs films grown on InP substrates. A typical growth trajectory of pseudo-dielectric constants $\langle\varepsilon_1\rangle$, $\langle\varepsilon_2\rangle$ is shown in Figure 13. The initial part of the trajectory, between the points marked as "start" and "coalescence", corresponds to the growth of a 3-dimensional pyramidal structure. This structure develops when one layer of atoms begins to develop before the preceding layer is complete. Ellipsometry detects this as a surface roughening. Such undesired growth results principally from an incorrect In-to-Ga beam flux ratio that results, in turn, from shutter opening transients. By contrast, Figure 14 shows a growth trajectory with no initial 3-dimensional growth. In this case, the initial flux ratio happened to be suitable for layer-by-layer growth even though the steady state flux ratio was incorrect and the growth eventually became 3-dimensional. From these two examples, it can be seen that real time ellipsometry is very sensitive to the growth pattern, and can be used easily to detect results of flux transients.

3.1.4   Real Time Film Thickness Measurements   An example of the application of the potential for ellipsometric thickness control in real time is shown in Figure 15. This data was derived from the unprocessed data shown in Figure 14 and the data analysis procedure described in Section 2.2.4. For this work, InGaAs was grown on a InP substrate. This latticed-matched epitaxy was chosen because it would avoid temperature-induced shifts of the pseudo-dielectric function and provide a clear demonstration of the proposed algorithm. The scatter in data evident in Figure 14 for the first 5.4 minutes was due either to a flux transient or to the fact that the thin film properties deviated significantly from their bulk properties. Between 5.4 minutes and 11 minutes the spiral developed smoothly and it was possible to extract a thickness measurement using the protocol referred to above. The application of this procedure is shown in Figure 15 which demonstrates that the thickness of the film increased linearly from near zero to 400 Å. This thickness data was developed in real time as α and β were measured. It is evident from this that when the Alpha Loop is closed real time thickness control will be realized.

3.2   Beta Control Loop

The Beta Control Loop, the loop that stabilizes functioning of the MBE machine and helps to ensure reproducible film growth, has been advanced through the efforts of numerous scientists and engineers. During the period of performance for this report, the Principle Investigator responsible for the development of this loop was Mr. Jeffrey Heyob. His report documenting progress in this area is reproduced in Appendix A.
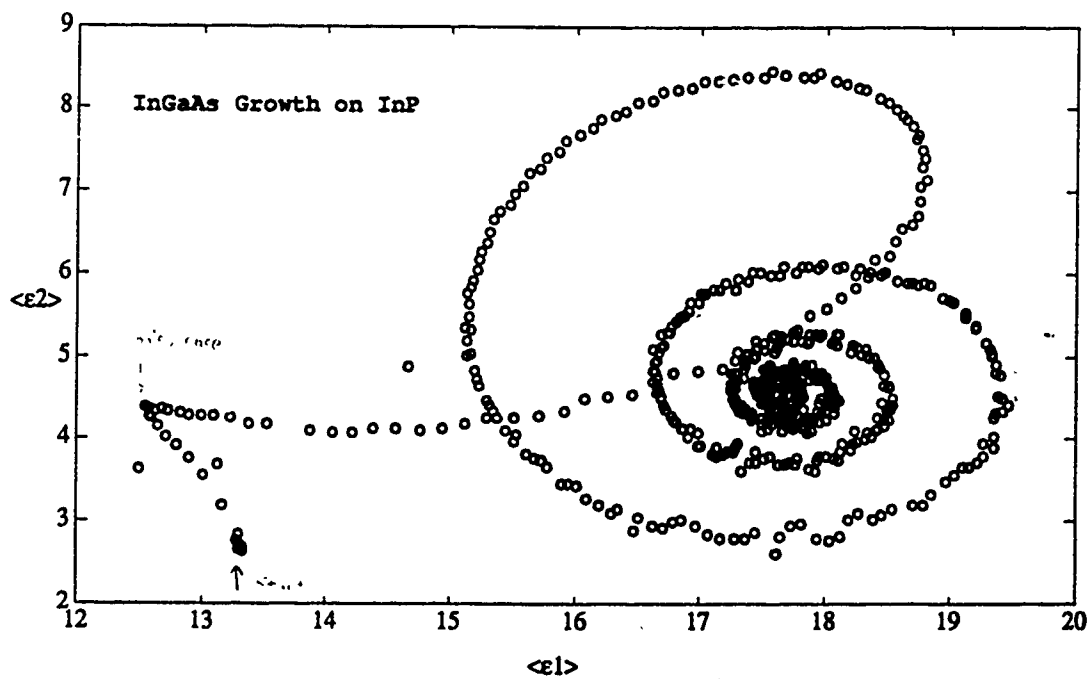
FIGURE 13 · **ELLIPSOMETRY TRAJECTORY OF InGaAs GROWN ON InP WITH INITIAL ERROR IN In/Ga FLUX RATIO**
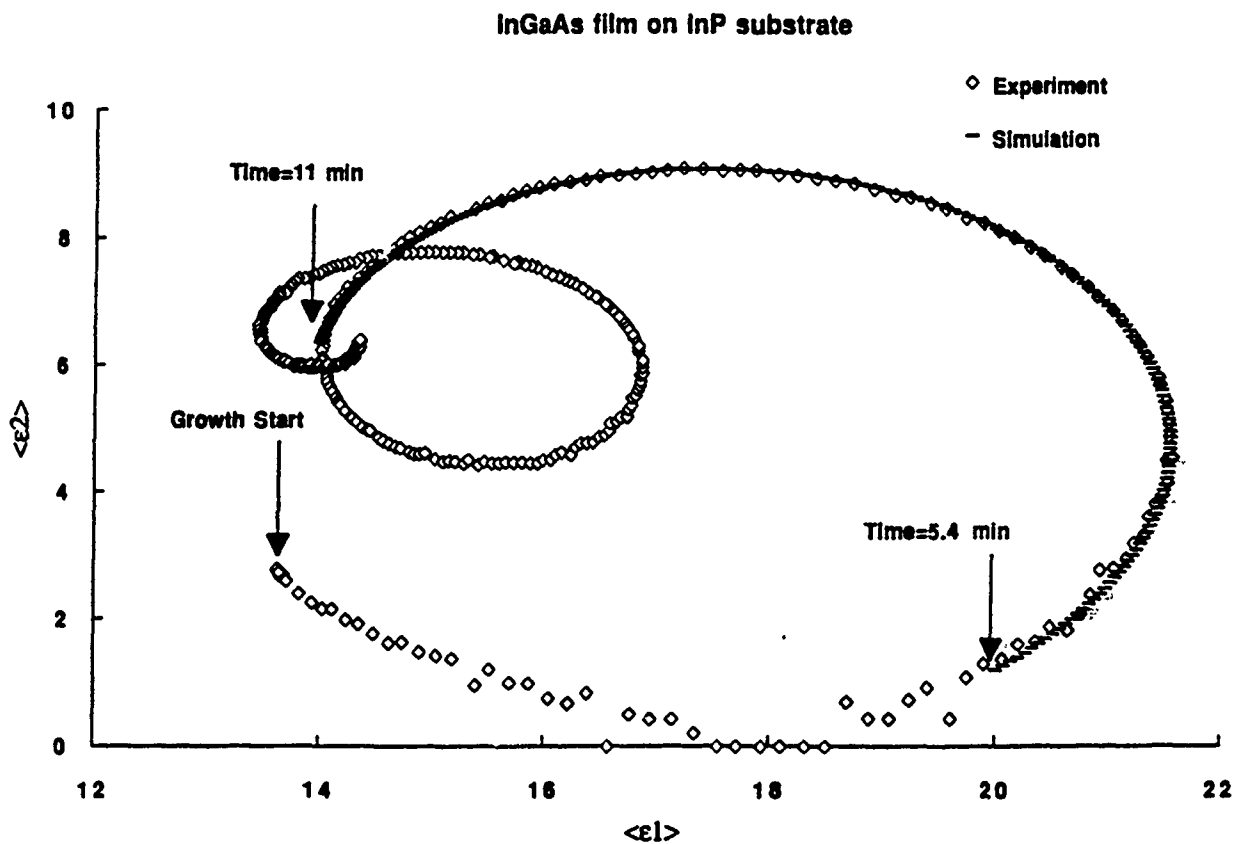
InGaAs film on InP substrate

FIGURE 14   ELLIPSOMETRY TRAJECTORY OF InGaAs GROWN ON InP

31
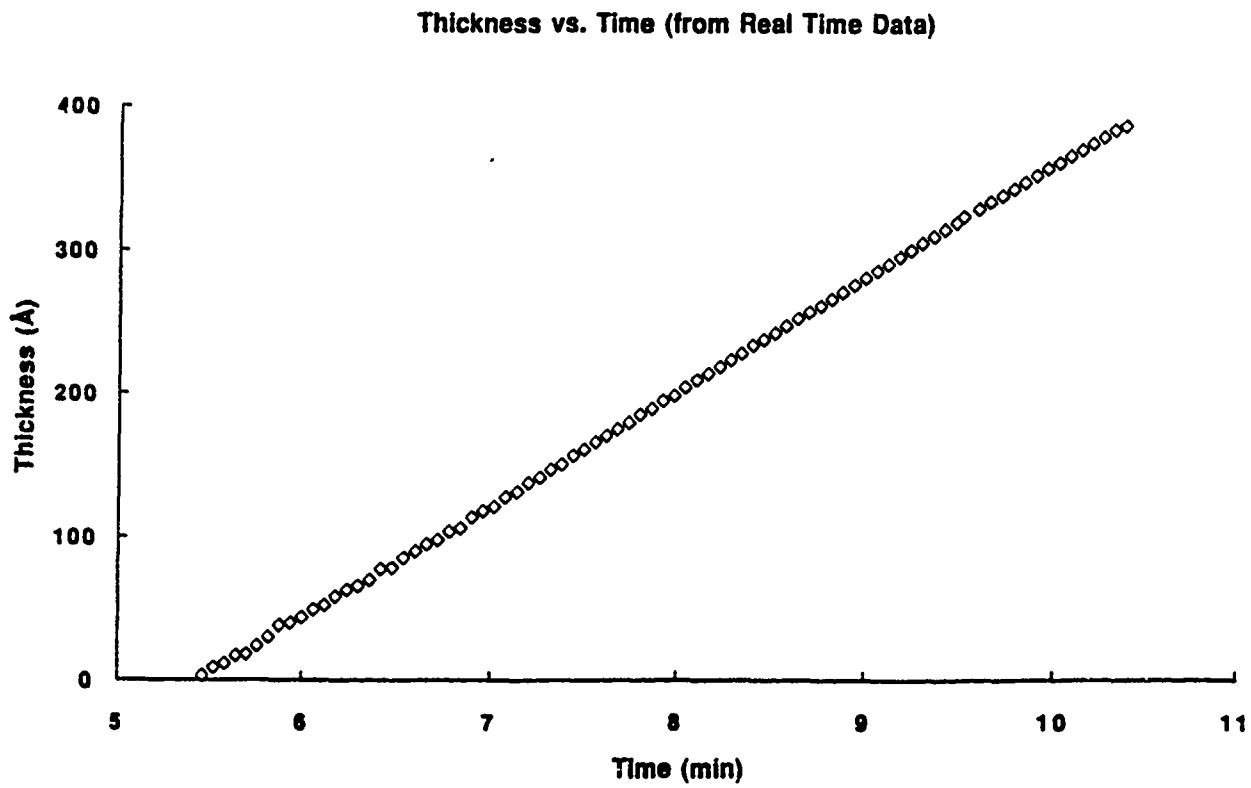
Thickness vs. Time (from Real Time Data)

FIGURE 15 **REAL-TIME THICKNESS OF InGaAs GROWN ON InP (derived from data of Figure 14)**

4.0 FUTURE RESEARCH PLANS

The Phase I effort has demonstrated the viability of MBE film deposition control under management of the Alpha and Beta control loops. In order to complete development of a fully automated deposition process, these two loops must be integrated into an MBE machine and interfaced through a Supervisor to work cooperatively. Beyond these original objectives, it will prove useful to incorporate additional supra-supervisory, self-directed control in the form of "Qualitative Process Automation" (QPA).

Specifically, the objectives of a Phase II effort would be:

i) achieve fully automated first generation QPA process control over semiconductor devices grown by molecular beam epitaxy; *

ii) beta test first generation QPA control system at the Air Force Electronics Laboratory and Sandia National Laboratory, both of which have indicated interest in incorporating the results of this program in their own film growth efforts;

iii) integrate complete WPML-developed QPA expert system for high-level supervisory capability, and transfer expanded capability to users of first generation QPA systems;

iv) develop a plan for commercialization and beta test the second generation QPA system to epi- toll manufacturers and integrated electronics companies.

The technical components of this proposed Phase II program divide conveniently into three research and development areas: process (state-driven) control, materials properties (goal-driven) control and QPA integration and supervision. Started under the current Phase I effort, the first two areas have now produced compelling evidence that completion of a Phase II effort will lead to a technical and commercial success.

The process control loop has been designed to achieve repeatability of the MBE process parameters. Initially, this development required the creation of a means for setting optimum conditions for the proportional/integral/derivative (PID) temperature controllers. That work was completed during the current Phase I effort, and appropriate control modules are now installed on the two MBE machines in the Materials Laboratory. In a Phase II effort, the Process Discovery Autotuner (PDA) required to automate this optimization process, would be interfaced with the PID

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* Since QPA also is a goal-driven control system, the goal-driven, real-time MBE control system, whose development was initiated under this Phase I effort, often is referred to as a "first generation QPA."

drivers. This PDA already has been successfully bench tested so that successful integration is virtually assured.

A second part of the process control loop relates to the Shutter Opening Transient Compensator. This control module is intended to eliminate beam flux transients, which result when shutters are opened, by providing prior compensation commands to the PID controllers. In a concept design version, this module also has been successfully bench tested using a preliminary compensation function. As reported above, experiments already have suggested that the compensation function might depend on other process parameters such as background fluxes and species. Their degree of influence would be assessed and, if necessary, accounted for in a modified function. Since these ancillary effects should influence the desired beam flux linearly, full shutter opening transient compensation is assured under a Phase II effort. This compensation method and the PID control method would be integrated in accordance with the plan outlined during the Phase I work.

Additional real-time control over the composition, thickness and properties of the growing film would be based on feedback to effusion cell heaters from processed ellipsometric measurements. An ellipsometer was installed on the VG-MBE machine during the current Phase I effort. Measurements were successfully made on films of Low Temperature-GaAs deposited on GaAs, and on InGaAs deposited on InP during their deposition. These data were successfully reinterpreted as inputs for generating appropriate control signals. During a Phase II effort, ellipsometry measurements and algorithms would be developed to include thickness and compositional control. The ellipsometry control scheme would be integrated into the complete MBE feedback control system. Since several of the control algorithms already have been successfully tested, completion of the feedback control software during Phase II presents a low risk.

Design of the overall control system was also completed as a part of the Phase I effort. As mentioned above, components of that design have already been incorporated into the in-house VG-MBE machine. As the number of control loops and options grow, this system will become increasingly complex. The Phase I design was modular so that individual control mechanisms could be introduced without disturbing those already in place. This integration approach will expedite continued development and enable the completion of a fully automated MBE deposition control system by the end of Phase II.

The product of a Phase II effort would be transferred to equipment manufacturers, device developers, and device manufacturers. The universality of the MBE control technology for these end users would be demonstrated both by the Electronics Laboratory at Wright-Patterson and by

Sandia National Laboratories. The Electronics Laboratory would provide important film recipes for control validation, and would be assisted by the Materials Laboratory in adapting the processing control system to two of their MBE machines. Sandia also would provide meaningful device recipes comprising film compositions, doping profiles and film thicknesses for a microwave waveguide divider. The prescribed films would be grown on the Materials Laboratory MBE machine. Sandia would fabricate devices from these films in order to verify the effectiveness of the integrated control system.

As the state- and goal-driven control loops are developed and integrated to produce a first generation QPA, a second generation QPA based on WPML's autoclave composite curing control system would be modified as needed and adapted to the MBE process to provide full QPA capability.* Data gathered and experience gained during this development, and data extracted from MBE machine health monitoring sensors would provide the inputs for the QPA expert system. The QPA would perform two functions. First, it would establish boundaries of the state space within which the first generation state- and goal-driven loops operate; i.e., it would establish the feedback response limits of these two loops. If the film thickness, for example, were to cross a boundary, neither of these loops would have the ability to assess either the significance or cause of that crossing. Therefore, feedback that would trigger an appropriate action would not occur. The QPA, on the other hand, would have been designed specifically to detect this boundary crossing and identify it as an "event" to which the QPA must respond. In this sense, the QPA system would have augmented the continuous sensor input and continuous control response of the first generation QPA feedback control loops with discrete inputs and responses. The input sent to the QPA would remain constant between events, and the QPA would respond only when an event occurs.

The second function the QPA would perform is determining, via an expert system, the appropriate response in case of an event. The QPA would emulate a human operator who would be aware of, in addition to the occurrence of an event, all other conditions, i.e. "health", of the MBE machine, available actions, and possible consequences, including secondary consequences. When completed, this full control capability would be demonstrated on two MBE machines in the Materials Laboratory and the Electronics Laboratory. Then, with the concurrence of the Materials Directorate, the QPA will be beta tested at and transferred to industrial users during a Phase II effort.

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* For an excellent review of this control philosophy see, LeClair, S., et al, "Qualitative Process Automation: Self-directed Manufacture Of Composite Materials," AI-EDAM 3, 125 (1989).

The future research outlined in this section relies heavily on the successes already obtained during the Phase I effort. These achievements virtually assure successful completion of a Phase II effort. Upon completion of that effort, a fully automated MBE deposition system will have been developed. It will be a system that approaches the ideal of providing an essential tool for the bandgap engineering of advanced electronic devices. In addition, the technology will have been developed in close cooperation with endusers. This will ensure a focus on practical and necessary electronic devices and materials, and will significantly expedite the wide dissemination of the critical control technology.

5.0 APPENDIX

PROGRESS IN BETA CONTROL LOOP DEVELOPMENT

TABLE OF CONTENTS

LIST OF FIGURES

SUMMARY

The refinement of the "MBE Control" program resident on a Macintosh IIfx microcomputer progressed in several facets toward the improvement of the Molecular Beam Epitaxy (MBE) process.

MBE flux stability was addressed beyond its controllability through temperature by a proportion-integral-derivative (PID) control-loop. Flux data analysis gave support to a hypothesis that some of the residual flux instability might be due to power supply harmonics or powerline disturbances driving long term Knudsen Cell thermal oscillations on the order ten minute periods and directly influencing flux stability. Preliminary tests have been run to quantify this hypothesis by improving the stability of the PID temperature controller and power supply that controls the energy input to the Knudsen Cell thermal control loop. The existing Eurotherm 825 PID temperature controller was compared with an upgraded Eurotherm Model 818, and the existing Eurotherm Model 831 phase-angle-fired Silicon-Controlled-Rectifier (SCR) was compared with a Sorensen Model 150-7 switching direct current (DC) power supply. The tests were conducted with the Indium Knudsen Cell on the Varian Gen II MBE system and show that the DC power supply can improve flux stability by 87% after the initial shutter opening transient. The improved 818 controller effects the flux stability by 75% with the SCR power supply. The 818-DC configuration shows the same 87% improvement as the 825-DC test, however, the inclusion of the 818 controller exhibits thermal compensation for the initial shutter opening transient for a 78% improvement of the overall flux stability.

Apple Computer's System 7 release and the corresponding "Think C" compiler upgrade to version 5 have been installed in the MBE development microcomputers for the expanded multi-tasking facilities and support for inter-application communication (IAC). Multi-tasking and IAC will allow the MBE instrument interfaces, the Process Discovery Autotuner, beam equivalent pressure calibration, MBE growth control, and other supervisory processes to be developed as

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separate programs that communicate with each other. Individual program development promises shorter design cycles and simpler program troubleshooting.

The simpler program troubleshooting extends from a consistent program design that involves four basic program blocks. An "Initialization" block that performs basic program start-up initialization of internal data structures, peripheral communication channels, and building the program's unique user interface. The "User Interface" block handles user input events for direct user control and observation of the program's operation. The "Inter-Application-Communication" (IAC) block handles the transmission of data and commands to-and-from all of the other multi-tasking programs in the MBE control system. The "Execution" block is the unique function of the particular program that depends on the initialization, user commands, and IAC data from other programs to perform its designed task. The grouping of program function into defined blocks allows reusability of general program functions; such as the IAC block which contains generic code to post and accept IAC transmissions. The basic structure of the user interface block would interpret user interface events and pass the information in these events to specialized routines for a particular program.

This modular approach in the development of the MBE control system provides a protected environment for each program's unique and often complex data structures, and also provides a consistent data communication channel to any other programs required for data inter-action in the multi-tasking MBE control environment. A program would be developed and debugged as a stand-alone program using simulated data to represent the external multi-tasking environment. When the program is installed as a functional unit of the MBE control system, a graphical window in its user interface would provide operator control to switch off the simulated data used for debugging and establish the connections needed for data exchange with other programs. The IAC connections between the various program modules are very flexible to allow making, breaking, and re-establishing data links with any combination of programs with as many as 128 simultaneous data links. This modular design through IAC data linking allows new or enhanced program modules to be incorporated into the MBE system as simple as loading the program and establishing

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the links. These links can provide a program's unique data to other programs within 1.5 milli-seconds, and if a program requires another program to reply to a special request, the reply is available in 30 milli-seconds on a Macintosh IIfx. Specific data flow through the system achieves better organization during special sequences of the MBE operation, such as during set-up, tuning, calibration, or growth, by having non-involved program modules idle. A more advanced sequence could have a supervisor program switch non-involved program modules off and re-start them when they are needed.

INTRODUCTION

The ''MBE Control'' program originated as a 'C' language computer program implemented on a Macintosh IIfx microcomputer and controlling a Varian MBE machine. The IIfx microcomputer replaced a DEC pdp11 minicomputer which suffered major damage during a storm induced power transient. The Macintosh IIfx microcomputer provided a cost effective and expedient replacement for the MBE computer control system. It also afforded an improved operator interface with extensive graphics capacity and access to the MBE control system program source code for research and development utilization not available with the DEC pdp11. The MBE control program has evolved into a control system using several interacting program modules in a multi-tasking environment on the Macintosh IIfx using Apple Computer's System 7 software and is currently operating on a second Vacuum Generator MBE machine.

Flux stability during the MBE growth process was the focus of research that led to the development of the "MBE Control" program which incorporates the Process Discovery Autotuner, Beam Equivalent Pressure calibration, flux compensation experiments, data logging, and other MBE set-up and growth functions. The relationship between flux and the multiple MBE Knudsen Cell temperatures required concentration on stabilizing the temperature of the Knudsen Cells. The volume of information needed to simultaneously stabilize all of these temperature control loops required computer automation of the process knowledge acquisition and utilization of this knowledge for optimum temperature control of the Knudsen Cells. The need for system customization, porting the system to new machines, and the ability to "drop-in" new instrument and sensor interfaces led to the implementation of modular programs and inter-application-communication.

METHODS AND PROCEDURES

Control refinement of the Molecular Beam Epitaxy process was effected by evaluation and action on the operational characteristics of the MBE machine and the MBE control system combination.

- Flux stability tests indicate disturbances beyond present PID control capability. The disturbance entry could be through the control-loop power supply which might be confirmed with substitution of an improved PID controller or power supply.

- Development lead time for new inclusions to the "MBE Control" program is absorbed by weaving software updates of several programmers into a single program. Inter-application communication among several independently developed and debugged programs offers to improve utilization of program development time.

- Recent data format developments are encumbered by the original flat data structure thereby requiring a flexible structure capable of handling complex data formats. Dissemination of the original flat data structure into specialized data structures within individual program modules would simplify data utilization.

- Data logging is increasingly important to accelerate machine control evaluation, but is hindered by in-complete data logging and excessive storage requirements. Complete data logging will need to be merged with real-time data compression.

RESULTS AND DISCUSSION

MBE flux stability was addressed beyond its controllability through temperature by the currently installed Eurotherm 825 proportion-integral-derivative (PID) control-loops with Eurotherm 831power supplies. Flux data analysis gave support to a hypothesis that some of the residual flux instability might also be due to power supply harmonics or powerline disturbances driving long term Knudsen Cell thermal oscillations on the order ten minute periods and directly influencing flux stability. Preliminary tests have been run to quantify this hypothesis by improving the stability of the PID temperature controller and power supply that controls the energy input to the Knudsen Cell thermal control loop. The existing Eurotherm 825 PID temperature controller was compared with an upgraded Eurotherm Model 818, and the existing Eurotherm Model 831 phase-angle-fired Silicon-Controlled-Rectifier (SCR) was compared with a Sorensen Model 150-7 switching direct current (DC) power supply. The tests were conducted with the Indium Knudsen Cell on the Varian Gen II MBE system. Figure 1 shows the 825-SCR configuration and a general lack of flux control with temperature deviation of ±0.5 °C and an overall flux deviation of 7e-9 Torr with more than 4e-9 Torr flux deviation after a shutter opening transient of 200 seconds. Figure 2 uses the DC power supply and shows the same ±0.5°C temperature deviation, overall flux deviation of only 1.5e-9 Torr, and less than 5e-10 Torr flux deviation after a 100 second transient. Figure 3 shows the 818-SCR configuration with a temperature deviation of ±0.1°C and a flux deviation of 1e-9 Torr after a 200 second transient. The overall flux deviation with shutter opening transient was 1.5e-9 Torr. Figure 4 is the 818-DC configuration with a temperature deviation less than ±0.1°C, an overall flux transient of 1e-9 Torr, and a flux deviation of 5e-10 Torr after a 100 second transient. Comparison of Figures 1-4 show that the DC power supply can improve flux stability by 87% after the initial shutter opening transient dies out. The improved Eurotherm 818 controller effects the flux stability by 75% while using the SCR power supply. The 818-DC configuration shows the same 87% improvement as the 825-DC test, however, the inclusion of the 818 controller exhibits thermal compensation for the initial shutter opening transient for a 78% improvement of the overall flux stability.
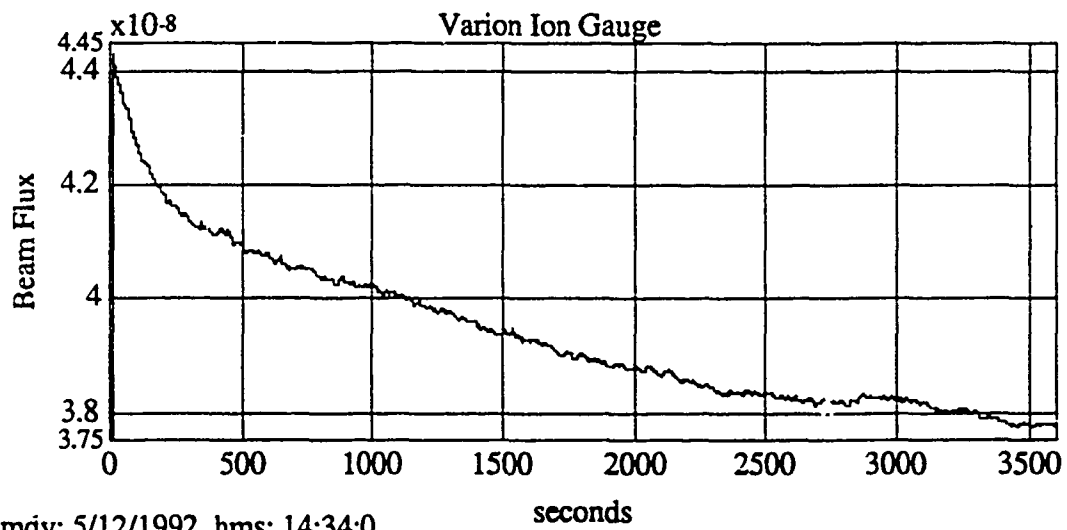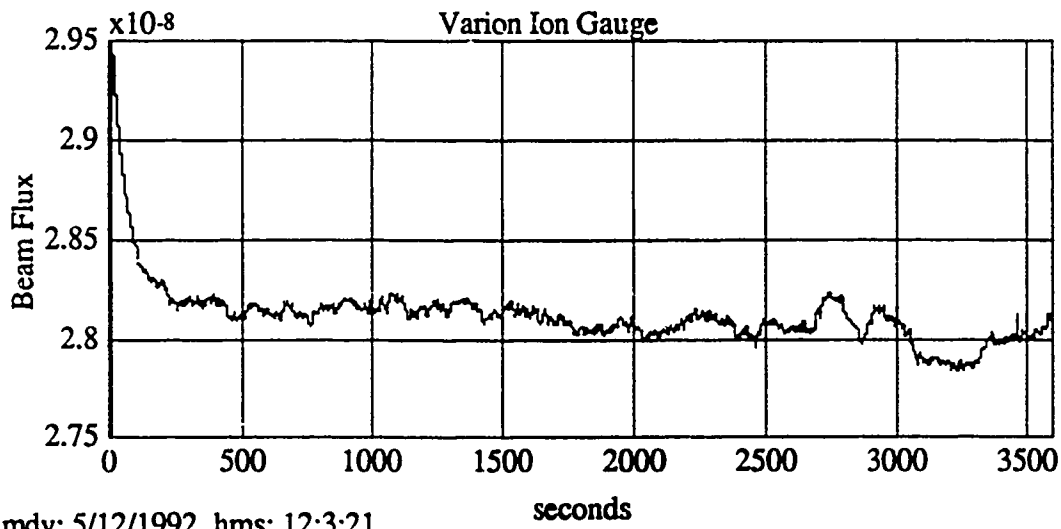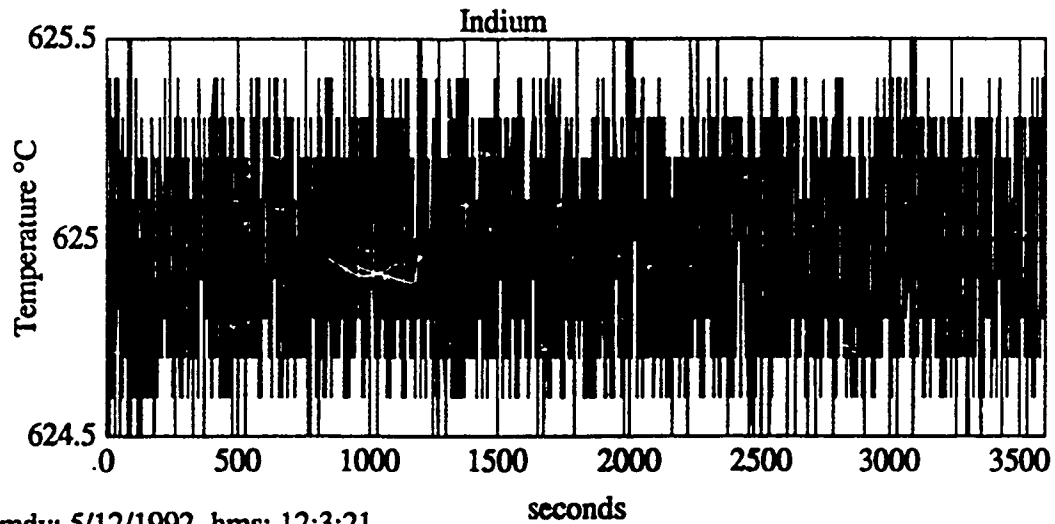
mdy: 5/12/1992, hms: 14:34:0
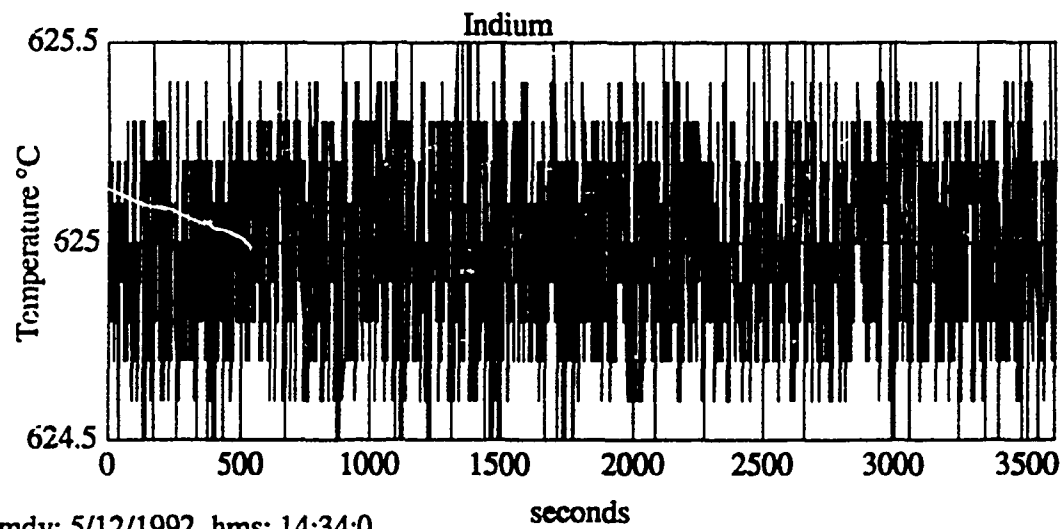
mdy: 5/12/1992, hms: 14:34:0

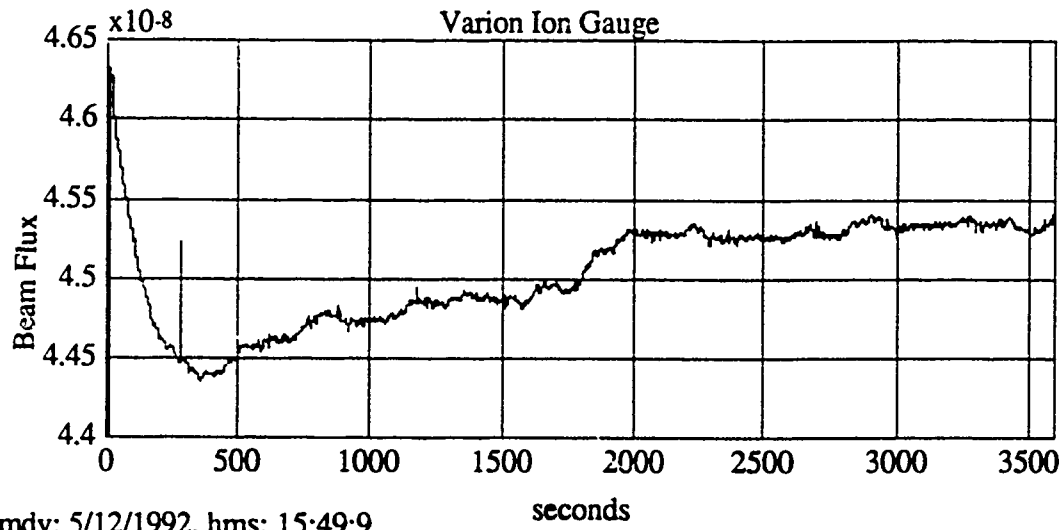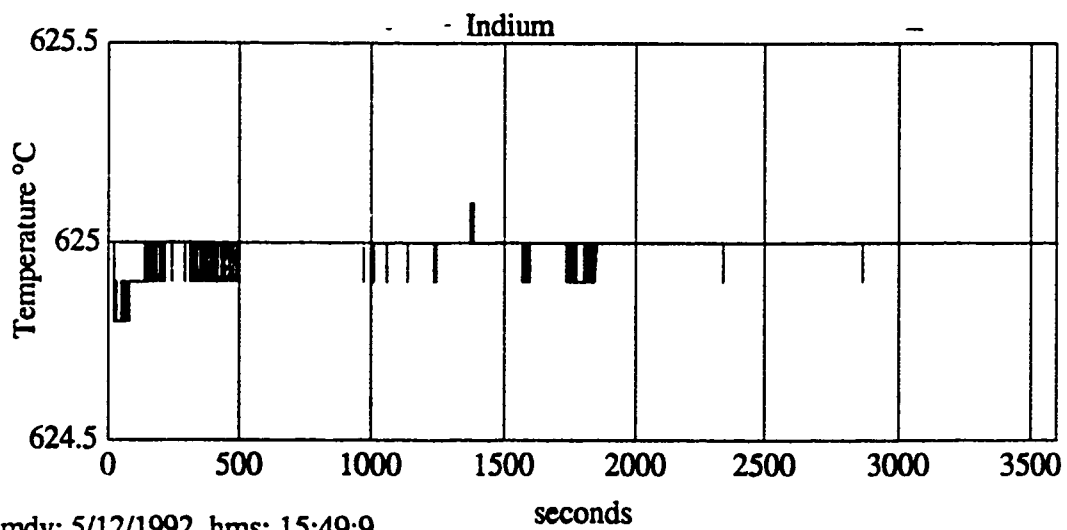**FIGURE 1. Indium with Eurotherm 825 and SCR Heater Supply**

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Varion Ion Gauge

mdy: 5/12/1992, hms: 12:3:21

Indium

mdy: 5/12/1992, hms: 12:3:21

FIGURE 2. Indium with Eurotherm 825 and DC Heater Supply

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Varion Ion Gauge

mdy: 5/12/1992, hms: 15:49:9

Indium

mdy: 5/12/1992, hms: 15:49:9
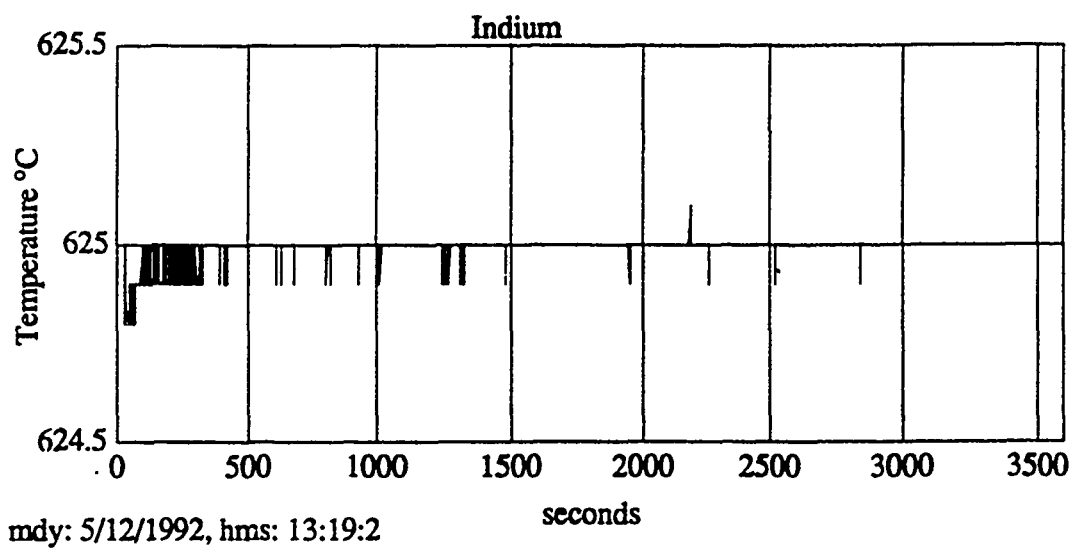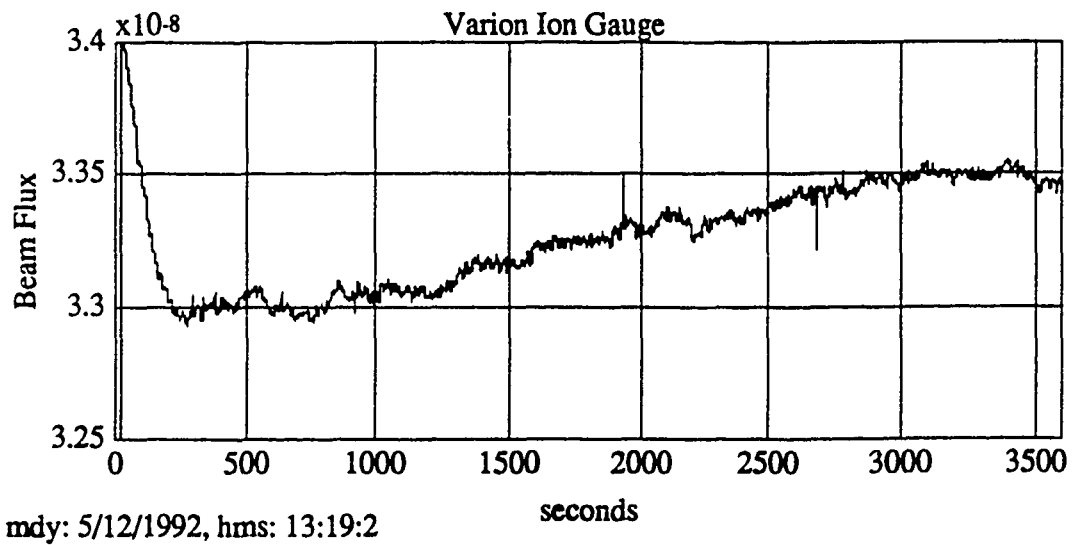
FIGURE 3. Indium with Eurotherm 818 and SCR Heater Supply

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Varion Ion Gauge

mdy: 5/12/1992, hms: 13:19:2

Indium

mdy: 5/12/1992, hms: 13:19:2

FIGURE 4. Indium with Eurotherm 818 and DC Heater Supply

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Apple Computer's System 7 release and the corresponding "Think C" compiler upgrade to version 5 have been installed in the MBE development microcomputers for the expanded multi-tasking facilities and support for inter-application communication (IAC). Multi-tasking and IAC will allow the MBE instrument interfaces, the Process Discovery Autotuner, beam equivalent pressure calibration, MBE growth control, and other supervisory processes to be developed as separate programs that communicate with each other. Individual program development offers shorter design cycles and simpler program troubleshooting. Additionally, IAC functions are accessed similar to the data interchange within the original "MBE Control" program.

Five program modules are presented in the following flowcharts to illustrate the similar components within each program that are essentially reusable code modules. The reused code modules are mainly the blocks that handle user interface events and IAC events, and to a lesser extent, the program initialization block. The internal data structure of each program provides efficient non-volatile storage of program cont : pre-sets, indexed referencing of data elements, and data element referencing by unique names. Operator and programmer interface windows are provided for efficient management of unique program control pre-sets.

The first program presented in Figure 5 through Figure 12 is the Plotter-Recorder which handles data plotting in strip-chart-like windows on the computer display. This program also performs full-time data logging with data compression. Figure 5 shows the basic functional blocks to initialize the program, manage a dedicated internal time-base, handle user interface events, handle IAC events, manage updates to the plotting windows and finally to manage the full-time compressed data log. Figure 6 expands the initialization block to show its component tasks with a unique assignment to launch other designated programs as a supervisory program. Figures 7 through 12 are similar expansions of Figure 5 to show the internal program logic.
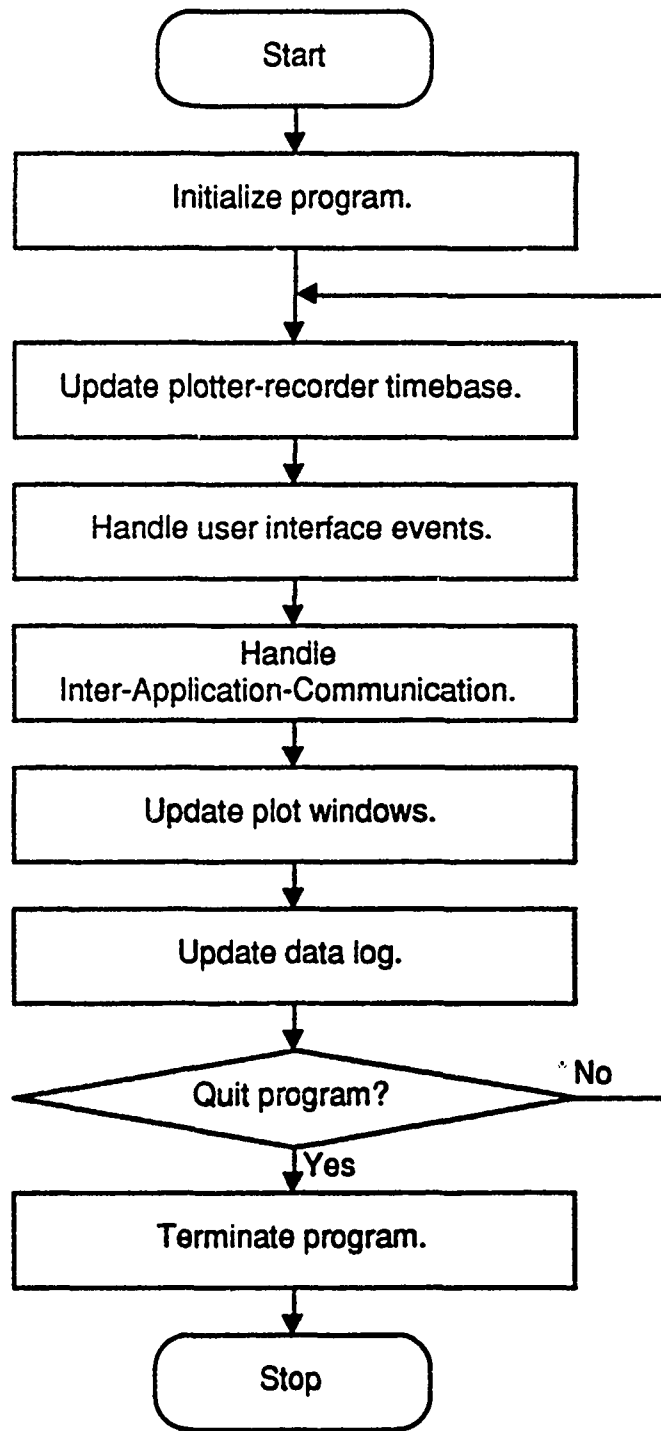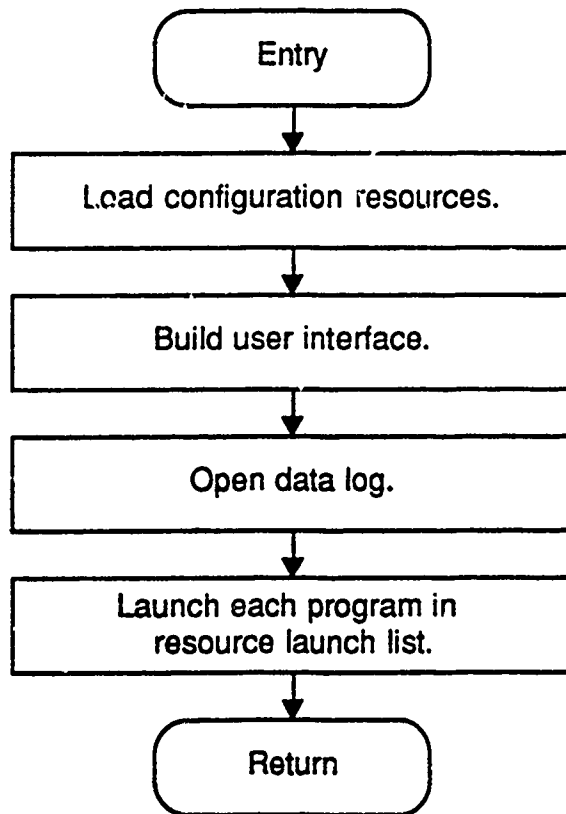
FIGURE 5. Plotter-Recorder Main Program Loop.

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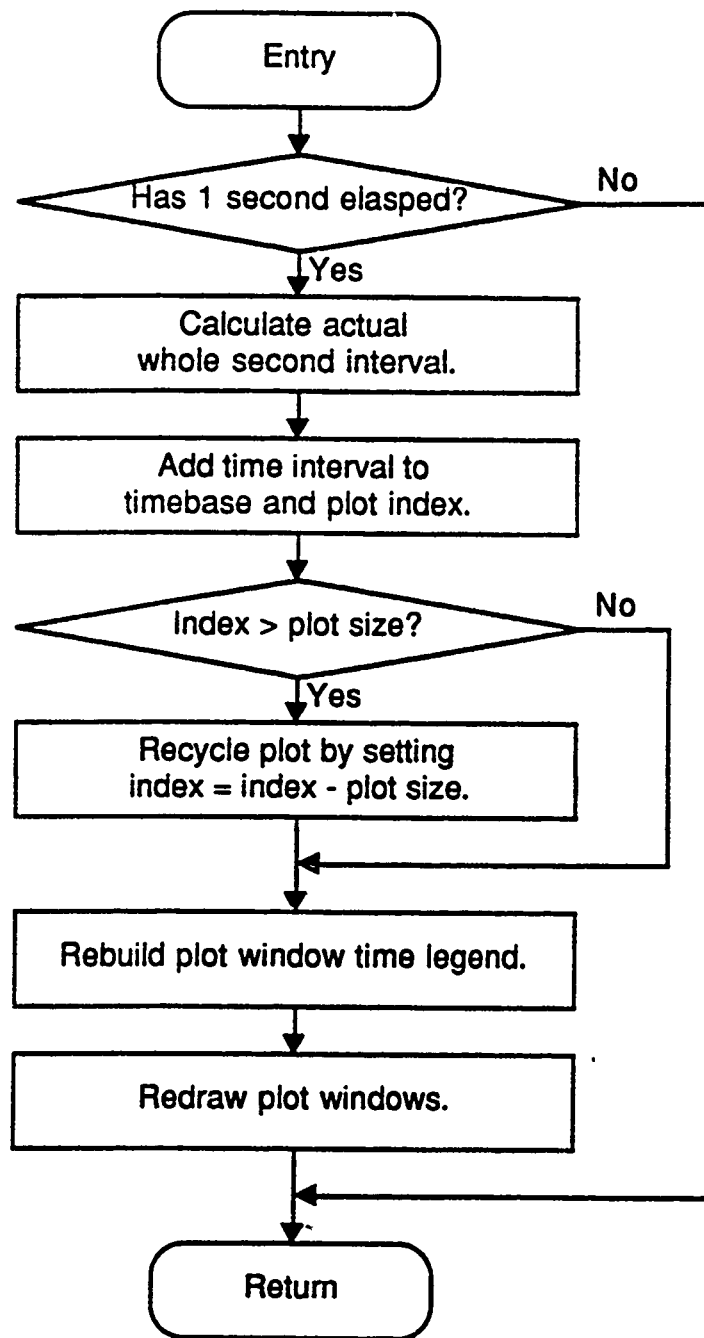**FIGURE 6. Plotter-Recorder Initialization.**

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FIGURE 7. Update Plotter-Recorder Timebase.
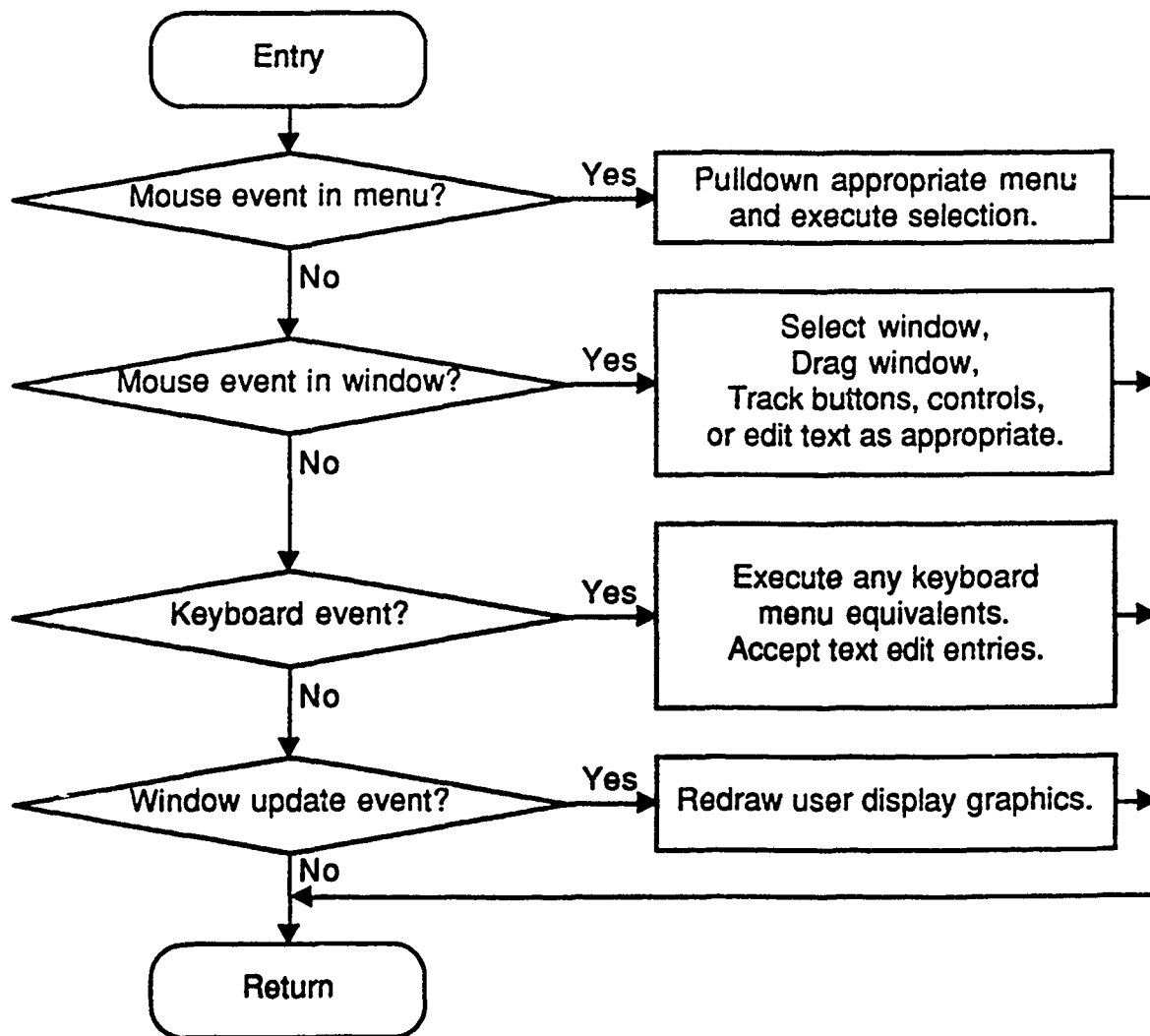
```
                    ┌──────────────┐
                    │    Entry     │
                    └──────┬───────┘
                           │
                           ▼
                        ╱─────╲                    ┌─────────────────────────┐
                      ╱ Mouse event ╲    Yes        │ Pulldown appropriate menu│
                      ╲ in menu?    ╱──────────────▶│ and execute selection.  │
                        ╲─────╱                     └─────────────────────────┘
                           │ No
                           ▼
                        ╱─────╲                    ┌─────────────────────────┐
                      ╱ Mouse event ╲    Yes        │      Select window,     │
                      ╲ in window?  ╱──────────────▶│      Drag window,       │
                        ╲─────╱                     │   Track buttons, controls,│
                           │ No                     │ or edit text as appropriate.│
                           ▼                        └─────────────────────────┘
                        ╱─────╲                    ┌─────────────────────────┐
                      ╱ Keyboard    ╲    Yes        │   Execute any keyboard  │
                      ╲ event?      ╱──────────────▶│   menu equivalents.     │
                        ╲─────╱                     │  Accept text edit entries.│
                           │ No                     └─────────────────────────┘
                           ▼
                        ╱─────╲                    ┌─────────────────────────┐
                      ╱ Window update ╲  Yes        │ Redraw user display graphics.│
                      ╲ event?      ╱──────────────▶│                         │
                        ╲─────╱                     └─────────────────────────┘
                           │ No
                           ▼
                    ┌──────────────┐
                    │    Return    │
                    └──────────────┘
```

FIGURE 8. Handle User Interface Events.

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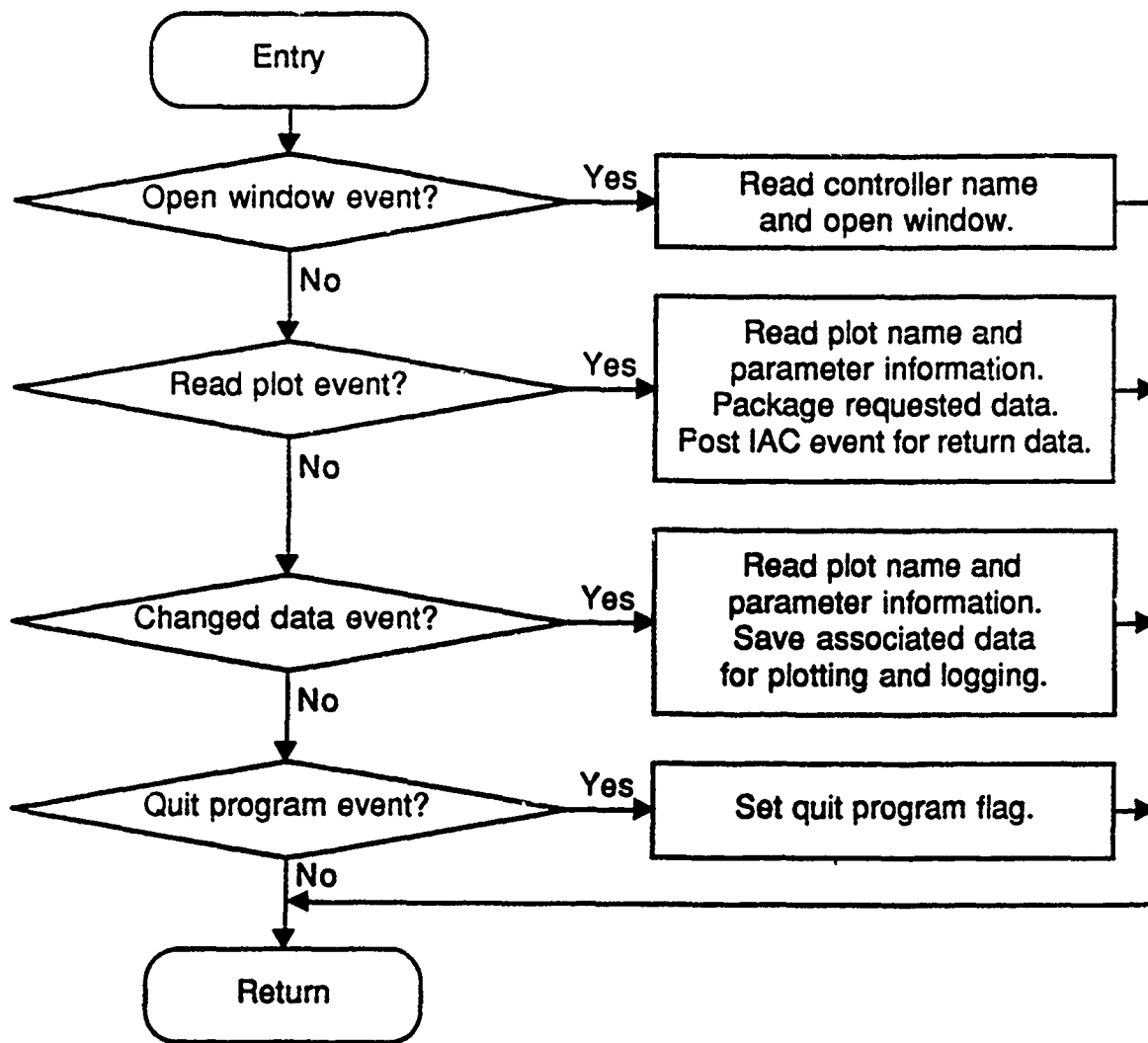
FIGURE 9. Handle Inter-Application-Communication.
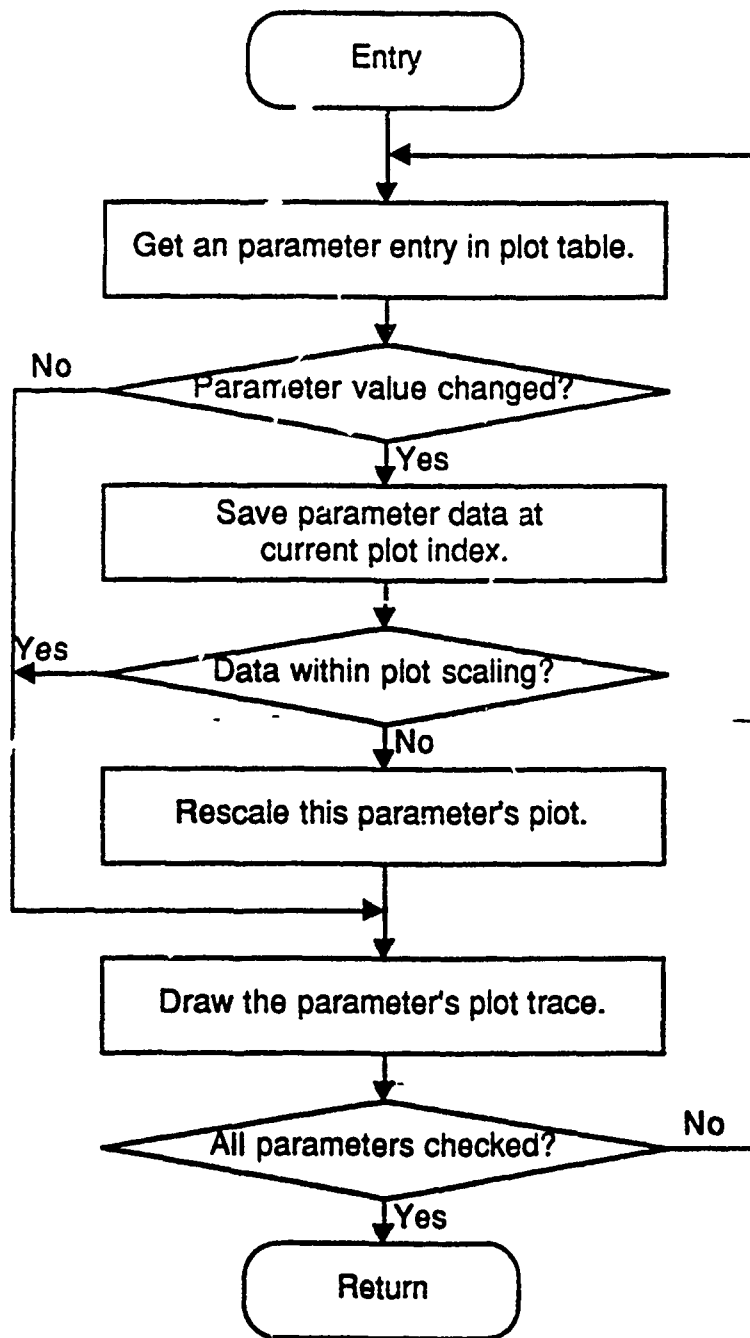
FIGURE 10. Update Plot Windows.
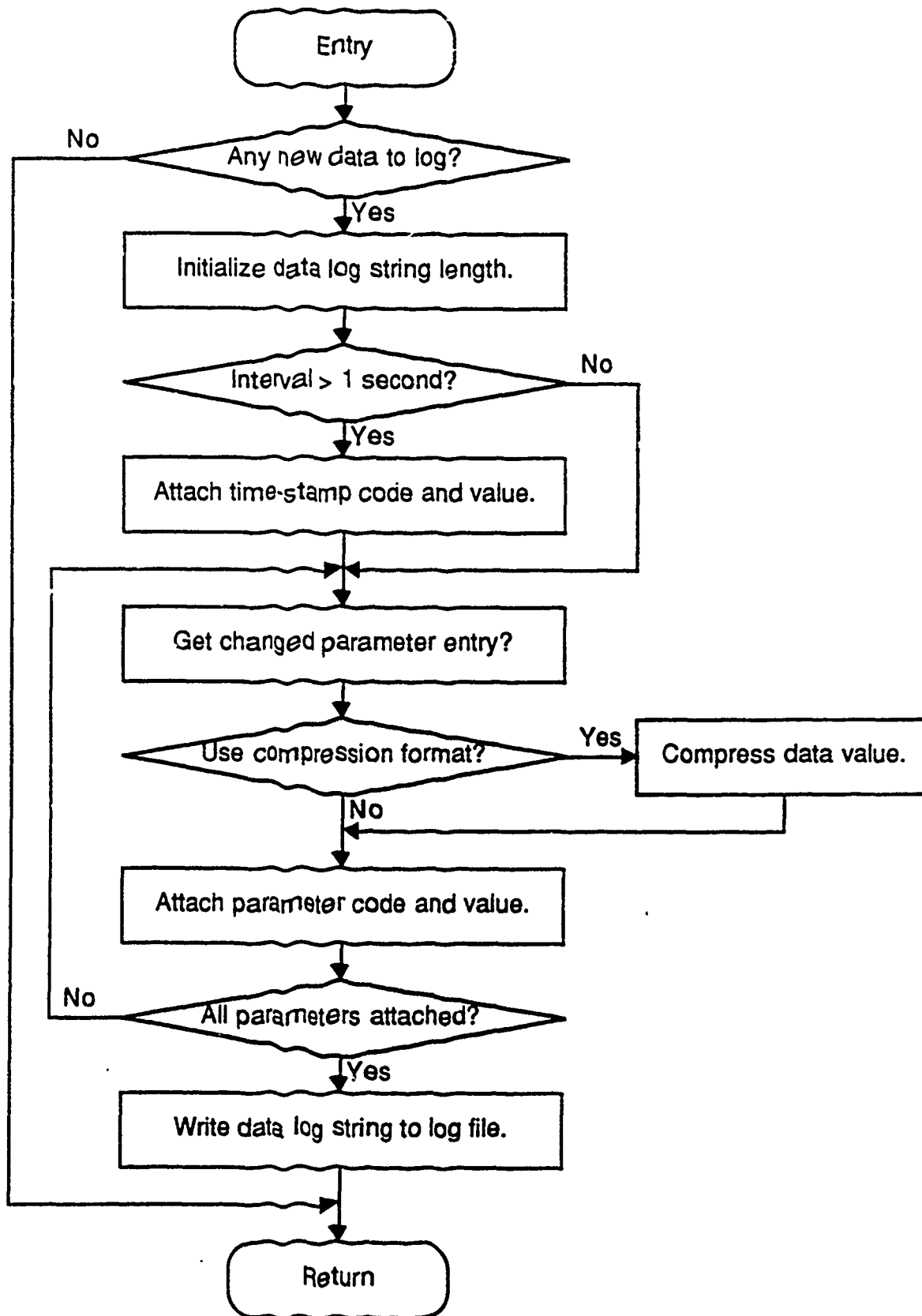
FIGURE 11. Update Data Log.

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```
          ╭─────────────╮
          │    Entry    │
          ╰──────┬──────╯
                 │
                 ▼
   ┌─────────────────────────────┐
   │     Close all plot windows. │
   └──────────────┬──────────────┘
                  │
                  ▼
   ┌─────────────────────────────┐
   │       Close data log.       │
   └──────────────┬──────────────┘
                  │
                  ▼
   ┌─────────────────────────────┐
   │ Send IAC 'quit' to each program │
   │   in resource launch list.  │
   └──────────────┬──────────────┘
                  │
                  ▼
   ┌─────────────────────────────┐
   │ Monitor operating system until all │
   │   programs actually quit.   │
   └──────────────┬──────────────┘
                  │
                  ▼
          ╭─────────────╮
          │    Return   │
          ╰─────────────╯
```
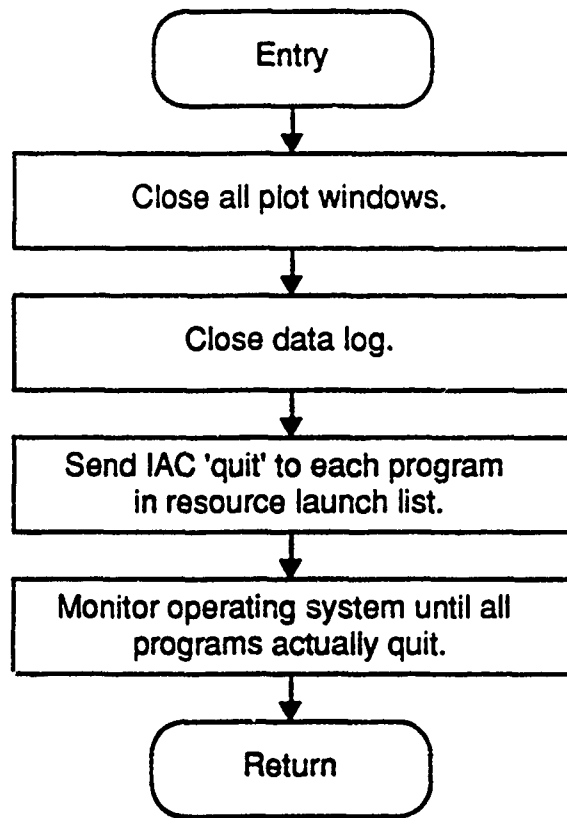
FIGURE 12. Plotter-Recorder Termination.

The second program is the Eurotherm controller interface program module shown in Figure 13. It follows the same programmatic format as the Plotter-Recorder program with initialization and then continual looping through User Interface and IAC event handling along with the unique functions of the program. Figure 13 shows the basic functional blocks to initialize the program, monitor in-coming serial data communications from the peripheral instrument channels, handle user interface events, handle IAC events, and issue new data commands to the peripheral Eurotherm instruments as requested through the user interface or through IAC events. Comparison of Figure 6 and Figure 14 shows the similarity of the program initialization routines with the exception of the program launch provision in Figure 6. Figure 18 handles the user interface and Figure 19 handles IAC events. They are virtually the same as Figures 8 and 9 which supports the concept of reusable code from earlier program developments.

The functionality of this program module as a communication interface with the peripheral Eurotherm PID controller instruments is shown in Figures 15, 16, and 17 for in-coming data communications. Figures 20, 21, and 22 illustrate the command encoding required to send instructions to the Eurotherm PID controller instruments. These six Figures 15-17 and 20-22 represent the unique functionality of the Eurotherm program module while the other Figures 13, 14, 18, and 19 are the general purpose elements of the program that set up its basic program components and simplify program development.
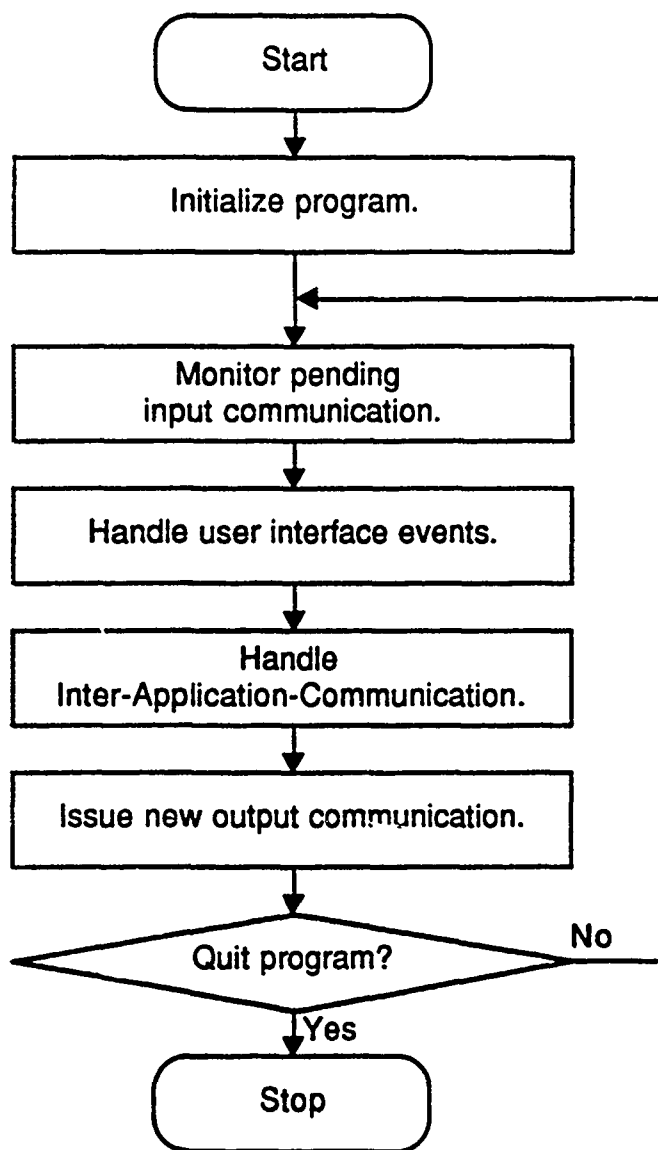
FIGURE 13. Eurotherm Main Program Loop.
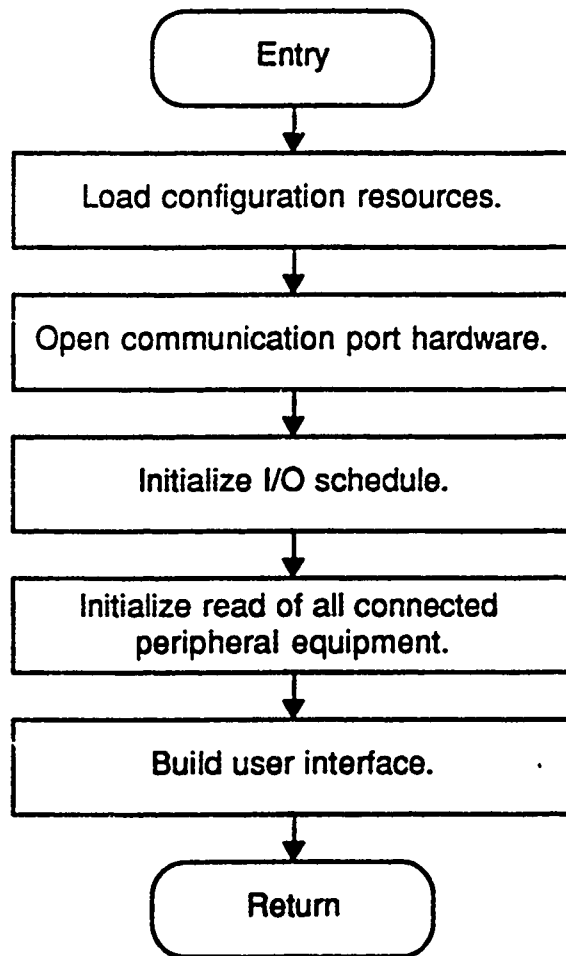
FIGURE 14. Eurotherm Initialization.

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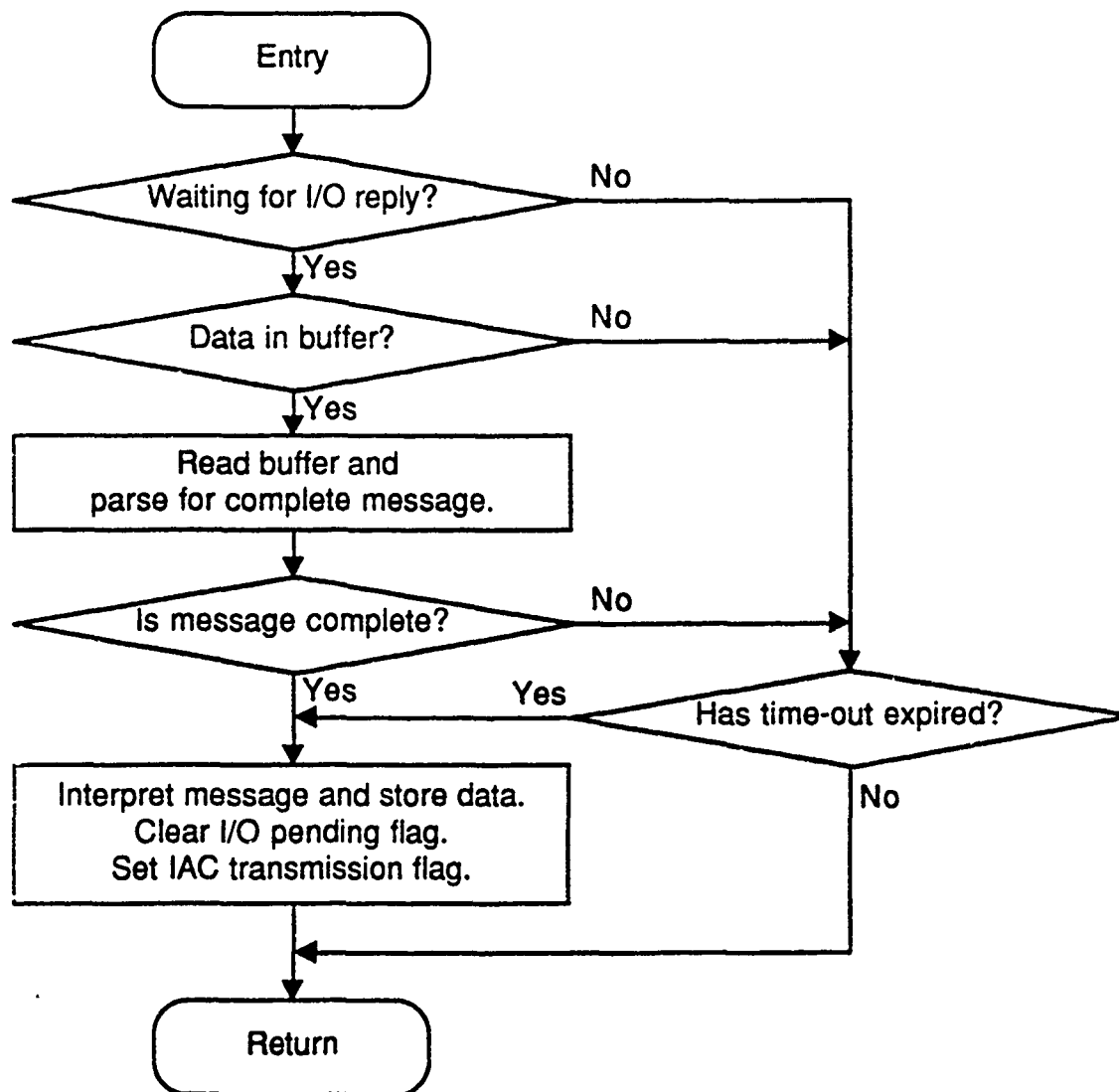
FIGURE 15. Monitor Pending Input Communication.

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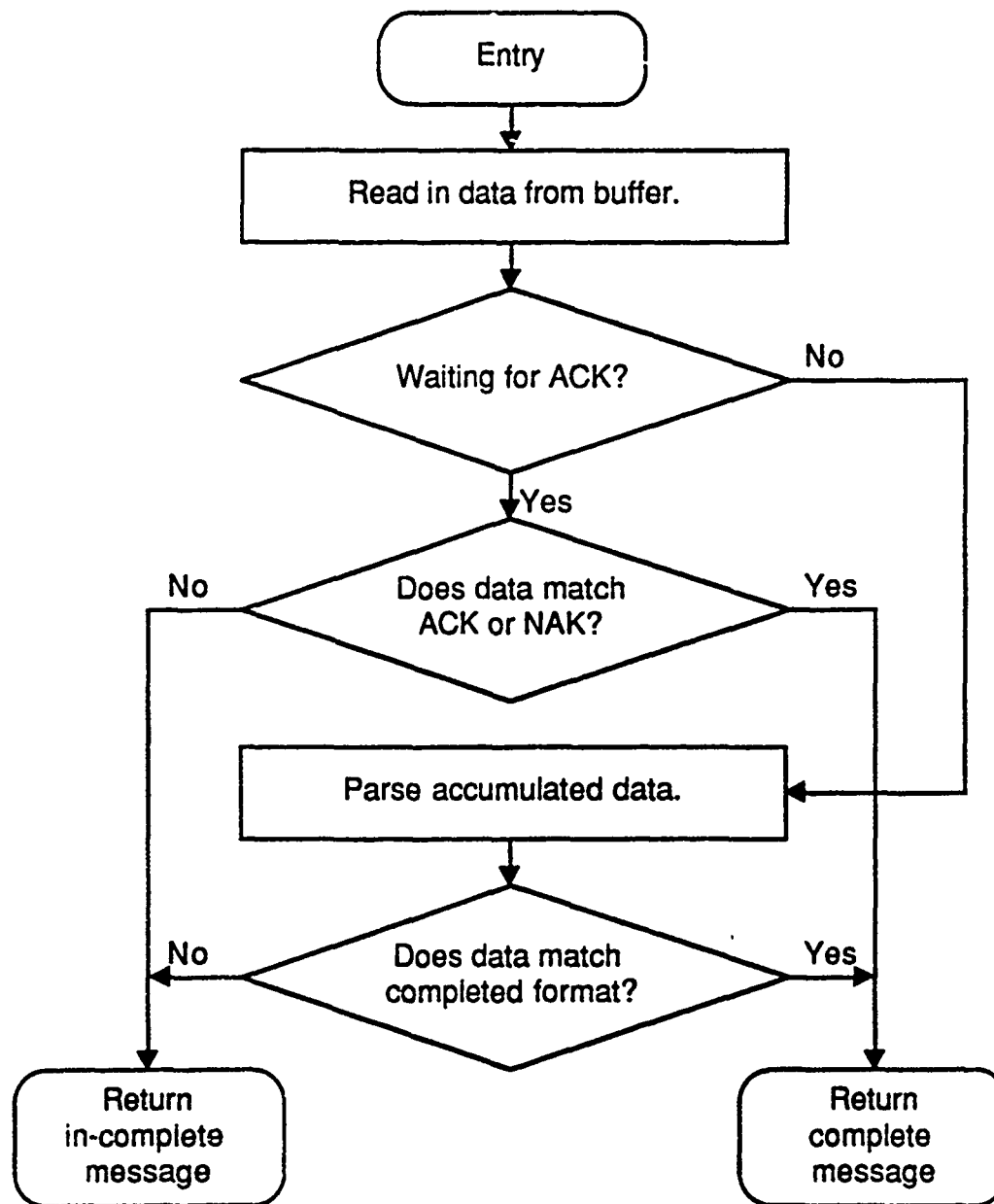
FIGURE 16. Read and Parse for Complete Message.
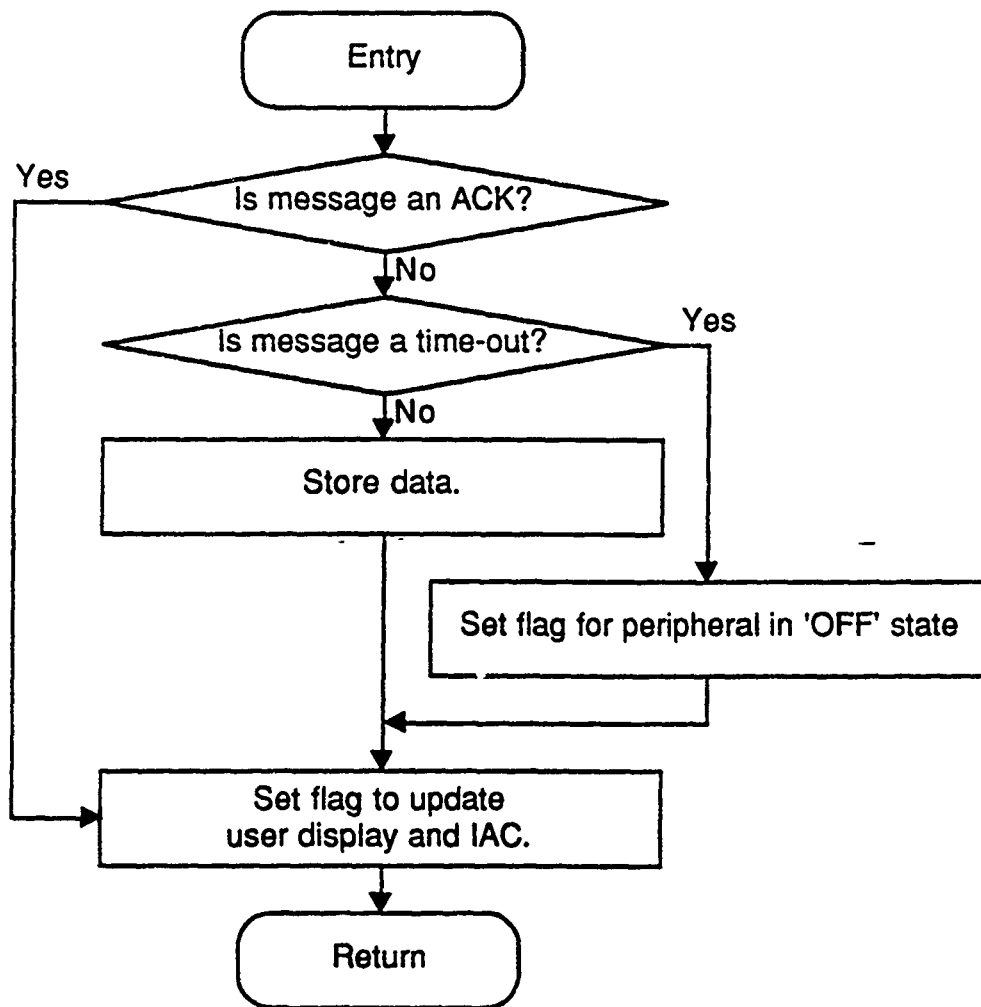
FIGURE 17. Interpret and Store Message.

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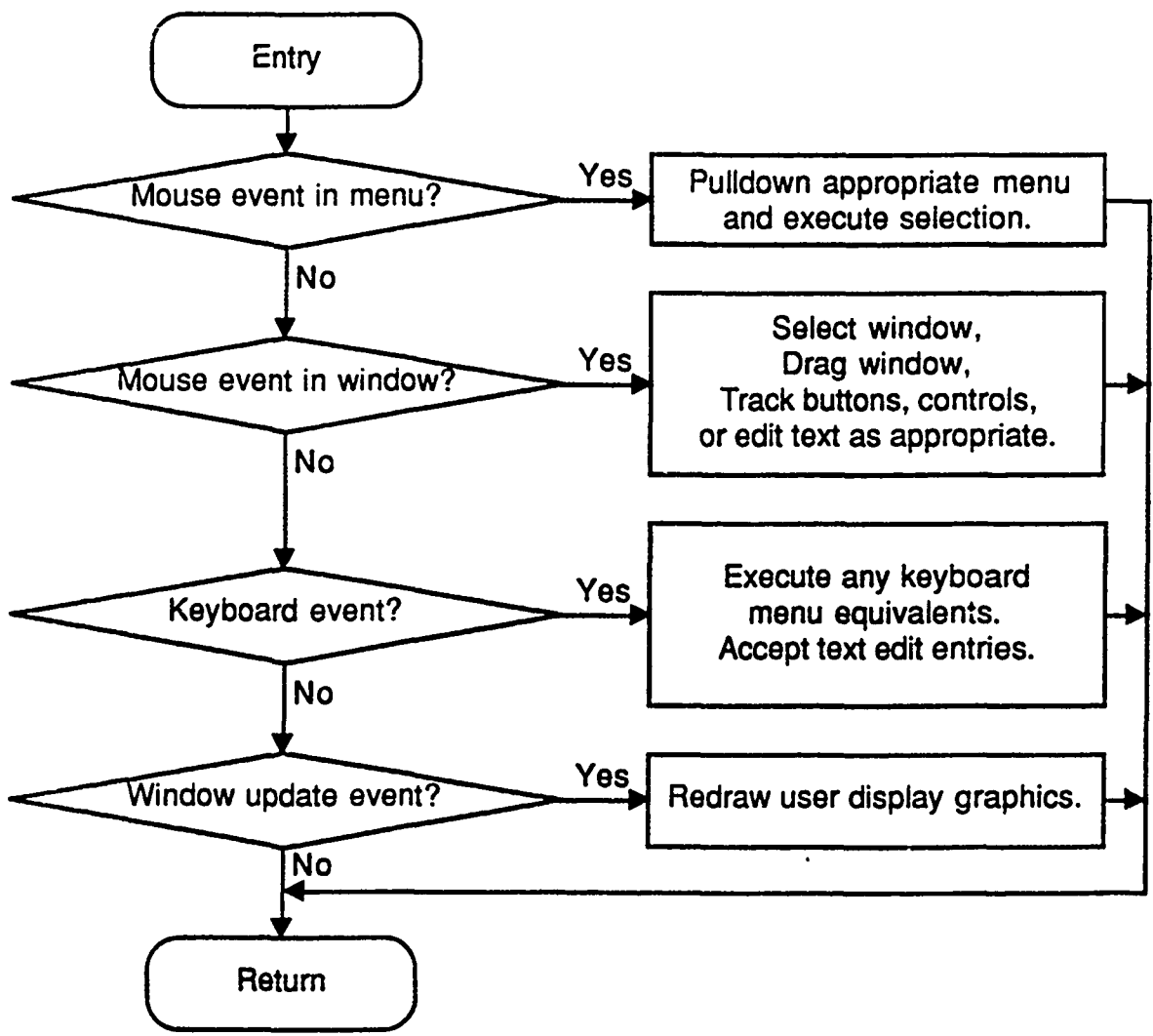
FIGURE 18. Handle User Interface Events.
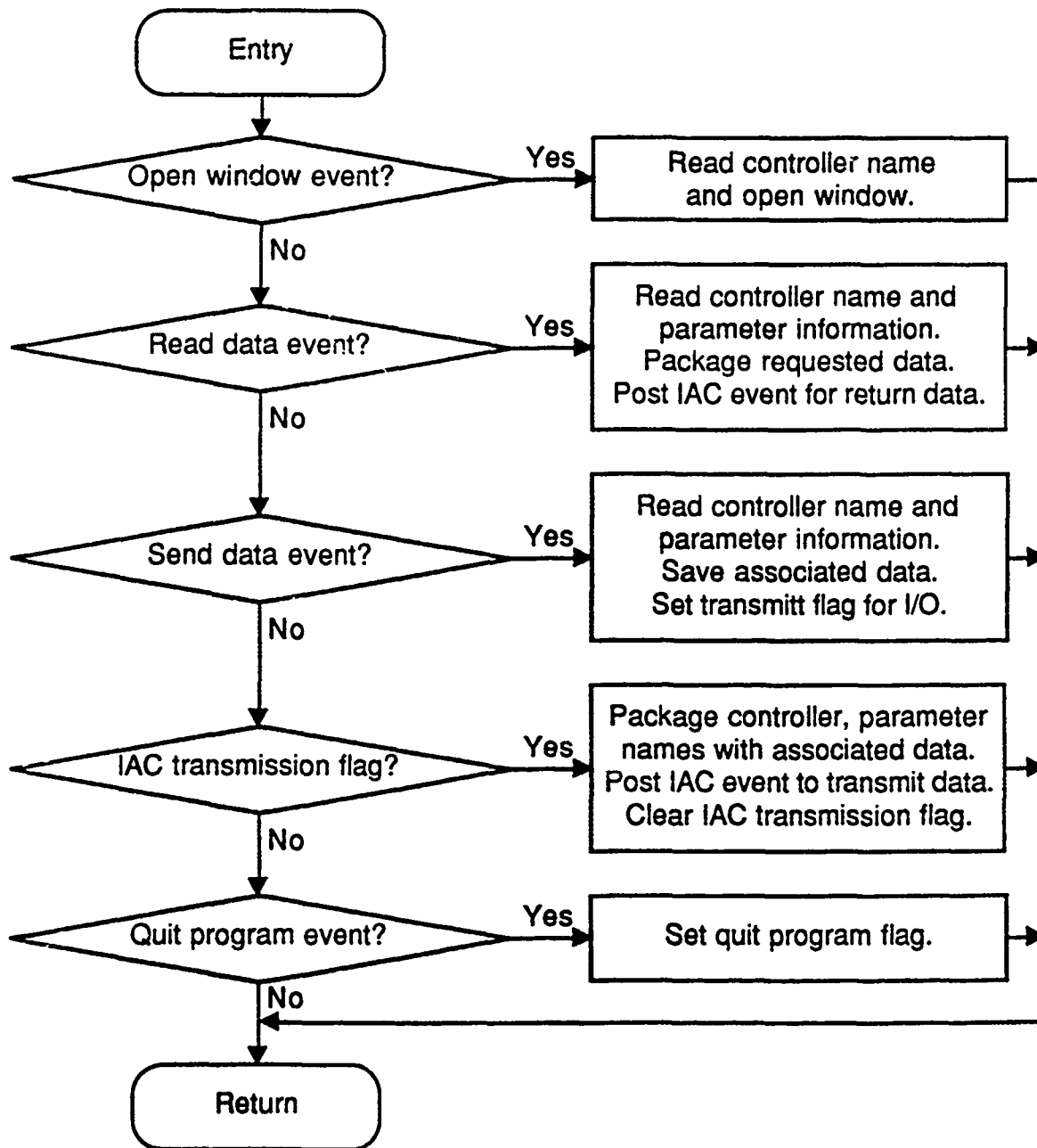
FIGURE 19. Handle Inter-Application-Communication.
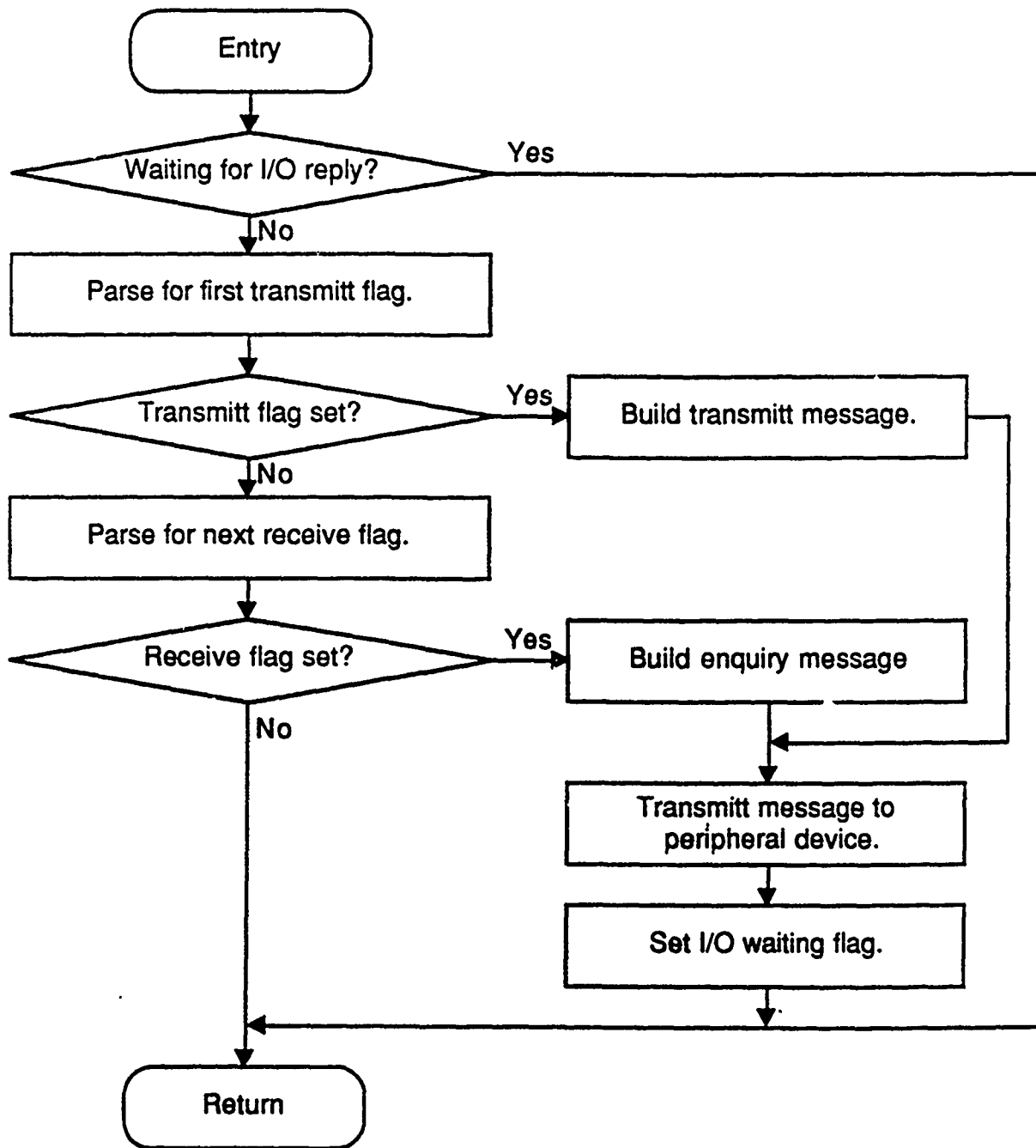
FIGURE 20. Issue New Output Communication.

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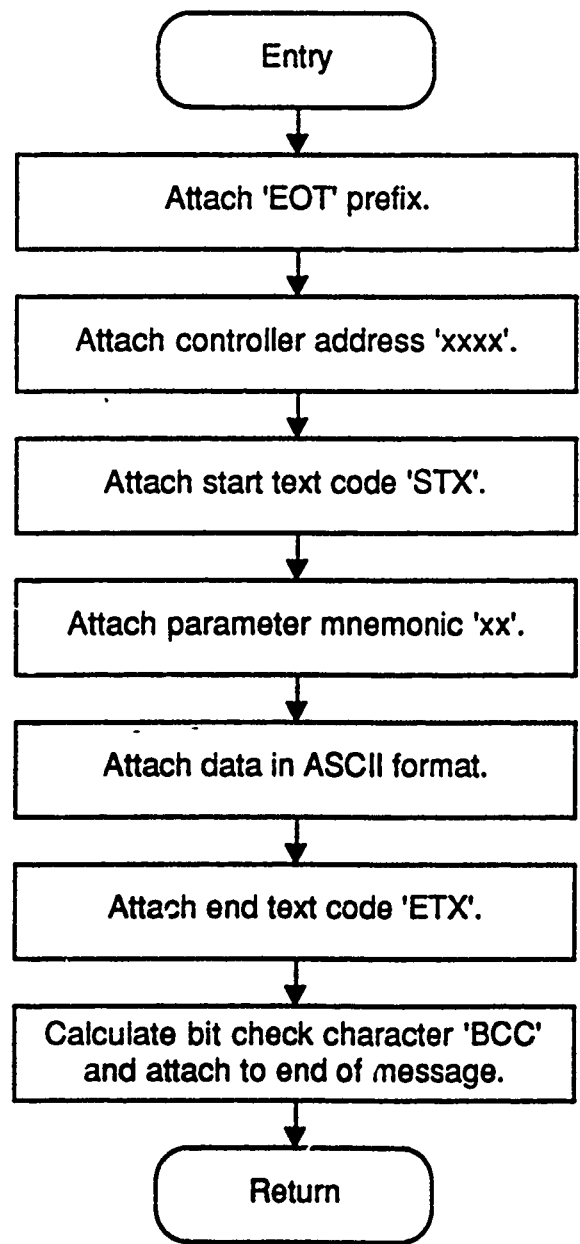
FIGURE 21. Build Transmit Message.
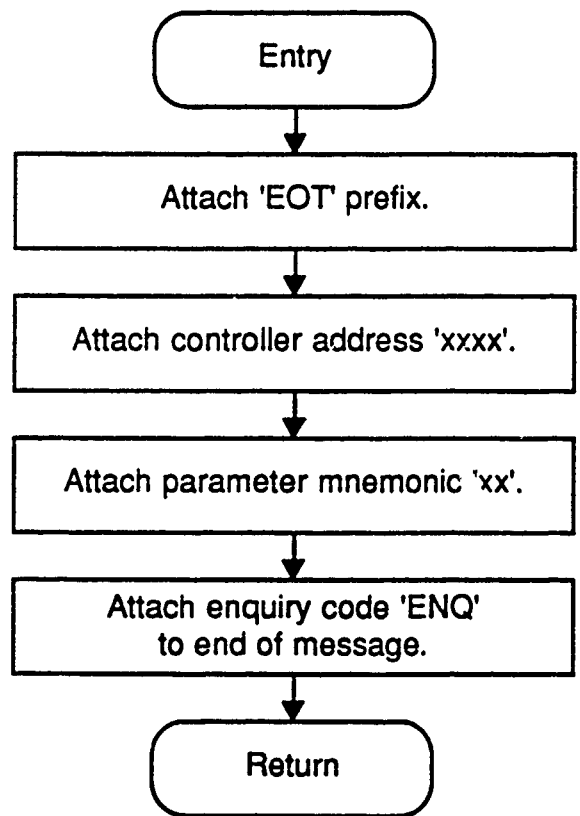
FIGURE 22. Build Enquiry Message.

The third program is the ShutterControl interface program module shown in Figure 23. It follows the same programmatic format as the Eurotherm program with initialization and then continual looping through User Interface and IAC event handling along with the unique functions of the program. Figure 13 shows the basic functional blocks to initialize the program, monitor the parallel data input interface for shutter feed-back sensors and cryo-shroud sensors, handle user interface events, handle IAC events, and write new state values to the parallel output shutter interface as requested through the user interface or through IAC events. Comparison of Figure 14 and Figure 24 shows the similarity of the program initialization routines for peripheral instrumentation program modules. Figure 26 handles the user interface and Figure 27 handles IAC events. As with the Eurotherm program, they are virtually the same as Figures 8 and 9 which supports the concept of reusable code from earlier program developments.

The functionality of this program module as a parallel input interface with the shutter feed-back sensors and the cryo-shroud sensors is shown in Figure 25. The sophistication in this interface is that it continually compares the current input channel reading with the previous reading and issues an input event for the user interface and IAC only when an input change has occurred. Figure 28 follows a simple procedure to respond to transmit command flags set up by either the user interface or IAC. Its sets the appropriate output channel signals to the commanded states and clears the transmit flag to prevent continual transmission. Figures 25 and 28 represent the unique functionality of the ShutterControl program module while the other Figures 23, 24, 26, and 27 are the general purpose elements of the program that set up its basic program components and simplify program development in a manner similar to the Eurotherm control program module.

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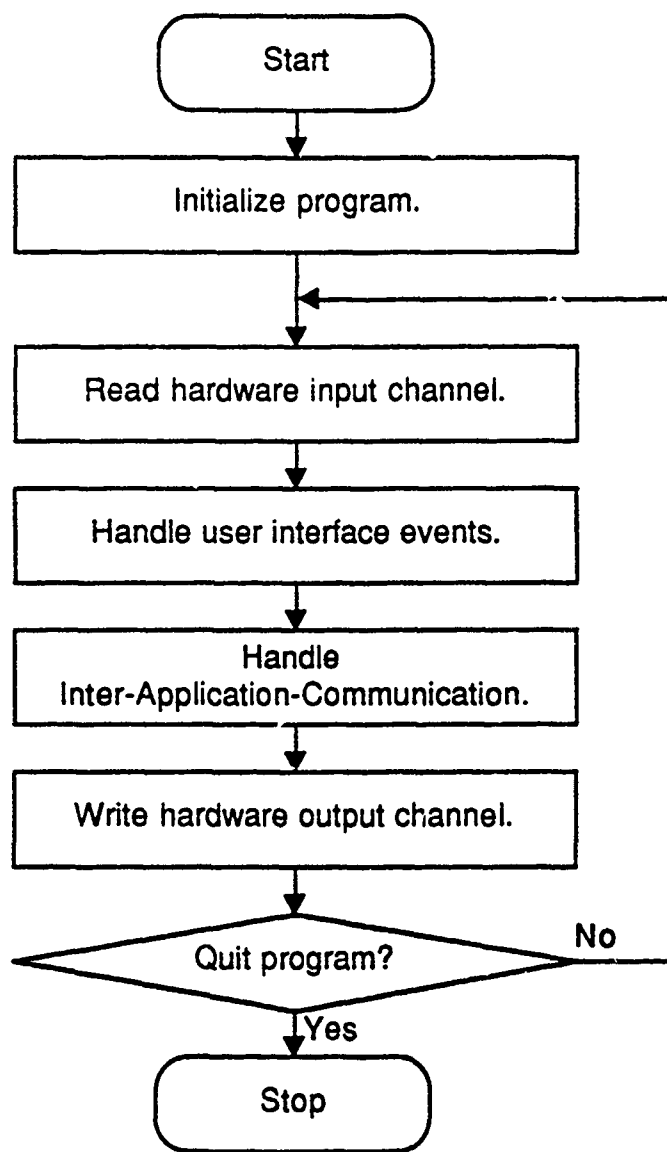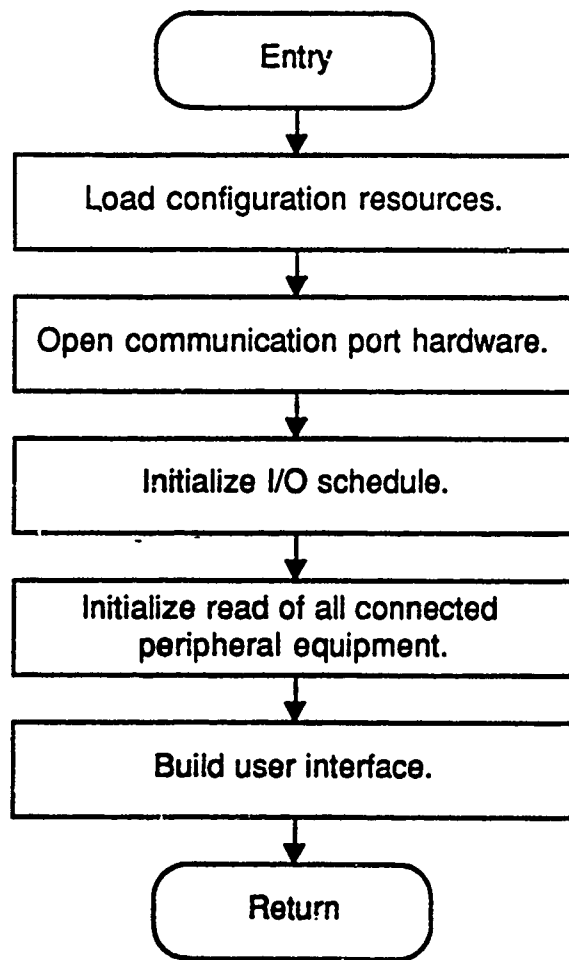
FIGURE 23. ShutterControl Main Program Loop.
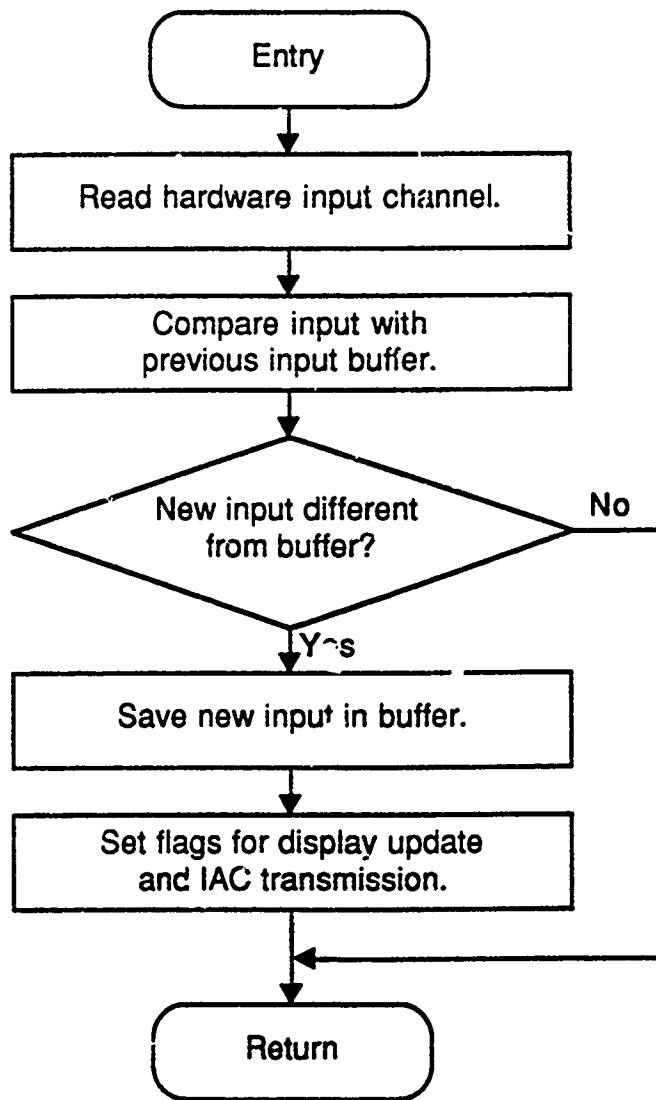
FIGURE 24. ShutterControl Initialization.
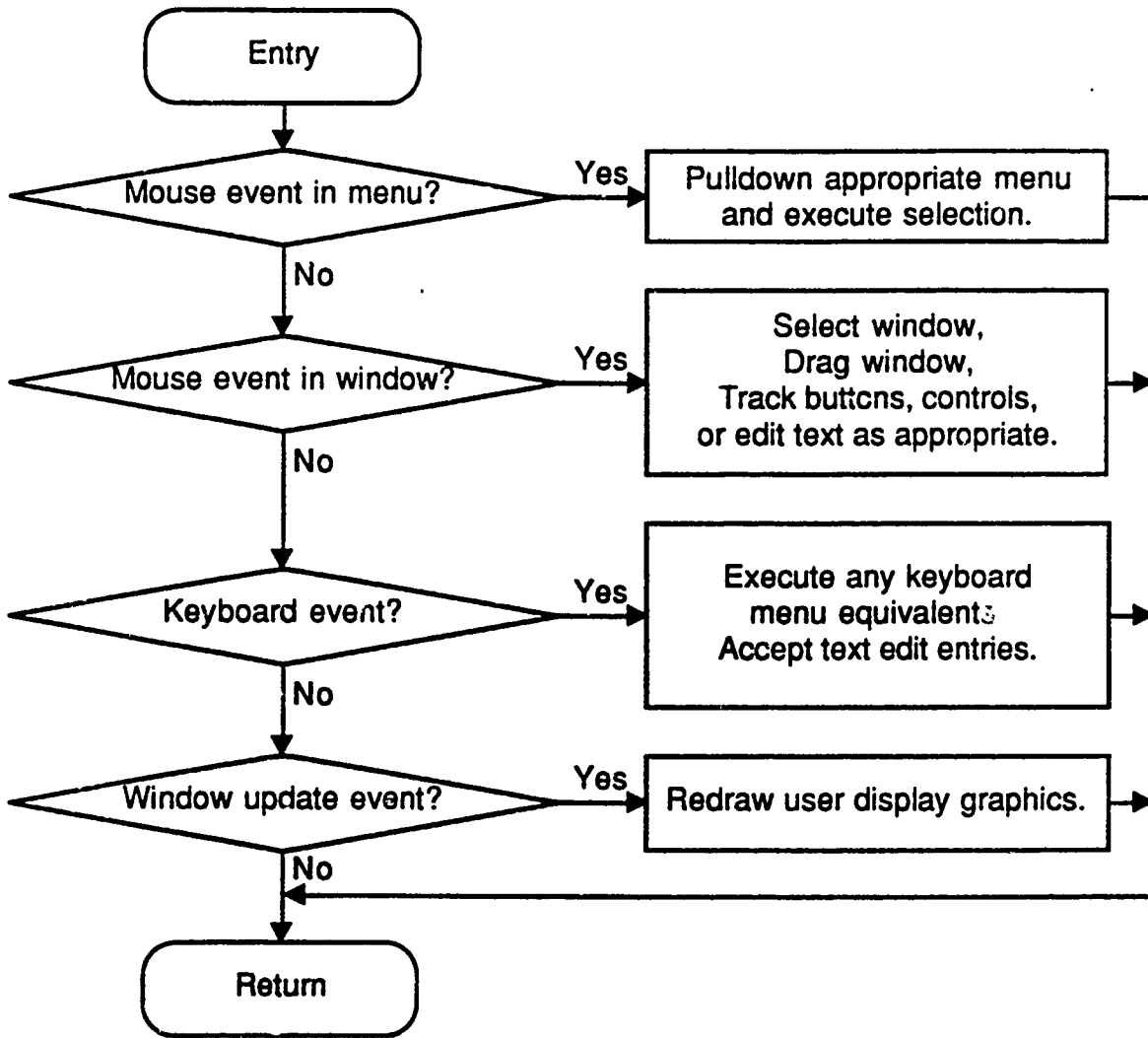
FIGURE 25. Read Hardware Input Channel.

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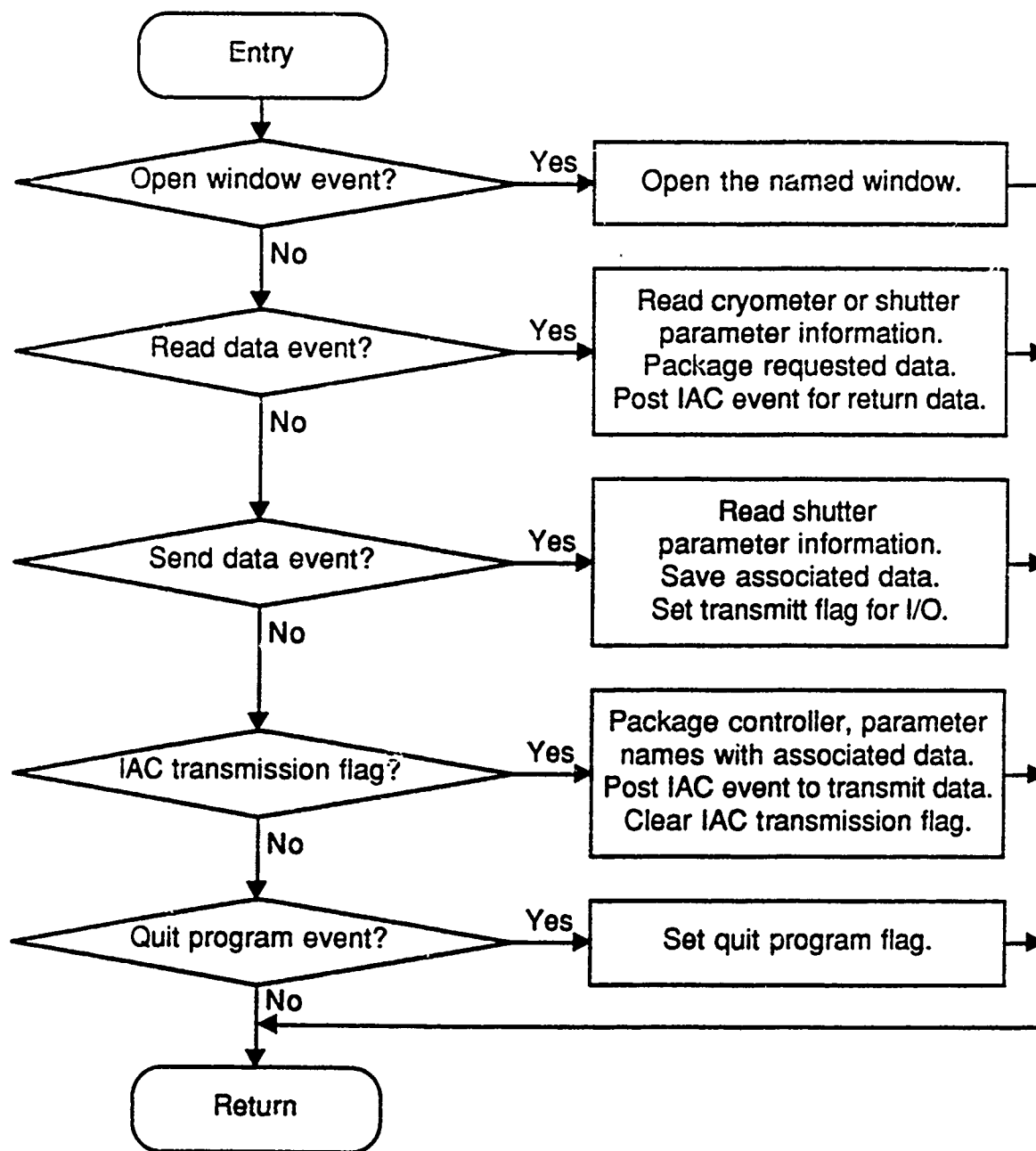**FIGURE 26. Handle User Interface Events.**

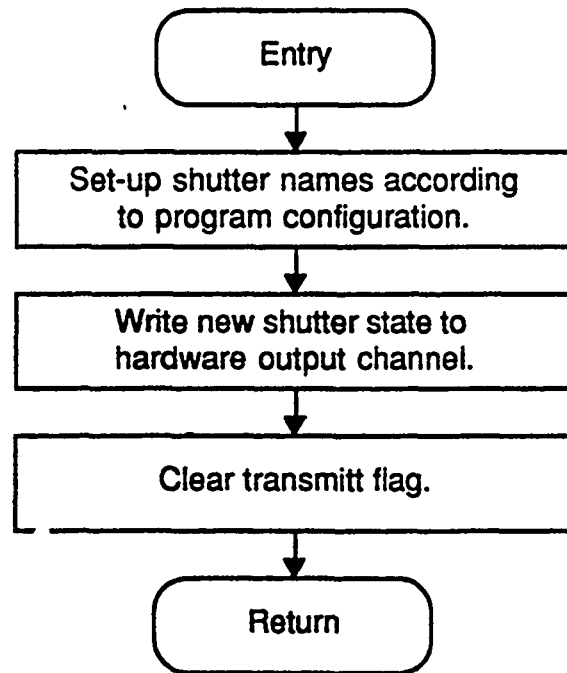FIGURE 27. Handle Inter-Application-Communication.

FIGURE 28. Write Hardware Output Channel.

The fourth program is the Ion Gauge interface program module shown in Figure 29. It follows the same programmatic format as the Eurotherm program with initialization and then continual looping through User Interface and IAC event handling along with the unique functions of the program. Figure 29 shows the basic functional blocks to initialize the program, monitor the serial RS-232-C interface for the Granville-Phillips ion gauge unit, handle user interface events, handle IAC events, and transmit an ON or OFF command to the Granville-Phillips ion gauge unit as requested through the user interface or through IAC events. Comparison of Figure 14 and Figure 30 shows the similarity of the program initialization routines for peripheral instrumentation program modules. Figure 32 handles the user interface and Figure 33 handles IAC events. As with the Eurotherm program, they are virtually the same as Figures 8 and 9 which supports the concept of reusable code from earlier program developments.

The functionality of this program module as a serial input interface is illustrated in Figure 31 with the complete message test loop and data field identification. This figure also shows the test for the peripheral instrument 'OFF' state by testing for a dedicated code. Figure 34 follows a simple procedure to respond to on/off command flags set up by either the user interface or IAC. Its builds the appropriate command string and transmits it and then clears the transmit flag to prevent continual transmission. Figures 31 and 34 represent the unique functionality of the Ion Gauge program module while the other Figures 29, 30, 32, and 33 are the general purpose elements of the program that set up its basic program components and simplify program development in a manner similar to the Eurotherm control program module.
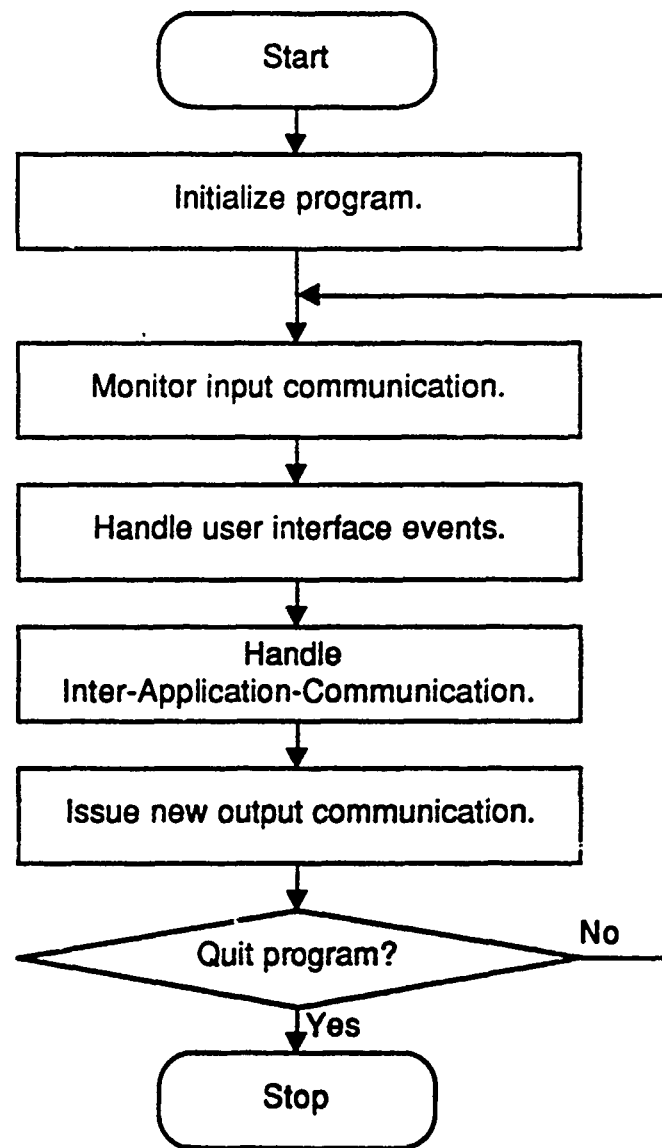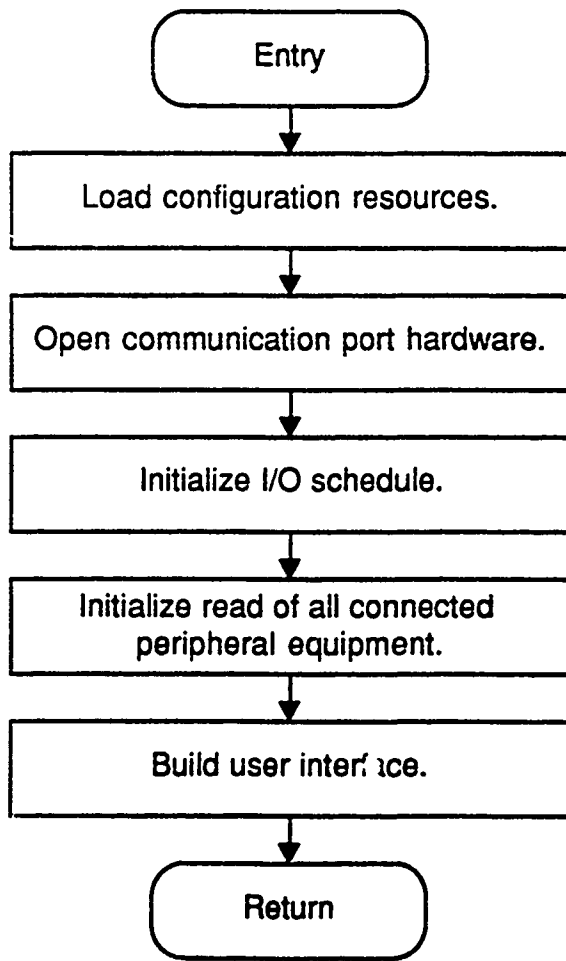
FIGURE 29. Ion Gauge Main Program Loop.
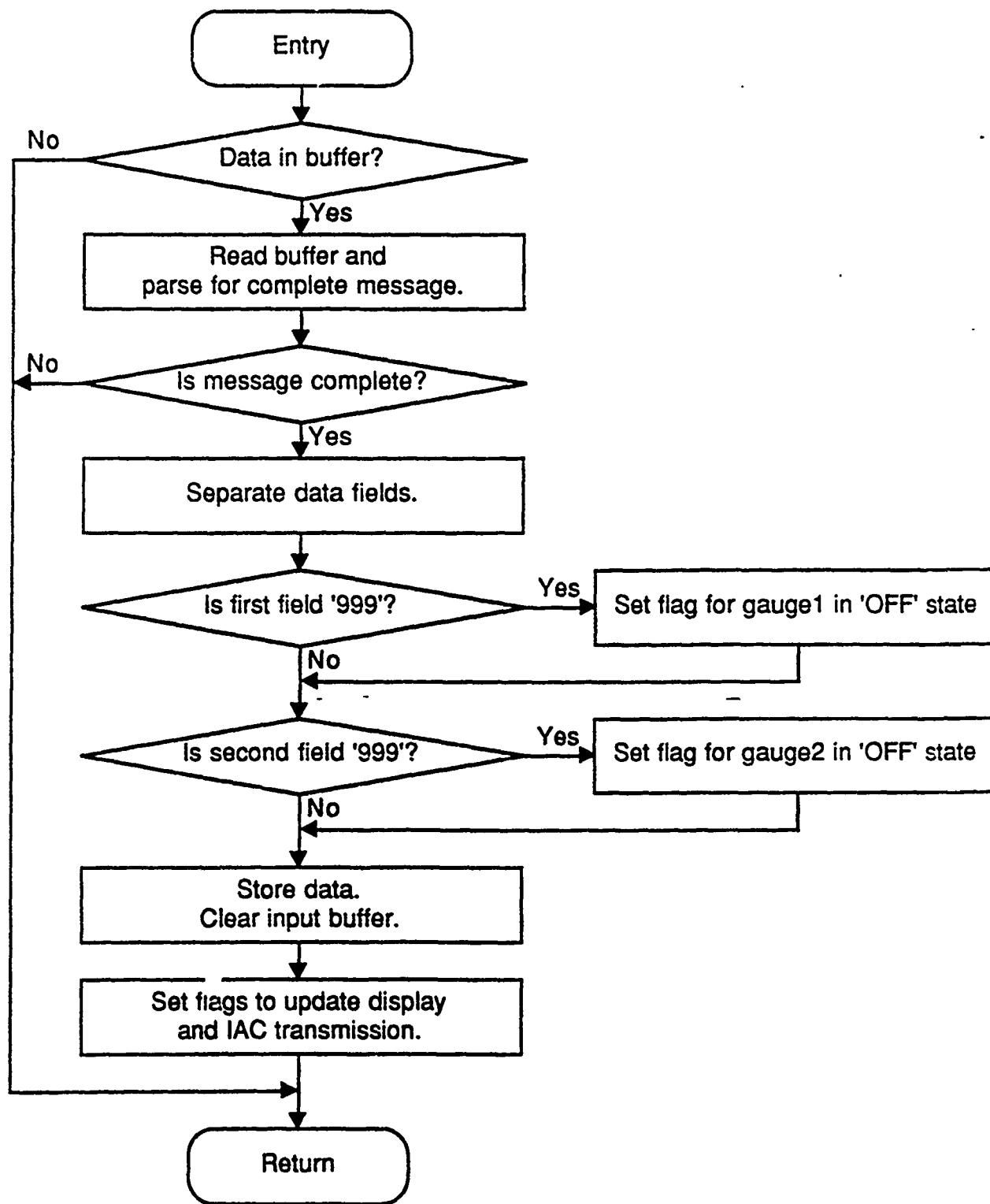
FIGURE 30. Ion Gauge Initialization.

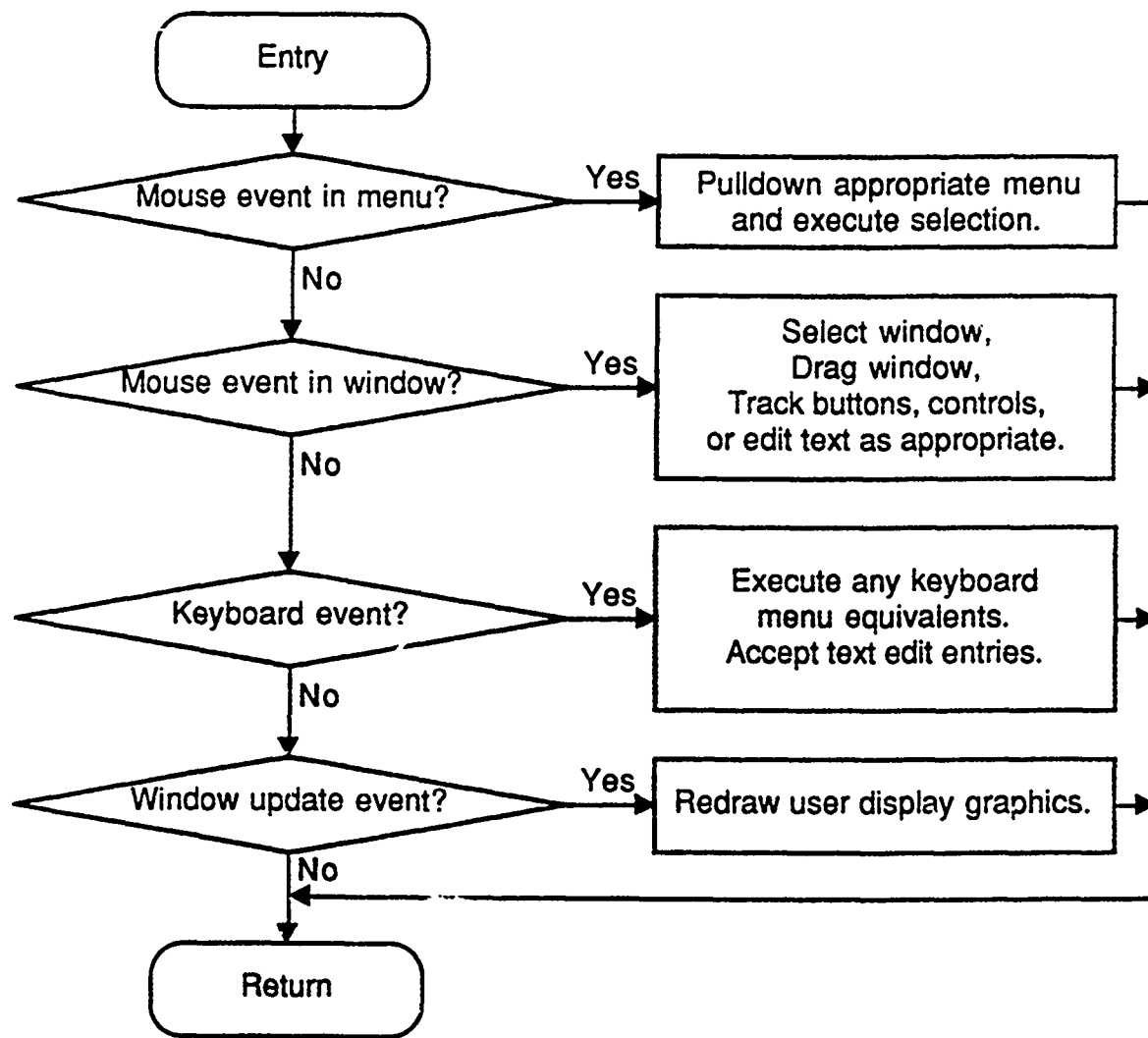**FIGURE 31. Monitor Input Communication.**

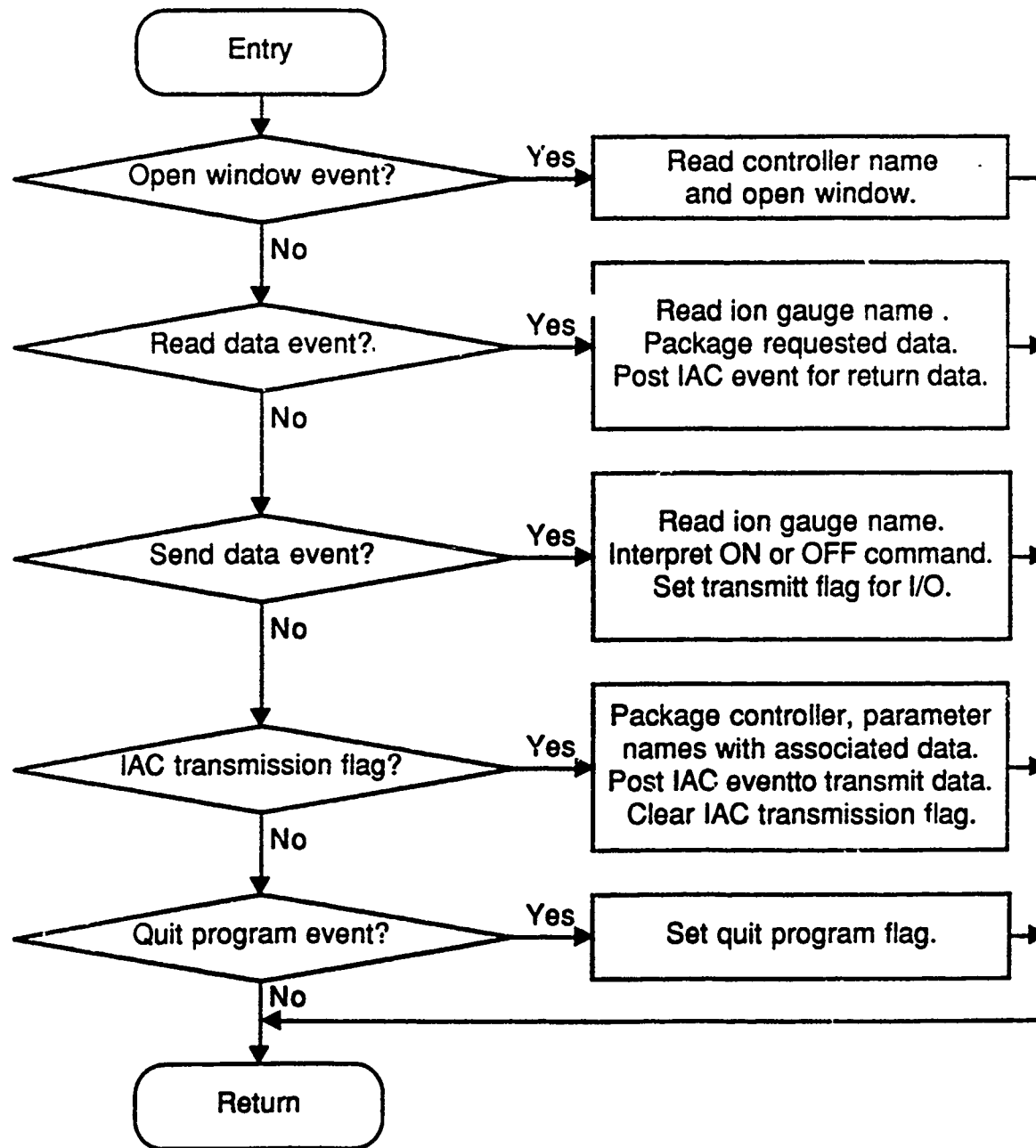**FIGURE 32. Handle User Interface Events.**

FIGURE 33. Handle Inter-Application-Communication.
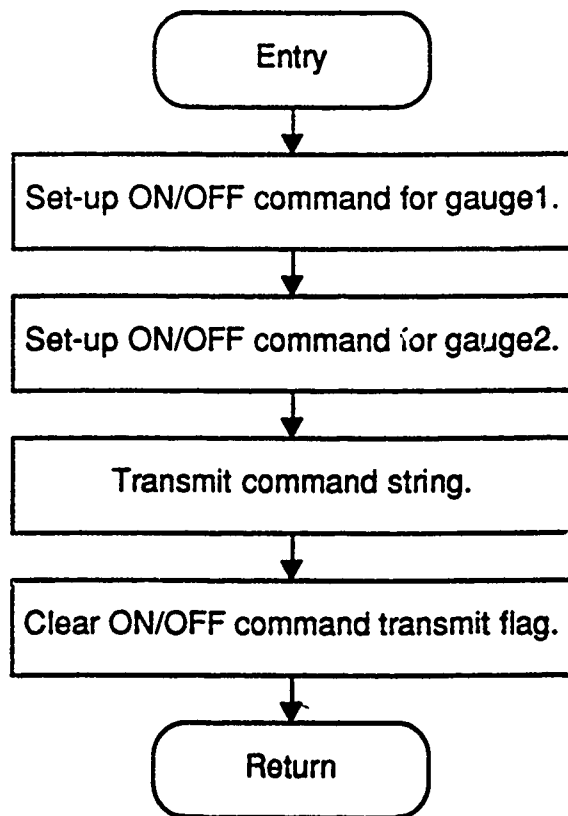
FIGURE 34. Issue New Output Communication.

The fifth program is the Process Discovery Autotuner program module shown in Figure 35. It follows the same programmatic format as the Eurotherm program with initialization and then continual looping through User Interface and IAC event handling along with the unique functions of the program. This program is different from the three previous programs that interface to peripheral instrumentation. It uses those programs as software interfaces to the actual instrumentation. Figure 35 shows the basic functional blocks to initialize the program, handle user interface events, handle IAC events, handle tuning sequence process manipulations for process parameter identification, and handle process control with the previously identified process parameters. Comparison of Figure 14 and Figure 36 shows the similarity of the program initialization routines with peripheral instrumentation program modules, but without the interface channel initialization. Figure 37 handles the user interface and Figure 38 handles IAC events. As with the Eurotherm program, they are virtually the same as Figures 8 and 9 which supports the concept of reusable code from earlier program developments.

The functionality of this program module as an autotuner is illustrated in Figure 39 with seven tuning modes tested and acted upon. During each tuning mode, a process monitor or command state is executed. The tuning mode is advanced to the next sequence when the process monitor target is achieved or the command completed. The last tuning mode operation is to assimilate the acquired process parameters into a readily executable format for the process step-control sequence illustrated in Figure 40. The process step-control sequence in Figure 40 uses the tuning acquired process parameters to anticipate the process response to a required process step-change. It calculates an optimum power input pulse to effect the process change and the controller PID terms needed to produce the power input pulse. Once the PID and setpoint changes are executed, the step-control sequence monitors the process as it approaches the intended setpoint and executes another process parameter based set of PID terms to impart process stability. Figures 39 and 40 represent the unique function of the Autotuner program module while Figures 35-38 are the general purpose elements of the program that set up its basic program components and simplify program development in a manner similar to all of the previous program modules discussed.
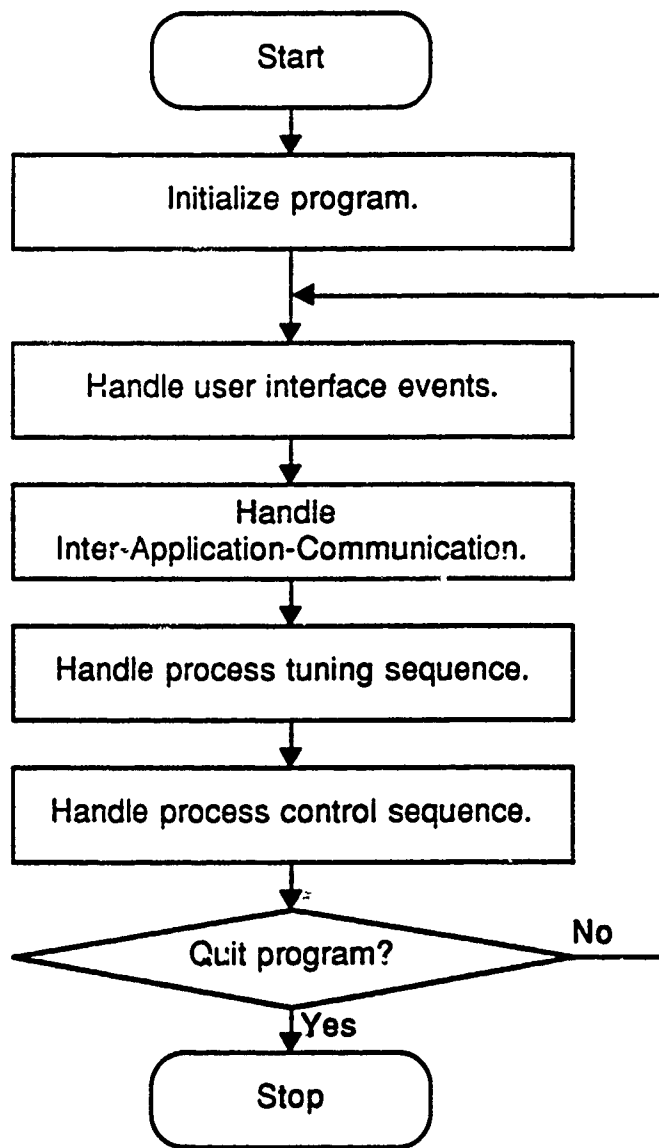
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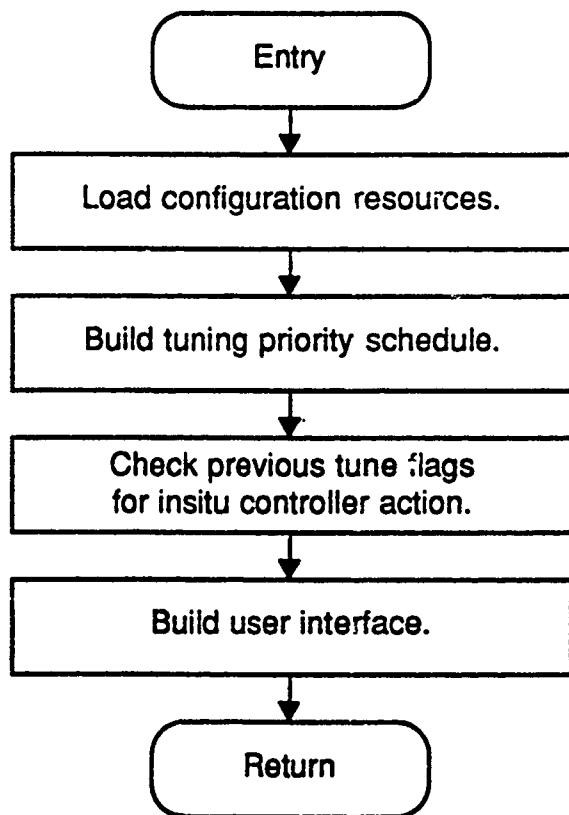**FIGURE 35. Autotuner Main Program Loop.**
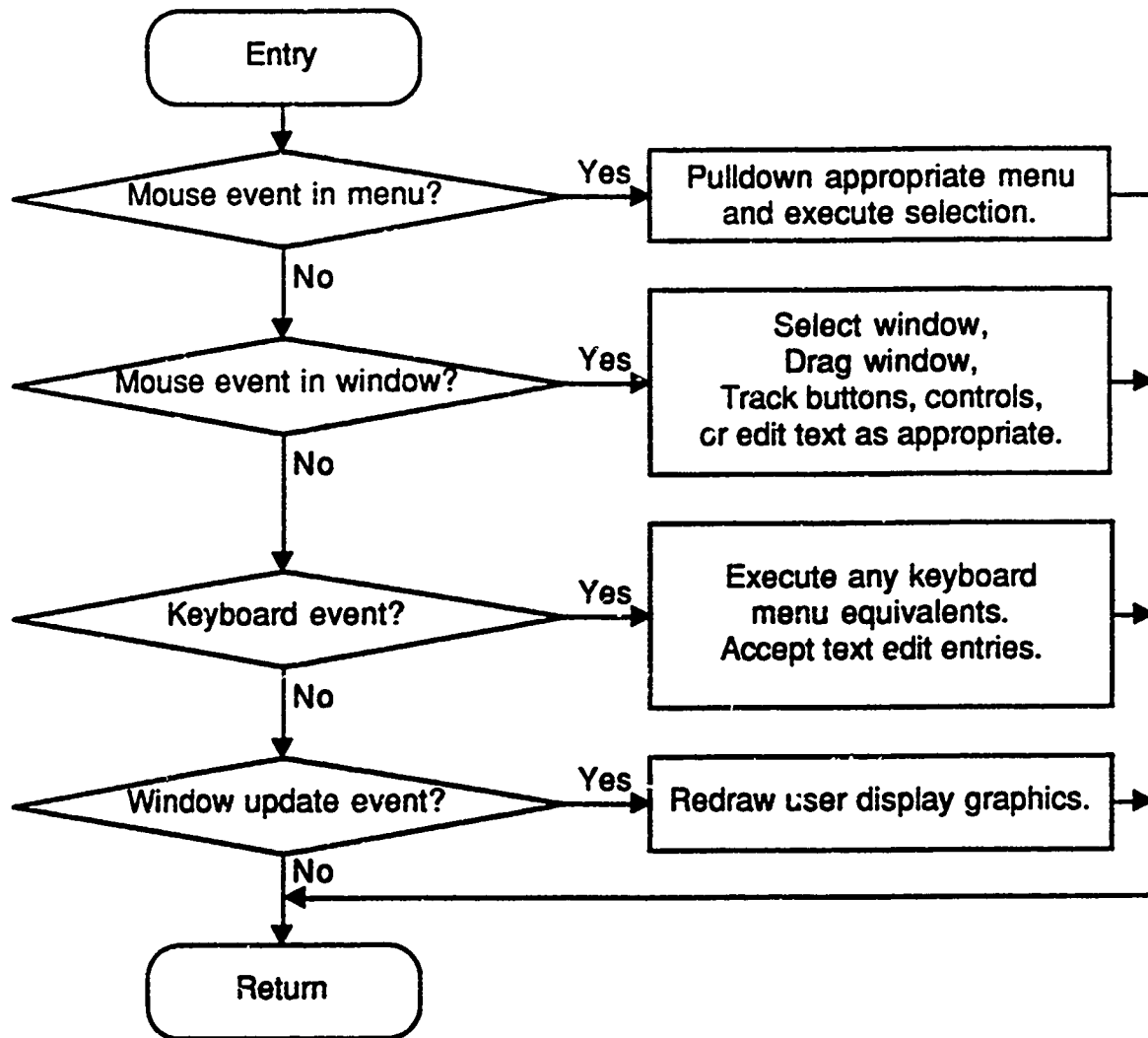
FIGURE 36. Autotuner Initialization.

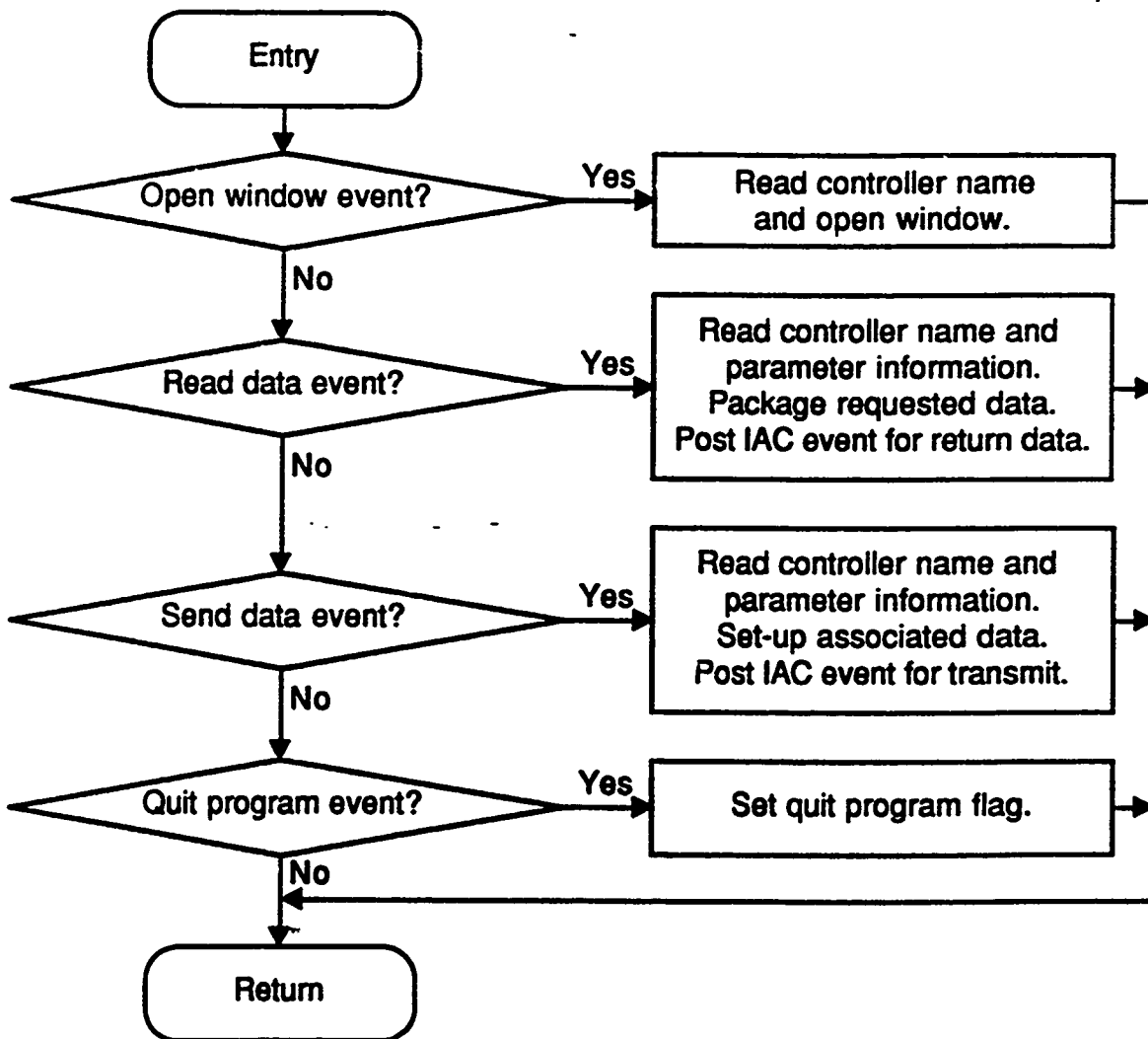FIGURE 37. Handle User Interface Events.

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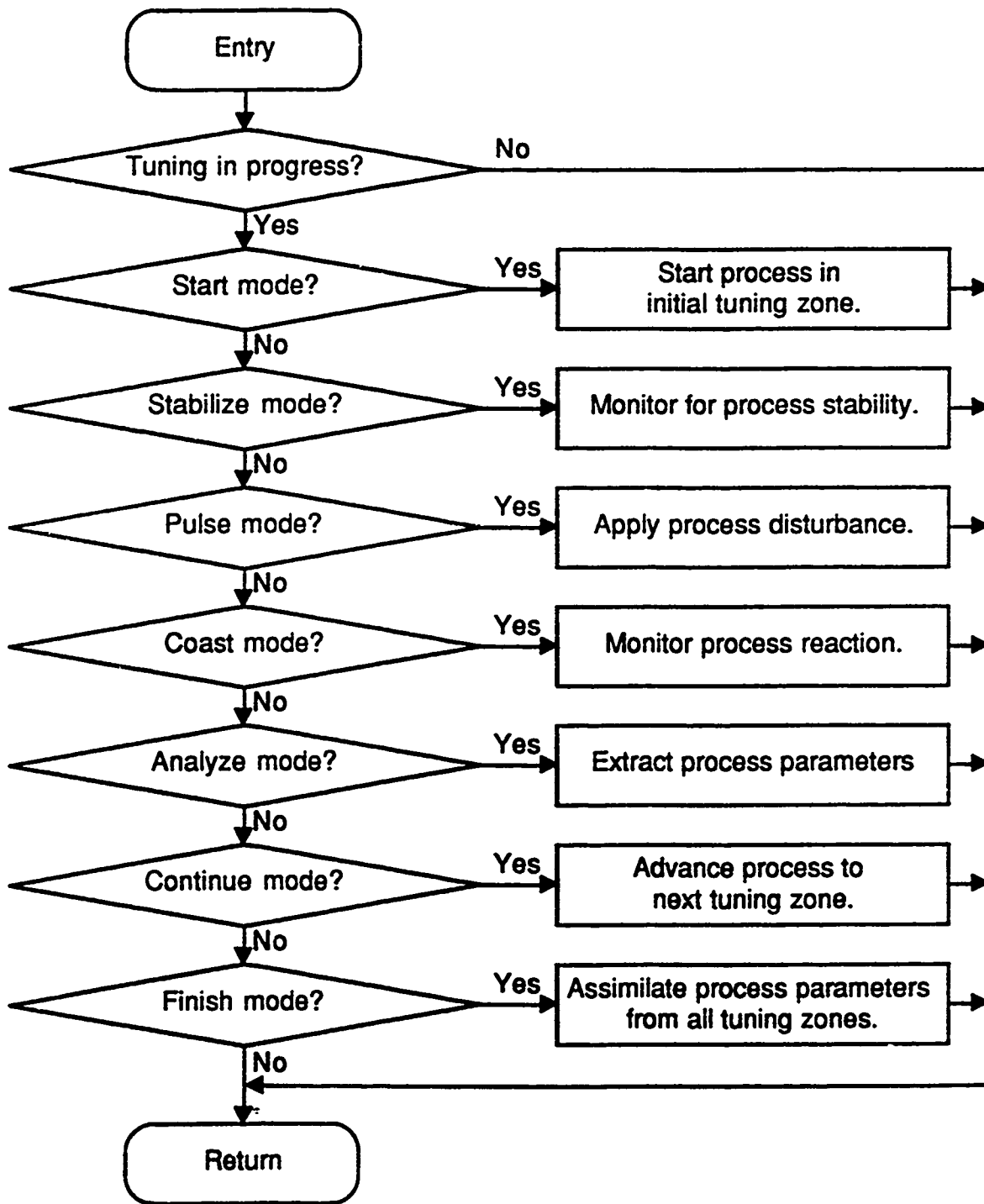**FIGURE 38. Handle Inter-Application-Communication.**
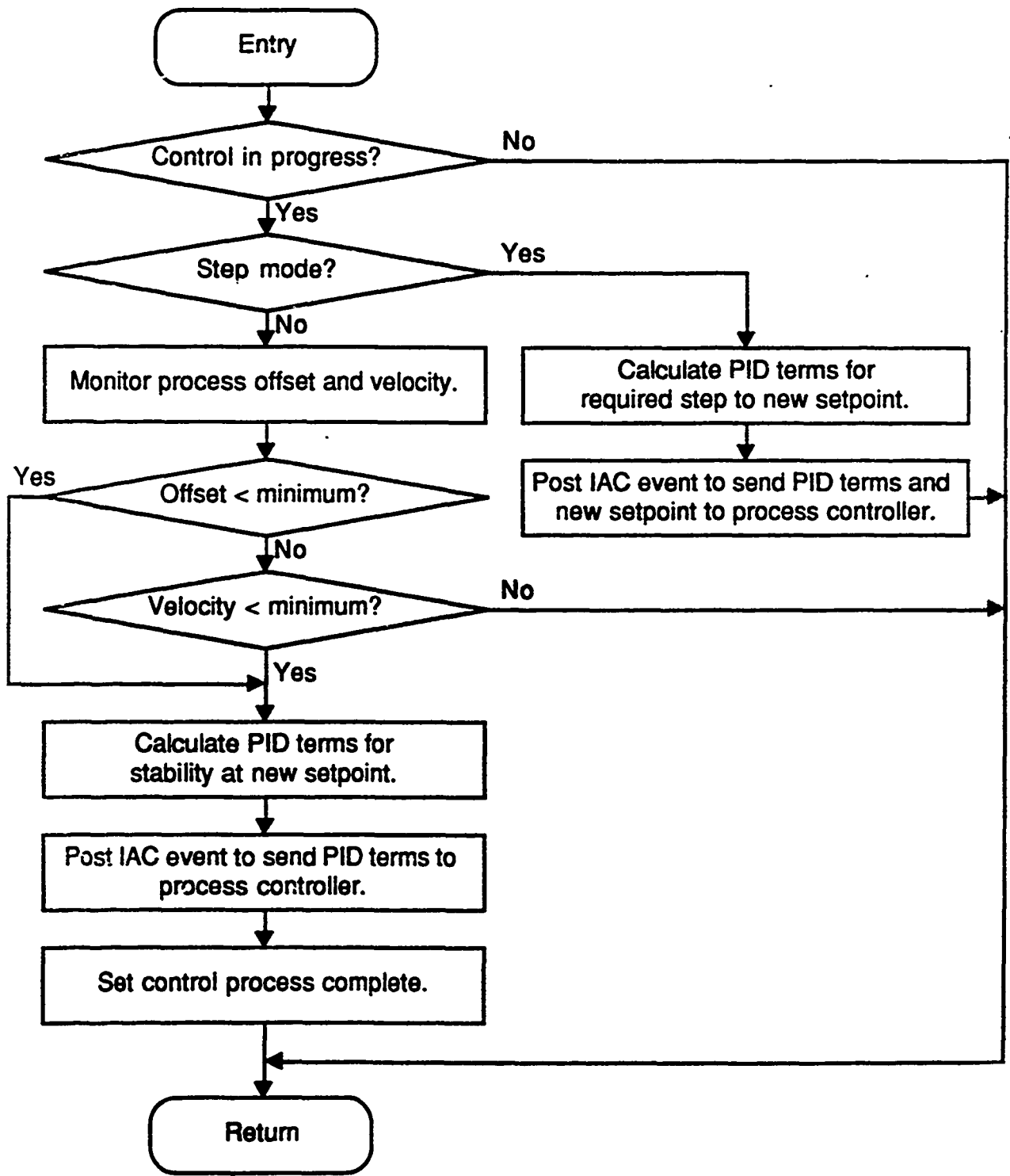
FIGURE 39. Handle Process tuning Sequence.

FIGURE 40. Handle Process Step-Control Sequence.

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The general program module organization and signal-data flow is illustrated in Figure 41. On the far left-hand side of the figure is the MBE machine representation. It shows the PID controllers for the Knudsen Cells and substrate holder, the Knudsen Cell shutters, cryo-shroud sensor, flux beam ion gauge, and ellipsometry instrumentation. Next to the machine elements are the instrumentation interface program modules with their respective hardware interfaces. These modules form the hardware link to the software based MBE control system. These interface modules link to the rest of the system through the Inter-Application-Communication (IAC) Bus. The modules on the right-hand side of the figure perform specialized control functions and may maintain their own private data files. At the top of the figure is a supervisor module which would be customized for a specific machine environment to issue commands to the appropriate control modules to automate MBE machine operation. All of the modules, whether they are for interface, control, or supervision, communicate to each other through the IAC Bus. The IAC Bus provides a flexible link between any two modules that does not specify any rigid data format. Data links can be created and deleted at any time and any number of times between any two modules. This flexibility allows new modules for instrument interfacing or control to be added to the MBE system as their need develops.

An example of signal-data flow for a specific activity in the MBE control system is shown in Figure 42. Knudsen Cell and substrate temperature control loop tuning is illustrated in Figure 42. The supervisor is shown at the top of the control hierarchy and is the initiator of the tuning sequence. The supervisor commands the Process Discovery Autotuner (PDA) Controller to perform the tuning operation. The tuner references its private PDA files, sends commands to close all shutters, commands the PID controllers through the tuning cycle, and analyzes the resultant process data from the data plotting module. Examination of this figure shows how the signal-data flow path involves only the communication necessary for the task assigned by the supervisor.
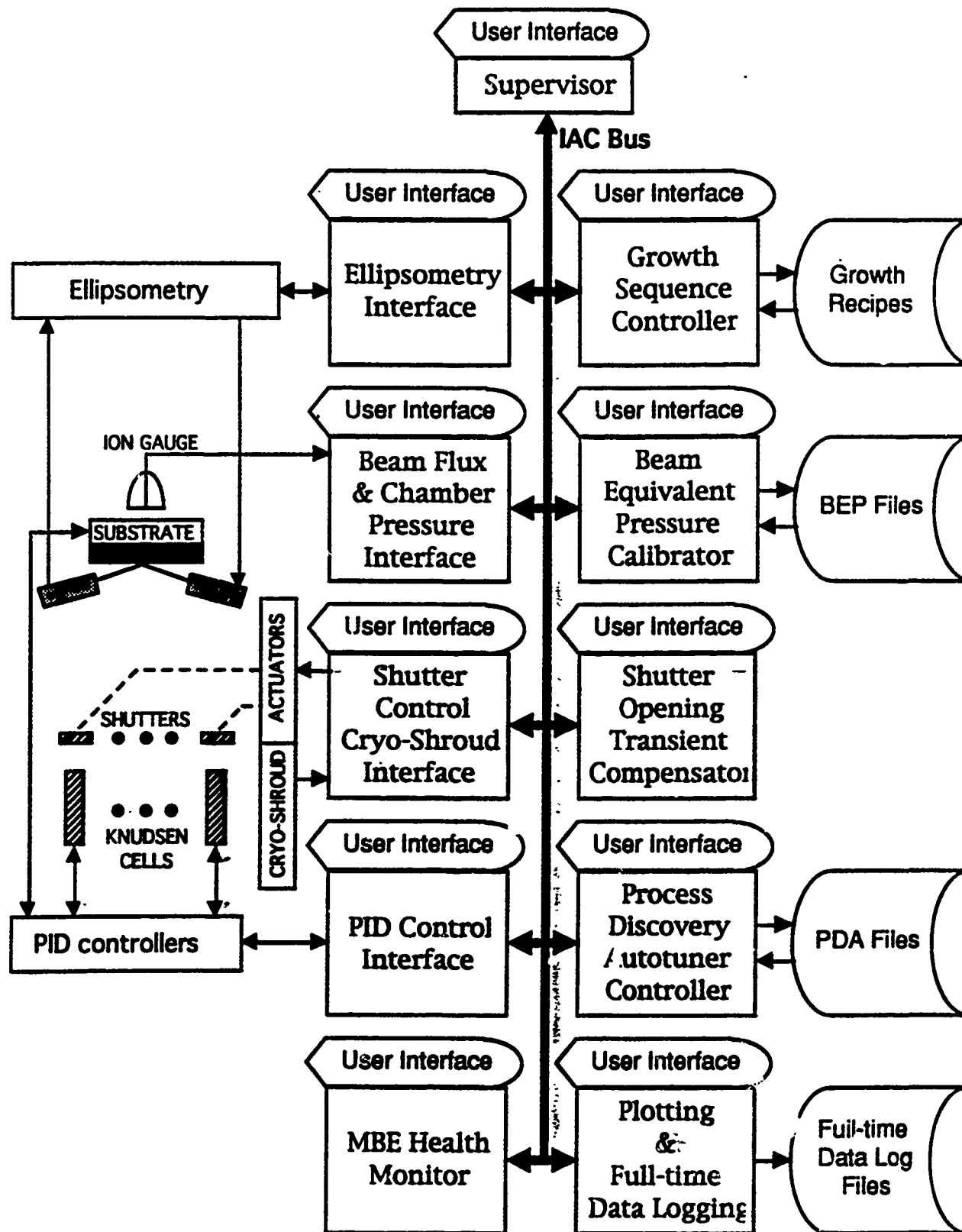
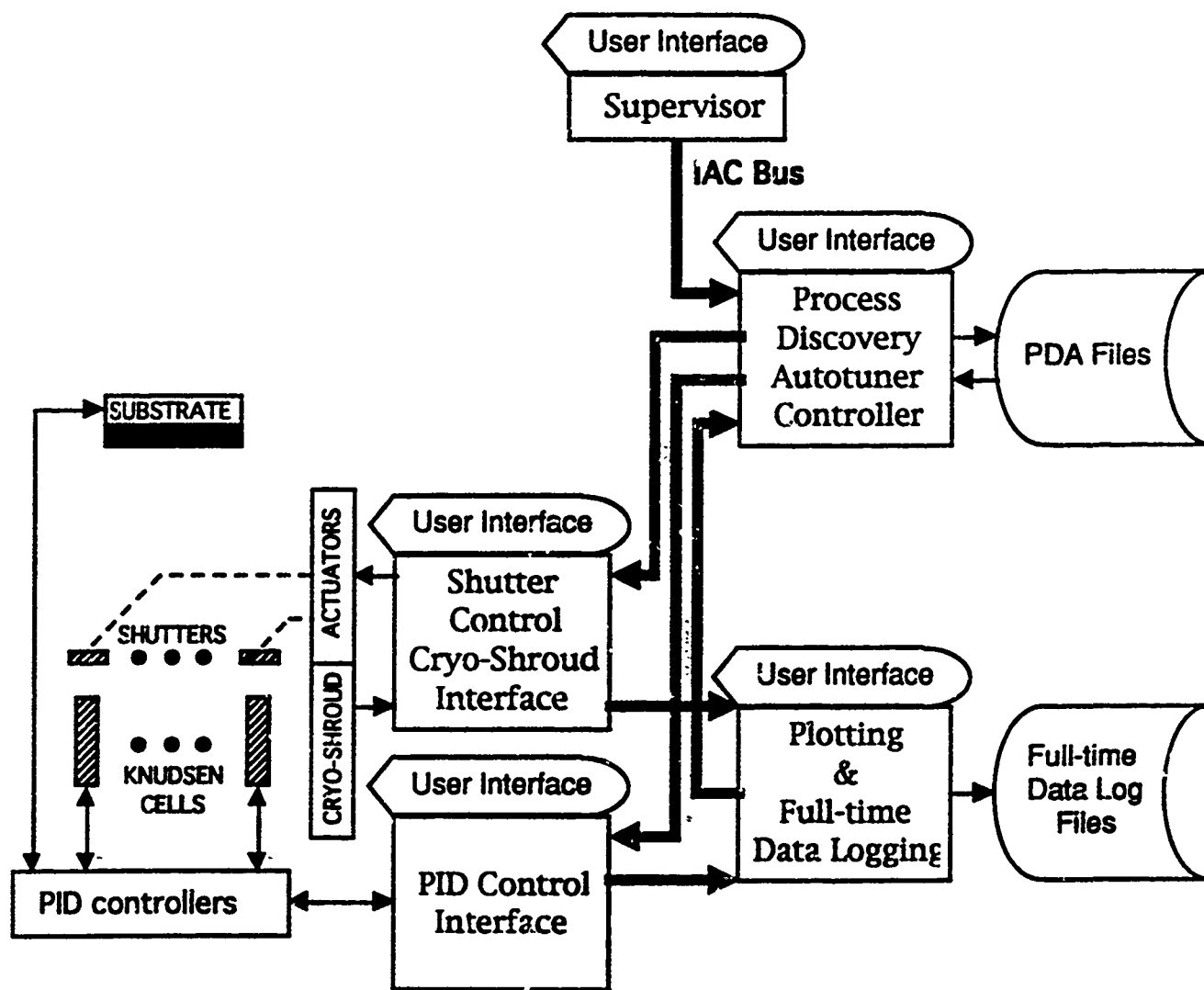**FIGURE 41. Modular Format of MBE Control System.**

FIGURE 42. Knudsen Cell/Substrate Tuning.

The efficiency of a computer control and data logging system is evident in Figure 43. The supervisor has commanded the Beam Equivalent Pressure (BEP) Calibrator to generate a new set of BEP files. The BEP Calibrator commands shutter operations directly, but commands Knudsen Cell temperatures through the PDA Controller which references its own private files for optimum temperature control through the PID control interface. The beam pressure data from the ion gauge is recorded in the plotting module which is coupled with shutter activity back to the BEP Calibrator to produce a new BEP file. This new BEP file is used to anticipate flux beam responses to shutter activity during the MBE growth sequence. Again, examination of this figure shows how the signal-data flow path involves only the communication necessary for the task assigned by the supervisor.

The supervisor module initiates and monitors the MBE growth sequence as shown in Figure 44. The Growth Sequence Controller (GSC) references its private files for the required growth recipe. The GSC controls the MBE growth process by manipulating Knudsen Cell and substrate temperatures through the PDA Controller which responds according to its PDA files. Growth is also controlled by the GSC by manipulating shutter states through the Shutter Opening Transient Compensator which responds according to data delivered to it by the GSC from the BEP Calibrator's private files. The command sequence from the GSC is regulated by recipe comparison to growth data received from the Ellipsometry Interface. In Figure 44, private data paths are maintained while the IAC Bus provides the signal-data flow path flexibility needed for the growth sequence control.
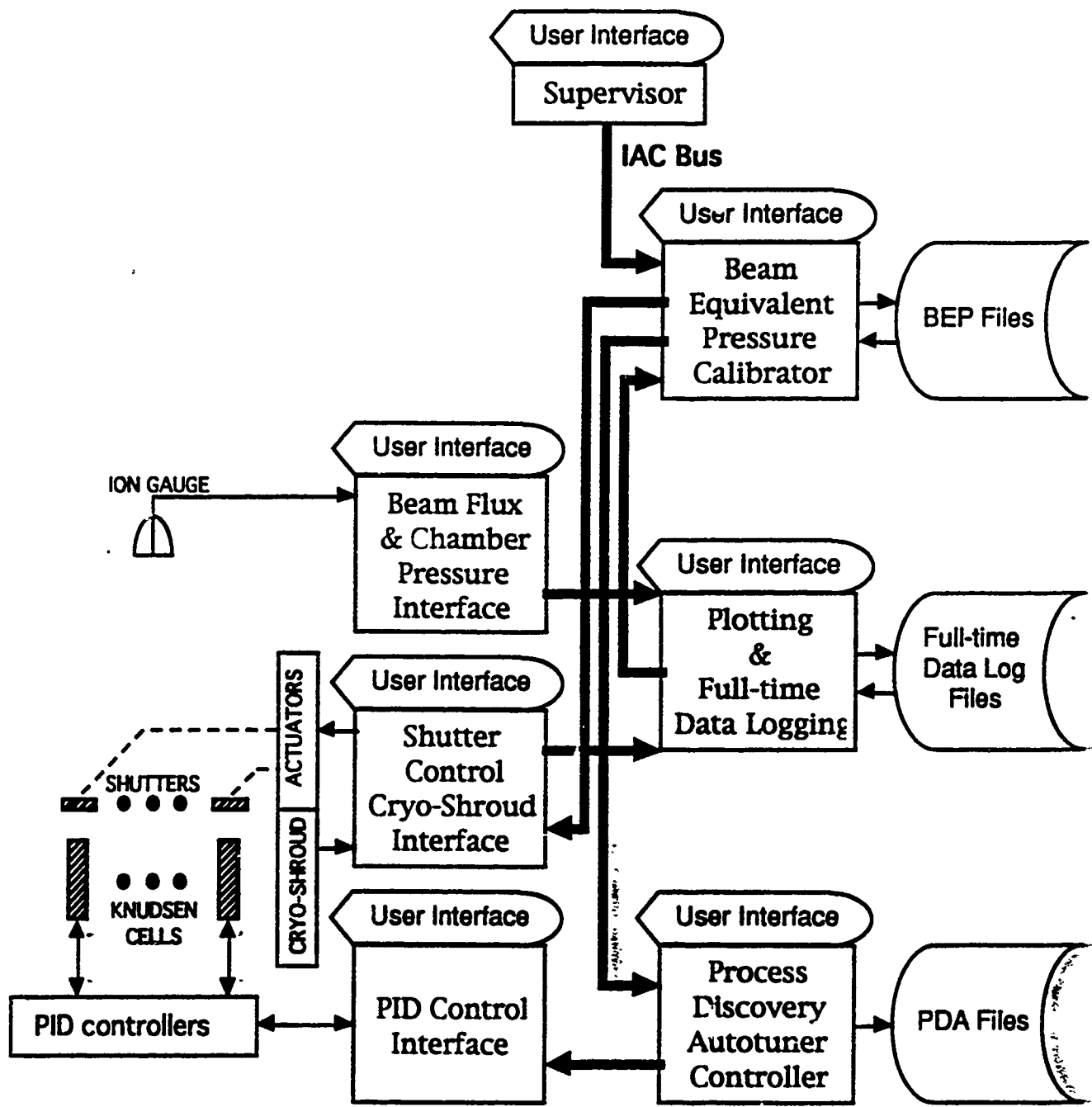
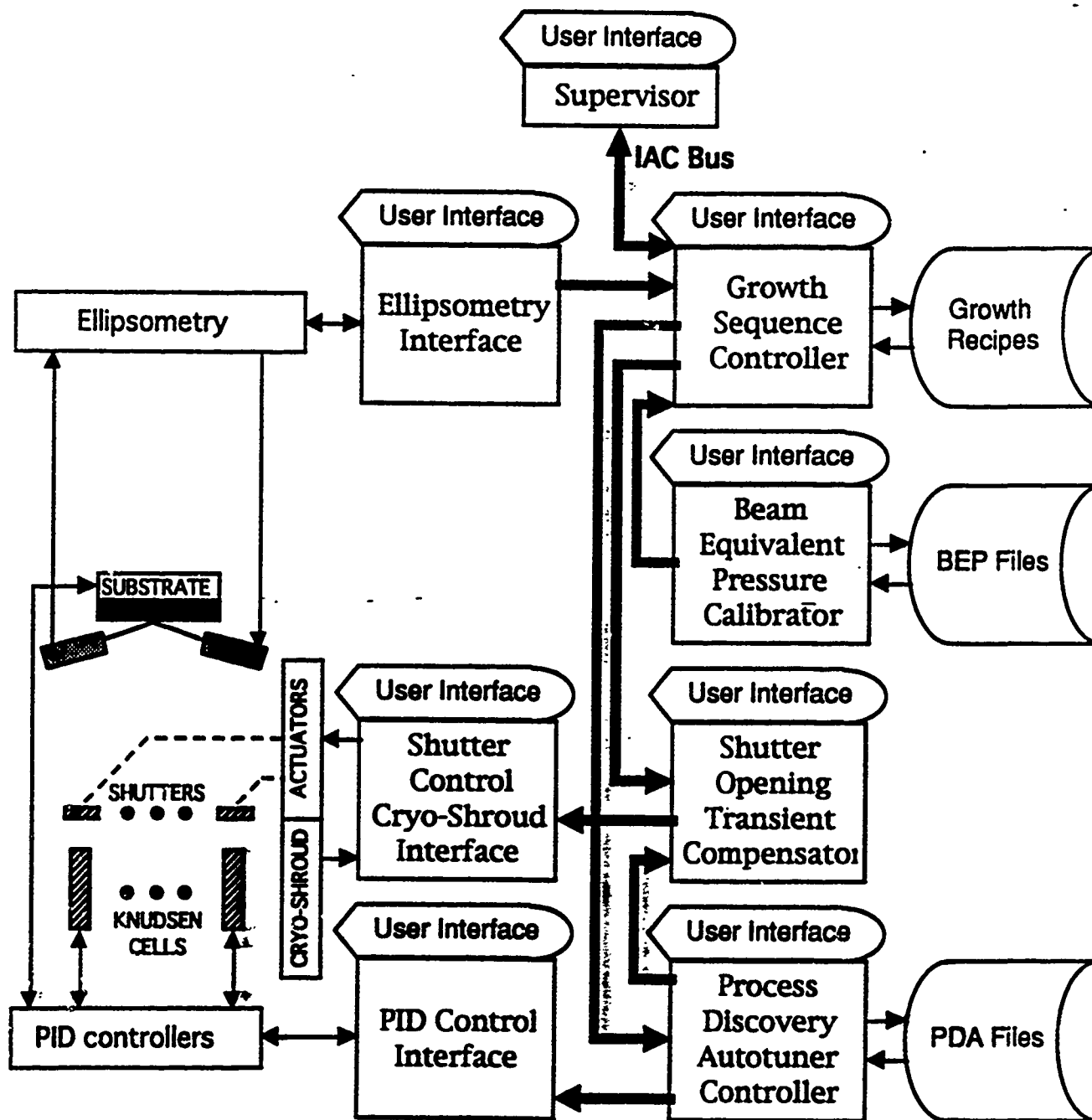**FIGURE 43. Flux Tuning.**

FIGURE 44. Growth Sequence Control.

Figure 45 shows one last vital communication path to insure the safety of an automated MBE system. This communication path is for system health monitoring. Vital MBE machine conditions such as safe Knudsen Cell and substrate temperatures, functioning cryo-shroud, and chamber pressure within range, require regular monitoring by the machine operator to insure the MBE machine integrity. However, unmanned situations occur daily and if a fault should occur, default action should be implemented. Figure 45 provides that default action with the MBE Health Monitor. The monitor would continually track the vital machine conditions and signal an expert system within the supervisor in the event of a fault. The supervisor in turn would attempt to notify the machine operator if the fault occurred during a growth sequence. If operator notification failed or no growth is in progress, the supervisor would proceed to reduce cell and substrate temperatures to pre-defined safe limits.

Figures 41-45 show the IAC Bus flexibility providing the mechanism for program module communication to many other program modules. A user interface function in each program module is used to establish communication links on the IAC Bus as simply as opening a file. As new modules are introduced and as new communication paths are needed, the IAC Bus connections can be readily established.
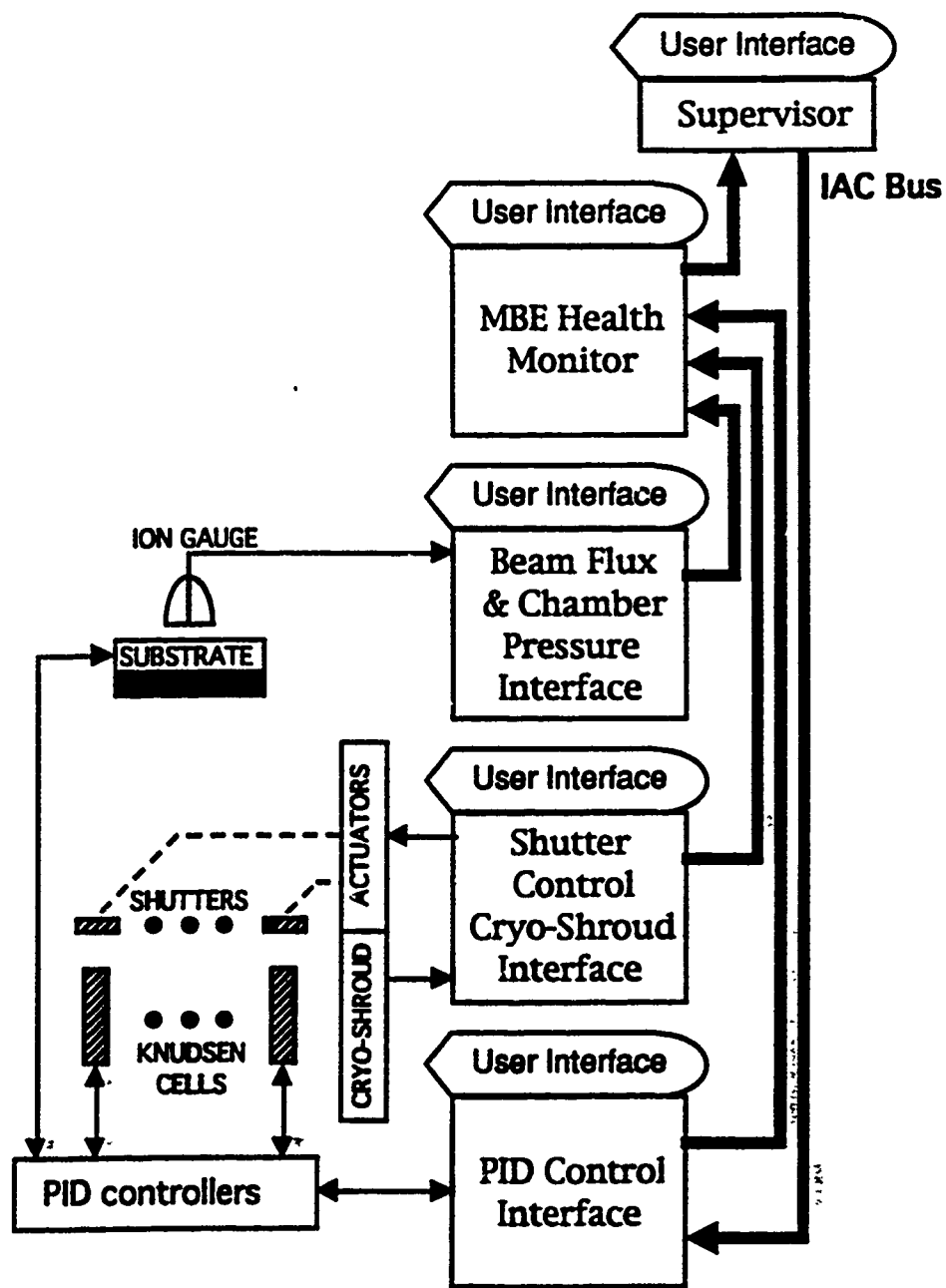
FIGURE 45. MBE System Health Monitor.

CONCLUSIONS

Progress was achieved in many small areas during this task. The refinements implemented on the Varian MBE system have also been installed on the companion Vacuum Generator MBE system at this site. Eurotherm data acquisition is well defined at this point and effort has been devoted to ion gauge flux data, shutter synchronization, cryo-shroud monitoring, and ellipsometry. Enhancements to the operator interface for the MBE control system have improved MBE functionality and testability through better control and data logging. Implementation of several IAC driven program modules has allowed collaborative MBE system programming to proceed more productively with the elimination of hidden program dependencies. The IAC implementation has also allowed stand-alone module debugging and variable configuration for multiple MBE system installations.

The flux stability, although improved by automatic PID tuning methods, shows that there is still thermal error reduction to be addressed by hardware refinements such as the soon to be installed Eurotherm 905 Knudsen Cell controllers. This thermal error reduction is carried forward as reduced uncertainty in the associated Knudsen Cell flux during the MBE growth process.

RECOMMENDATIONS

Flux stability needs continued evaluation through Knudsen Cell thermal control-loop tuning, control hardware refinements, and flux measuring instrumentation. Implementation of automatic continuous data logging with real-time compression is needed to collect the volume of data required for accurate system evaluation. Continued implementation of multi-tasking IAC driven programs will allow collaborative MBE system programming to proceed more productively with shorter design cycles and portability to other MBE configurations.