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PROGRESS TOWARD A COMPREHENSIVE  
CONTROL SYSTEM FOR MOLECULAR BEAM EPITAXY

**AD-A259 724**



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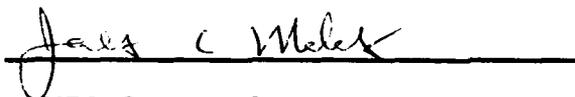
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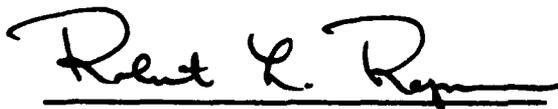
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13. ABSTRACT (Maximum 200 words) A hierarchical control system for improving the manufacturing capability of the thin-film semiconductor growth process, Molecular Beam Epitaxy, is under development at the Air Force Materials Directorate. The focus of the first level is to improve the precision and tracking of the variables, flux and substrate temperature. The second level consists of an expert system that uses sensors to monitor the status of the product in order to generate a process plan in real time. The third level features a continuously evolving neural network model of the process which is used to recommend the recipe and command inputs to achieve a desired product goal. All three levels require models of the process which are updated using automatic process identification experiments. The three levels of the system are described and experimental data is used to illustrate the impact of select modules.					
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## 1. Introduction

Future Air Force weapon systems, whether new platforms or upgrades to existing ones, will require more capable and sophisticated electronics and electro-optic systems to maintain qualitative superiority over potential adversaries. These future electronic and electro-optic devices will rely more and more on materials grown in epitaxial thin-film forms. Thus, the major DOD Microwave and Millimeter Wave Monolithic Integrated Circuits (MIMIC) program is aimed at providing vastly improved, low cost and highly reliable entire circuits on one chip for numerous DOD applications. This GaAs based technology has and will continue to lead to enormous increases in analog device capability in the microwave applications areas. Much of the current technology is based on ion implantation into bulk GaAs wafers, but an ever increasing number of applications are turning to devices such as High Electron Mobility Transistors (HEMT) and Heterojunction Bipolar Transistors (BHT) which are made entirely from epitaxial III-V semiconductor films grown on substrates such as GaAs and InP. Projections for future quantities and costs of starting materials for such device fabrication are very large. In addition to the MIMIC program, an increasing number of digital high speed circuits based on this epitaxial film and device technology are appearing and there is an increasing interest in electro-optic devices such as focal plane arrays using epitaxial superlattice films which have been found to have very attractive properties. Thus, a substantial and growing need for production level quantities of a variety of III-V semiconductor epitaxial films can be identified.

To achieve a substantial production level capability that can provide these low cost, reproducible, uniform, and tailorable thin-film structures will require advances in sensors of the growth process and integration of these sensors into an on-line real time process controller. Techniques such as Molecular Beam Epitaxy (MBE) and Metallorganic Chemical Vapor Deposition (MOCVD) do not currently utilize on-line process control and are subject to the variations and capabilities of the operator who sets machine parameters in advance of the growth run and hopes for a predictable product.

A comprehensive plan for improving the manufacturing capability of the thin-film semiconductor growth process, Molecular Beam Epitaxy (MBE), has been developed at the USAF Materials Directorate. Current results from the implementation of this plan are discussed in this report.

The primary objective of this MBE manufacturing research program is to improve the consistency and quality of materials grown with MBE. Although the selection of qualities most important to optimize depends on the type of thin-film being grown, the following qualities are generally important:

- 1) Layer Thicknesses
- 2) Alloy Concentration
- 3) Dopant Concentration
- 4) Impurity Levels
- 5) Interfacial Sharpness
- 6) GaAs or AsGa Antisites (Ga occupies As location or vice versa)
- 7) Vacancies (Missing atom)
- 8) Dislocations (Missing line of atoms)
- 9) Oval Defects

Methods for improving the qualities #1, #2, #3 and #5 are presented.

A secondary objective of this research is to reduce the manpower requirements for operating the process. The MBE process is extremely complex and the best operators tend to have many years of experience. At the same time, operation of the MBE machine involves extensive setup and repetition of tedious tasks. Automation of many of these tasks not only reduces the burden on the operator, but also improves the accuracy of data.

The improvement effort conceptually divides into three areas: improvement of flux control, real time control using an expert system with advanced sensor feedback, and material system modeling for the purpose of developing new recipes quickly. A three feedback loop control system which parallels these areas, shown in Figure 1, will ultimately control the MBE process. The feedback loops will be referred to as the Inner Loop, the Self-Directed Control Loop and the Ex Situ Loop.

The **Inner Loop** is designed to optimally control the process variables, flux and substrate temperature. The flux cannot be sensed in real time currently, but the Knudsen Cell temperature can. A PID controller is used to control the Knudsen Cell temperature. Improvements that the Inner Loop provides include Adaptive Gain/Bandwidth Control, model based compensation of shutter opening transients and Flux Setpoint Control. For each of these features, metrics of the process must be accurately known. By conducting automated system identification experiments during setup, the models for each Knudsen Cell for temperature and shutter input and the temperature-to-flux relationship for each Knudsen Cell are calibrated. The goal of the Inner Loop is to provide transient free, highly stable flux, even in the case of overlapping events, i.e. events which do not fully decay before being repeated.

A real time, expert system will control the process based on instantaneous material quality feedback, i.e. composition at the surface, growth rate and surface morphology. This feedback loop is called the **Self-Directed Control Loop** because the quality of the material is used to select the next actuation. This

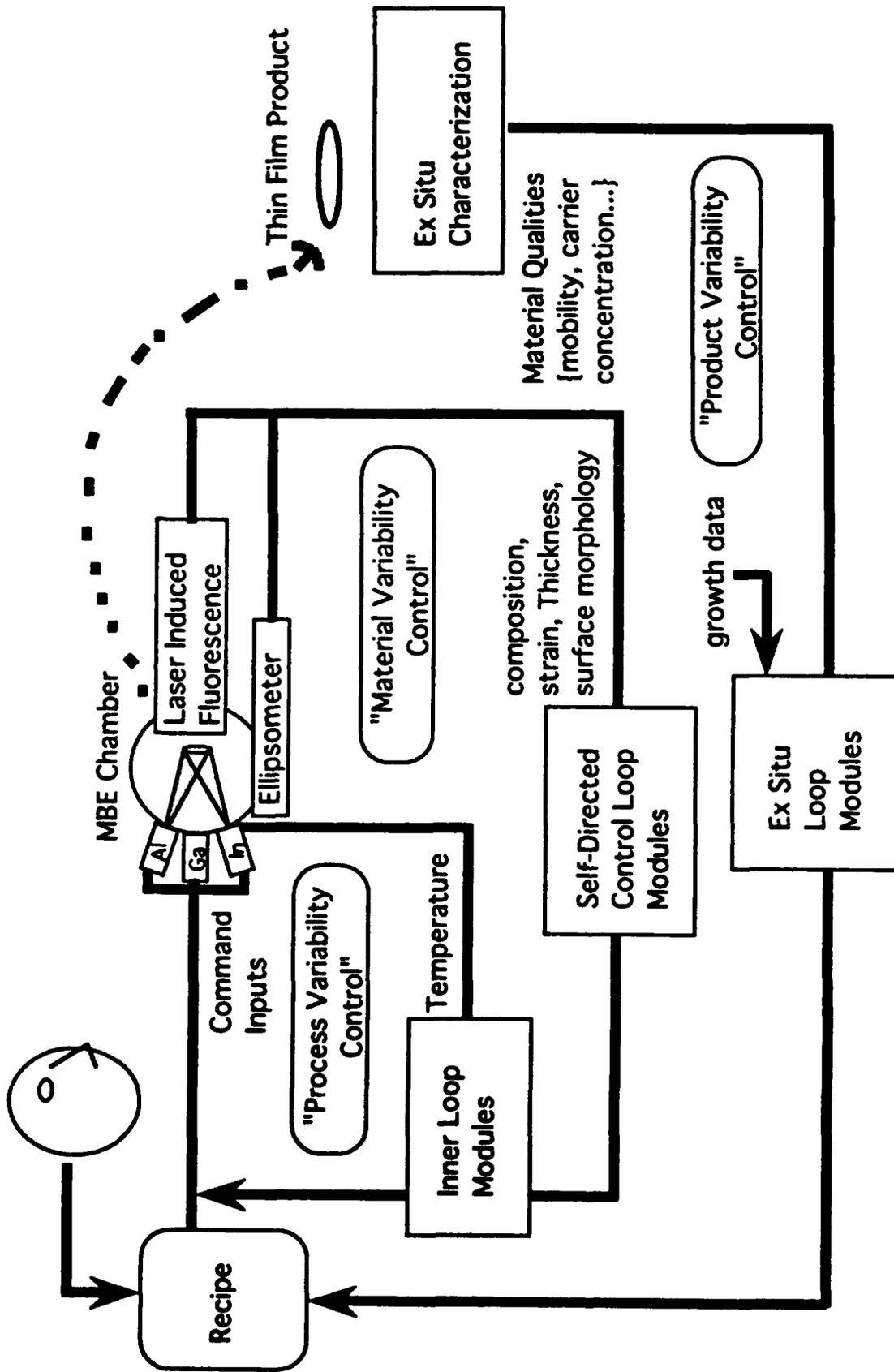


Figure 1: The three feedback loops of the MBE control system

system will tailor each growth run, overcoming process disturbances, to exactly obtain the thin-film specified by the recipe to the limit of sensor accuracy and process variable controllability.

The Self-Directed Control Loop can at best produce the recipe specified, because the product qualities of the thin-film being targeted (e.g. electron mobility, carrier concentration, transmissivity) cannot be monitored during the growth. The **Ex Situ Loop** is used to feed back these product qualities via a neural network model. This loop is called the Ex Situ Loop because the information fed back is from Ex Situ characterization of the thin-film. The Ex Situ Loop is used before each growth run to recommend the recipe and MBE machine inputs.

Together these three feedback loops will form the next generation control system for the MBE process.

## 2. Inner Loop

The principal control inputs to the MBE process are the temperatures of the source and substrate furnaces and the shutters. These inputs are used to generate flux beams. The stability of these flux beams is reflected in the consistency and accuracy of the product. The Alloy Concentration and Dopant Concentration, qualities #2 and #3 above, will vary in the depth direction if these fluxes are not consistent. Also the fluxes will affect Layer Thicknesses, #1. Inconsistency in the flux will probably even effect the crystallinity and defect levels, #5, #6, #7 and #8. The ideal flux waveform is square as shown in Figure 2. The typical flux waveform shown in Figure 2 contains a transient which is due to a reduction in the radiant heat reflected from the shutter after shutter is opened. Contributions from noise and inadequate compensation also cause the flux to oscillate.

A combination of hardware and software improvements can greatly improve the flux performance. An error analysis was conducted to determine the sources of error in the source temperature control loop.[1] A major component of error was identified to be from the Eurotherm 825 Controller. The steady state performance of the 825 controller was compared to the steady state performance of an 818 controller. Figure 3a and Figure 3b compare the temperature stability between the 825 and 818. The 818 controller is clearly superior. Flux stability, however, is more important. Figure 4 shows that the flux stability with the 818 controller is twice as good as with the 825 controller. The major cause of the oscillation in the 825 temperature signal is attributable to its internal 20kHz switched mode power supply. The 818 is also superior to the 825 in data acquisition speed and in that it has a tuning capability. Eurotherm now markets a 905 Controller which is even better than the 818. The Materials

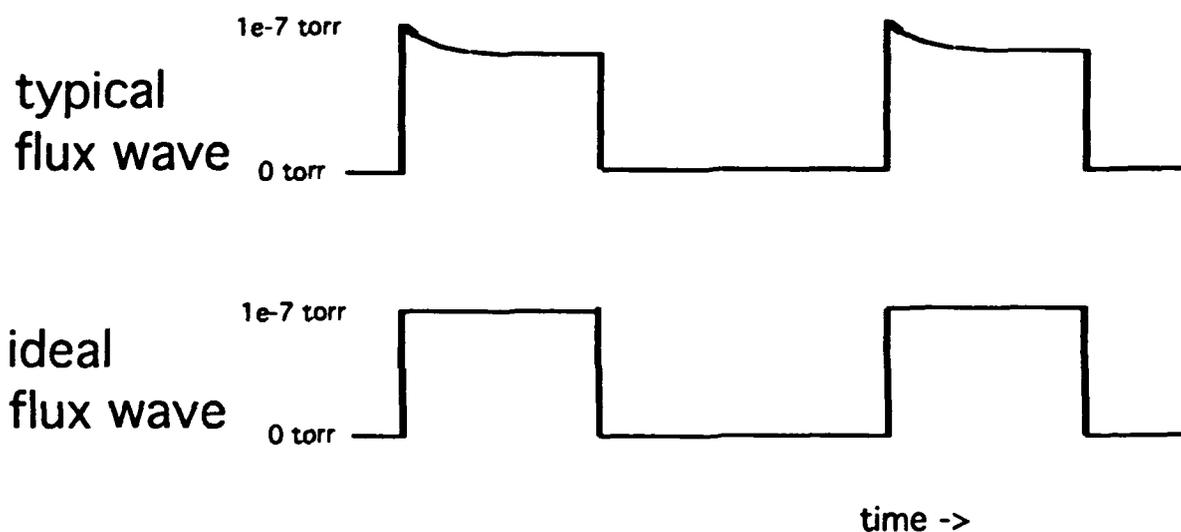


Figure 2: Comparison of a typical flux waveform with an ideal flux waveform.

Directorate is in the process of upgrading all existing 825 controllers on its Varian MBE machine to 905 controllers.

The effectiveness of the compensator whether it is a 818, 825 or 905 depends on how well it is tuned. An automatic process identification system called the Process Discovery Autotuner and an Adaptive Gain/Bandwidth Controller have been developed to utilize the control capability of the PID controllers effectively.[2][3] The Process Discovery Autotuner determines the characteristics of all the Knudsen cells over their entire operating ranges. This information is used by the Adaptive Gain/Bandwidth Controller to select ideal PID controller parameters depending on the situation. Under static conditions the Adaptive Gain/Bandwidth Controller operates as a gain scheduler (i.e. the P, I and D parameters chosen depend on the temperature) Under dynamic conditions the PID Controller is manipulated so that a temperature change is completed as quickly as possible. The Process Discovery Autotuner and the Adaptive Gain/Bandwidth Controller have been implemented and tested on a test cell. A

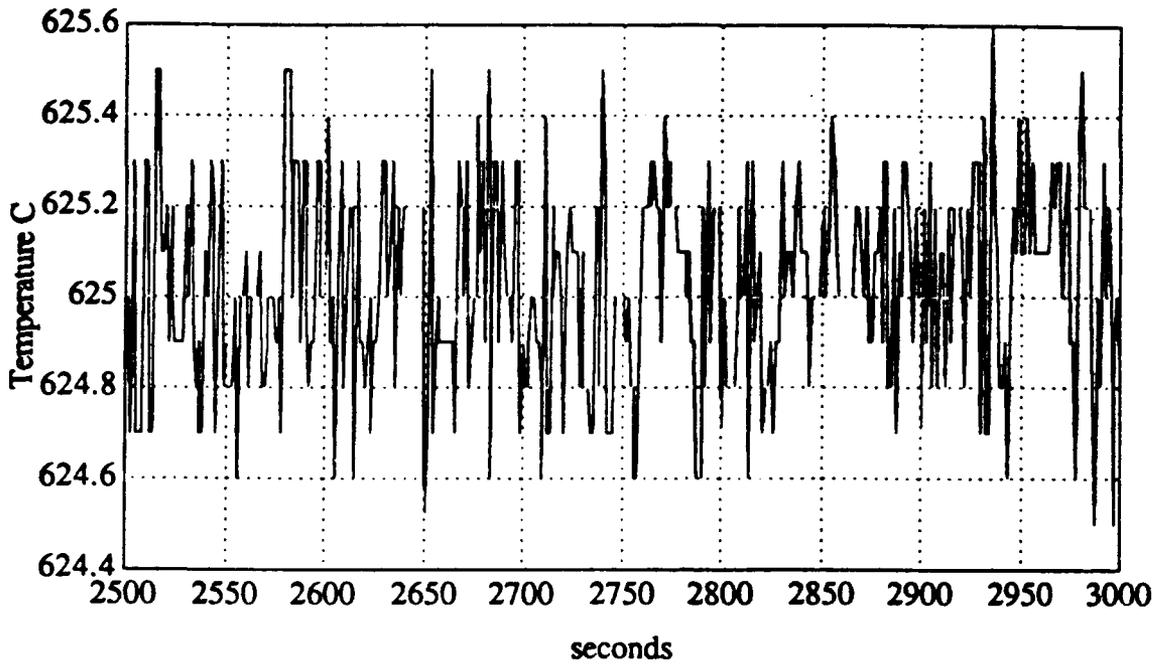


Figure 3a: Thermocouple temperature stability with the 825 PID Controller

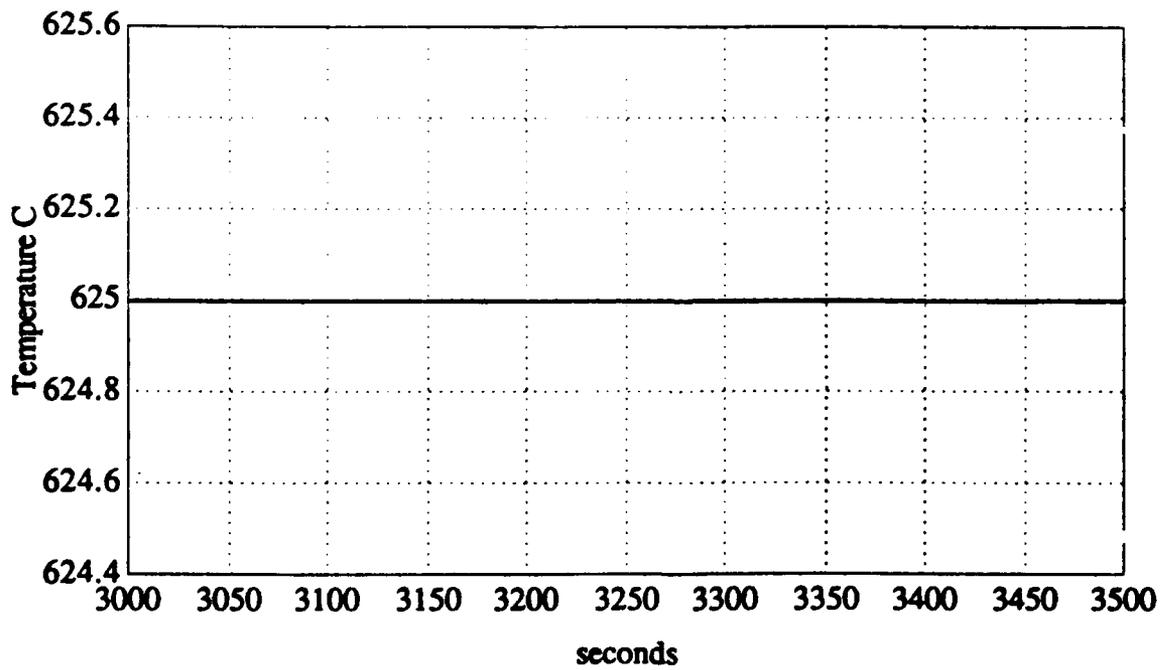


Figure 3b: Themocouple temperature stability with the 818 PID Controller

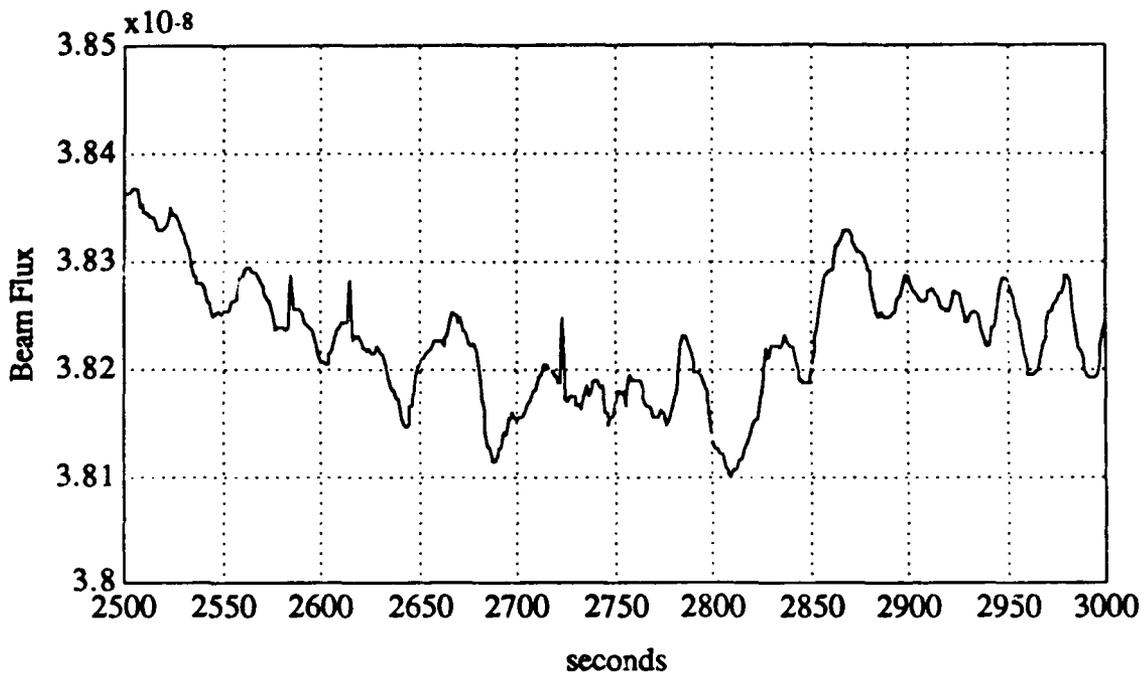


Figure 4a: Flux stability with the 825 PID Controller

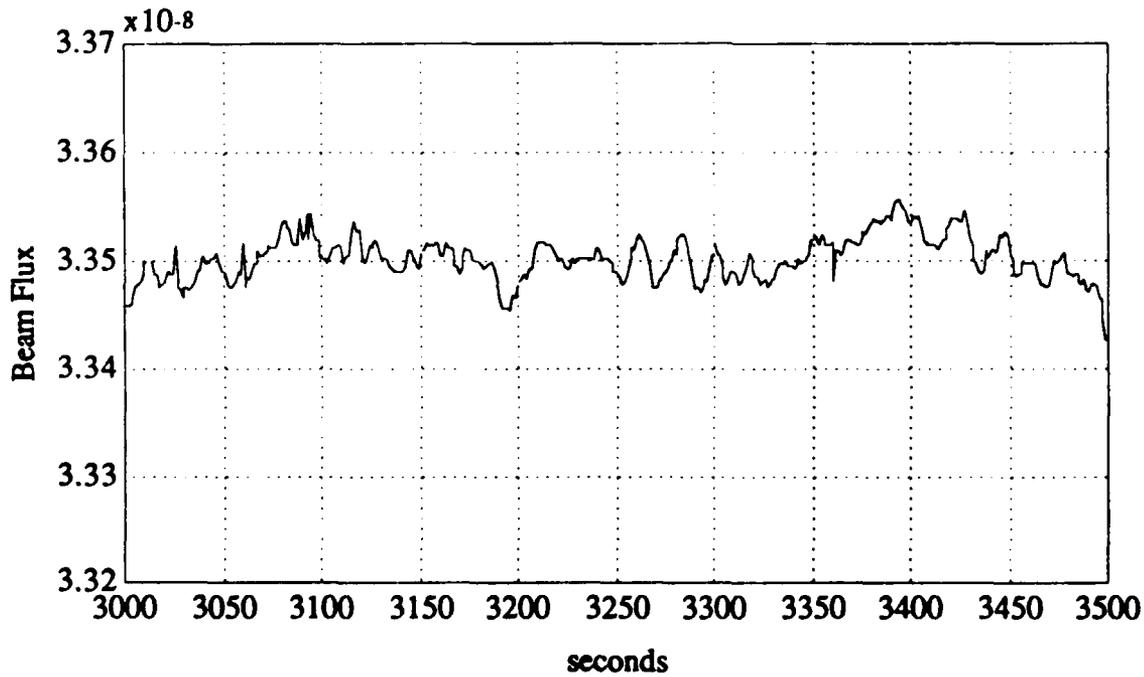


Figure 4b: Flux stability with the 818 PID Controller

thorough analysis of their capability is included in Reference 2. Implementation on an MBE machine is nearing completion.

An open loop compensator called the Shutter Opening Transient Compensator complements the Adaptive Gain/Bandwidth Controller. When the shutter is opened (or closed) the load on the Knudsen Cell furnace changes resulting in a flux transient as in the typical flux waveform in Figure 2. The surface of the material, from which the flux emanates, changes temperature immediately upon shutter opening whereas it takes a period of time before the PID controller realizes a change has taken place (because the thermocouple cannot be placed directly on the actively evaporating surface) and increases power. There is then a delay period before this increase in power reaches the melt surface (because the heating coils are not immediately at the melt surface). Although the PID controller maintains the thermocouple temperature at the setpoint, the melt surface temperature and the flux stabilize at lower values than with the shutter closed because of the increased thermal load.

The Shutter Opening Transient Compensator anticipates the additional thermal load and begins sending additional power to maintain a constant flux in advance of shutter opening. This type of compensation has been explored by other groups, however has not been incorporated into a MBE Control System.[4][5] To be integrated with other components of the control system, the Compensator must be robust enough to work with a variety of cell sizes and materials.

The Shutter Opening Transient Compensator, similar to the Adaptive Gain/Bandwidth Controller, relies on automatic process identification experiments such as measurement of the response of the Knudsen Cell to shutter opening. This information is used by the compensator to calculate a series of temperature setpoints so the correct energy to maintain the surface temperature of the melt is delivered each second.

Figure 5 compares the flux with and without Shutter Opening Transient Compensation. This experiment was conducted using the Indium cell. Equation 1 describes the compensation curve used which was derived using a Laplace Transform Analysis.[6] The process identification experiments were conducted manually. The first experiment is to measure the response to a shutter opening. The second is to measure the response to a setpoint change.

$$\Delta T_{\text{feedforward}} = \frac{\Delta T \times \Delta F_D}{\Delta F_P} \left( 1 + \frac{(t_P - t_D)}{t_D} e^{-\frac{t}{t_D}} \right) \quad (1)$$

where

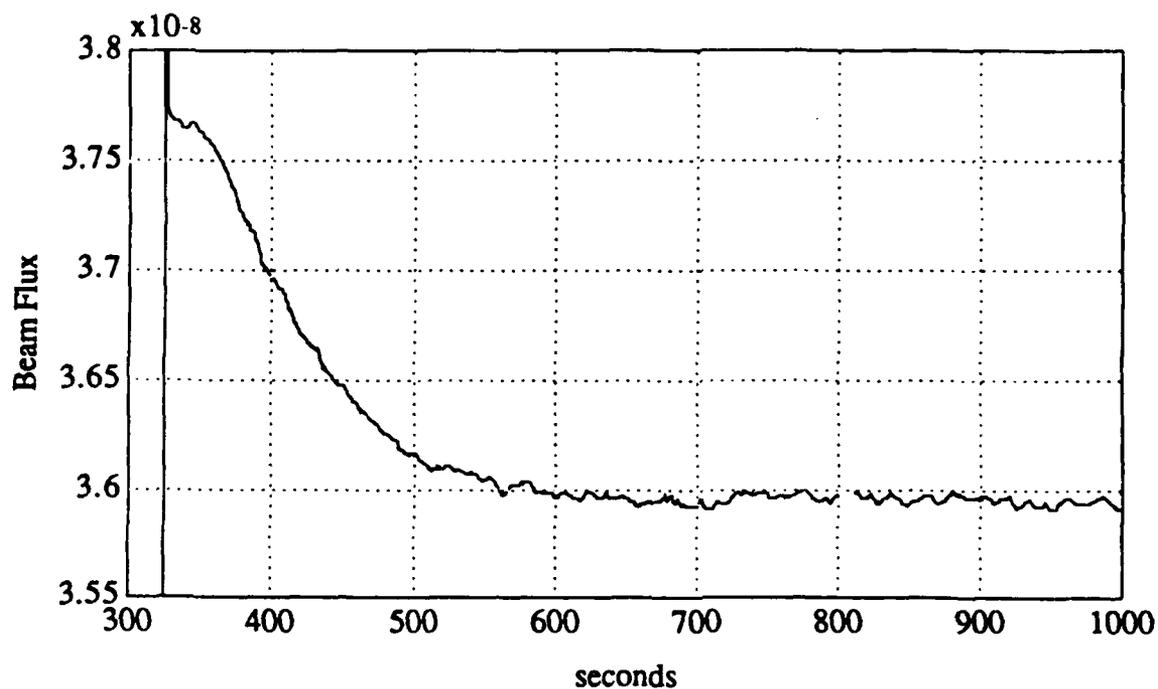


Figure 5a: Flux at shutter opening without Shutter Opening Transient Compensation

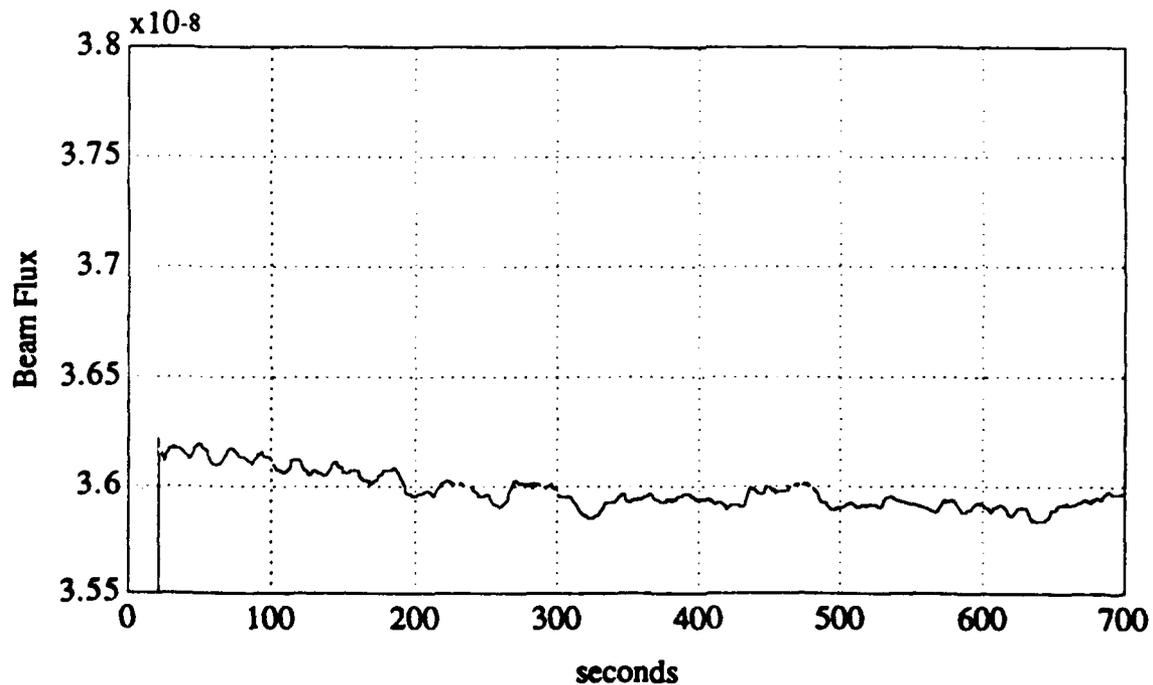


Figure 5b: Flux at shutter opening with Shutter Opening Transient Compensation

- $\Delta F_D$  - Total change in flux from experiment 1.
- $\Delta F_P$  - Total change in flux from experiment 2.
- $\Delta T$  - The temperature setpoint change for experiment 2.
- $t_D$  - The time constant for the response in experiment 1.
- $t_P$  - The time constant for the response in experiment 2.

The relationship of the flux to setpoint temperature for all the Knudsen Cells over their entire range, commonly referred to as the Beam Equivalent Pressure (BEP) curve, is also measured during Process Identification. The Flux Setpoint Controller uses this information so that the operator only needs to specify the desired flux rather than a temperature setpoint. A history of these curves can be used to track the level of material left in each Knudsen cell.

The purpose of the Inner Loop is to enable the MBE machine to produce consistent and accurate fluxes which will greatly improve the Self-Directed Control Loops ability to consistently produce the specified recipe. The interaction of the modules of the Inner Loop and Self-Directed Control Loop is shown in Figure 6. In the hierarchy, the Self-Directed Control System is one level above the Inner Loop.

### 3. Self-Directed Control Loop

The Self-Directed Control Loop uses information from sensors which monitor the material behavior (composition, thickness, etc., of the thin-film) to control the growth of the thin-film. The practicality of such control depends on the availability of advanced sensors and knowledge to adjust the process trajectory *in situ* given the process state.[7] This knowledge is stored in a rule base and is acted upon by an inference engine as shown in Figure 7. This system can be thought of as an expert system which interacts with a machine rather than a person.

A Self-Directed Control System, called the Alpha Controller, which uses the Reflective High Energy Electron Diffraction (RHEED) Sensor to monitor film growth rate and surface roughness has been demonstrated to control the process.[8] This system was designed to improve the control of constituent layer thicknesses and interface sharpness. This system demonstrated the principle of self-directed control on MBE, but was not practical for a production environment. RHEED may cause carbon absorption in the thin-film as well as some surface damage. Alternate sensor technology is needed for the Self-Directed Control Module of the MBE Control System.

Optical sensors are currently being investigated at the Wright Laboratory to fill this void.[9] In contrast to RHEED, the operation of an optical sensor is

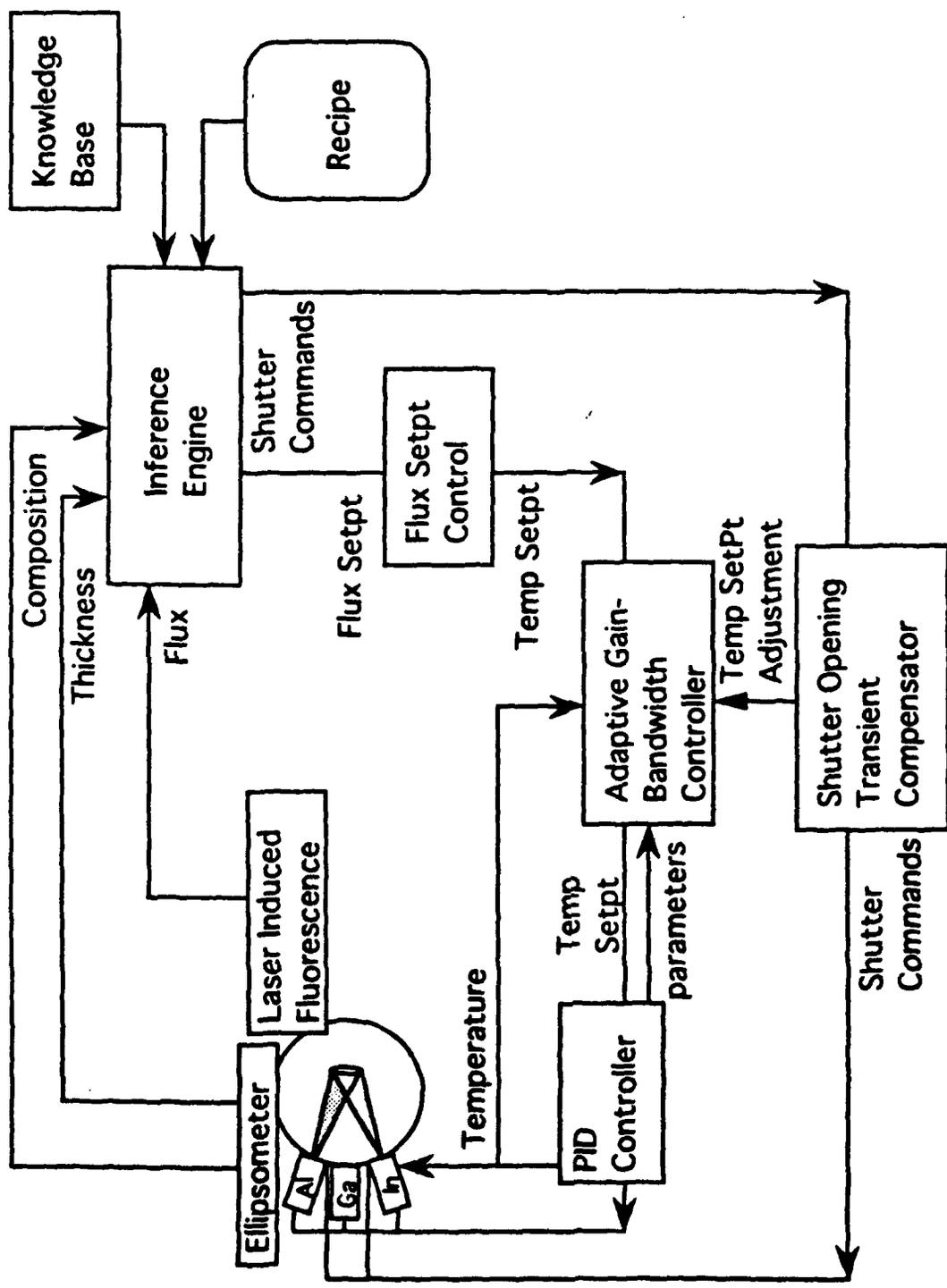


Figure 6: Interaction of the Inner Loop and Self-Directed Control Loop modules

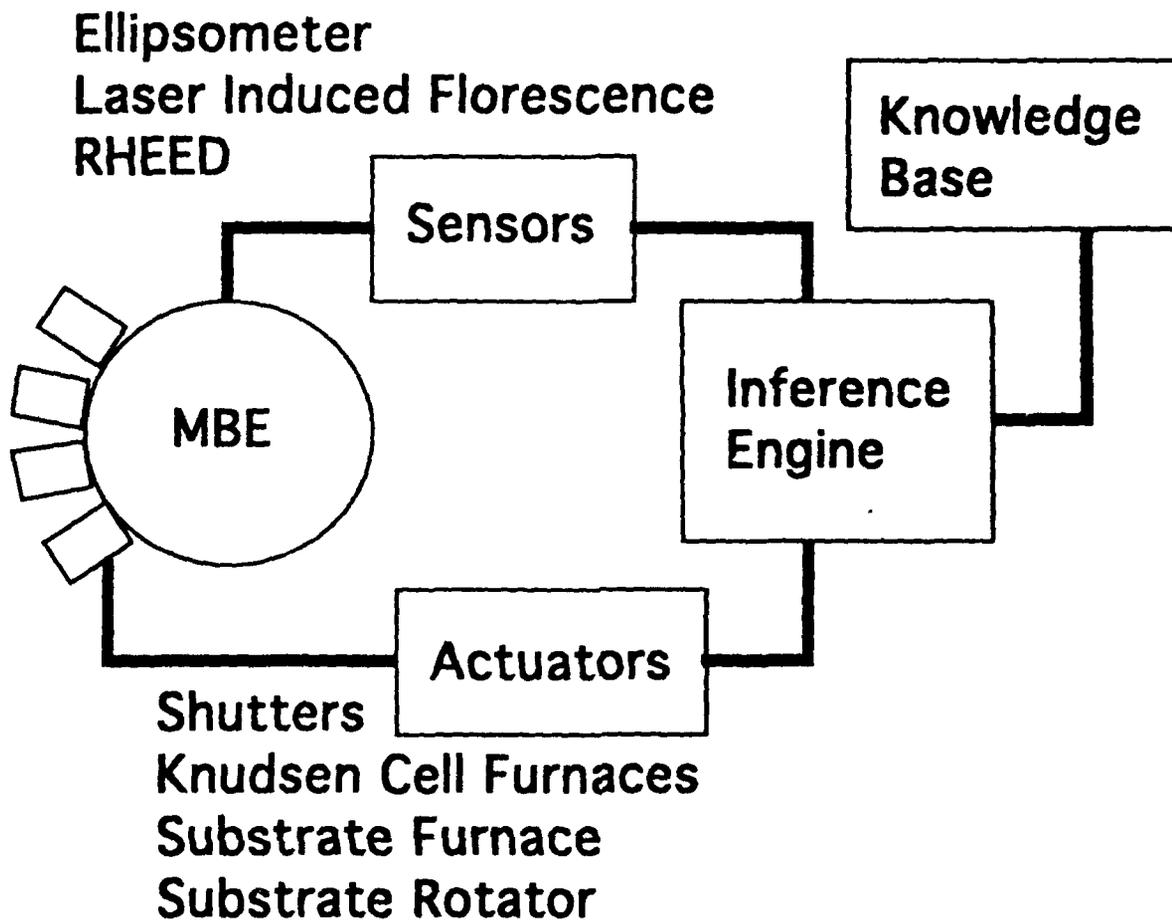


Figure 7: The Self-Directed Control Loop

unlikely to affect the growth in any way. One technique, Ellipsometry, potentially can provide real time information on the composition, thickness, strain, surface morphology and surface temperature. If multiple wavelengths of light are used then more than one piece of information can be obtained at the same time. Another optical technique, Laser Induced Fluorescence, can be used to measure the flux of various elements with high accuracy during the actual growth process.

A new inference engine and knowledge base have been developed using the C programming language and the Macintosh Computer to replace the Alpha Controller which was written on an IBM clone using the FORTH programming language. A demonstration of this system running a simulation of the MBE process is shown in Figure 8. The recipe is described in the top right corner. Four signals are plotted: Aluminum (Al) temperature, Gallium (Ga) temperature, composition and Layer Thickness. A process disturbance is invoked in this simulation; the amount of material in the Al Knudsen Cell is suddenly changed from 100 to 95 units. The simulator determines that since there is less material in the Al cell, the Al flux will also be less. Less Al flux causes the composition, the proportion of Al to all Group III molecules, to decrease. The expert system is monitoring the instantaneous composition. Since the target composition is  $Al_{0.5}Ga_{0.5}As$ , the expert system recommends an action to restore the composition, "Increase Al temperature". Eventually the target composition is restored.

The Layer Thickness which is the number of monolayers deposited in the current constituent layer is reinitialized and a new set of shutters is opened after each layer is completed. In Figure 8, when Layer Thickness was reinitialized after 40 monolayers, the Si shutter was opened.

Although the Self-Directed Control Loop is capable of growing the recipe specified, obtaining the desired product behaviors is not ensured because product behaviors can only be measured post process. For instance, the mobility of a material can only be measured using *ex situ* characterization techniques. In the case of an IR Detector the frequency of light to which the material is most responsive can only be measured using *ex situ* characterization techniques. A third loop, the Ex Situ Loop, is included in the MBE Control System to make the connection between the desired product qualities and the command inputs in order to speed up the development process for new materials.

#### 4. Ex Situ Loop

A secondary but important motivation for the Ex Situ Loop is to learn new facts and trends about the growth process. For example a trend relating Vacancies formation, Quality #6, and the control inputs may be identified.

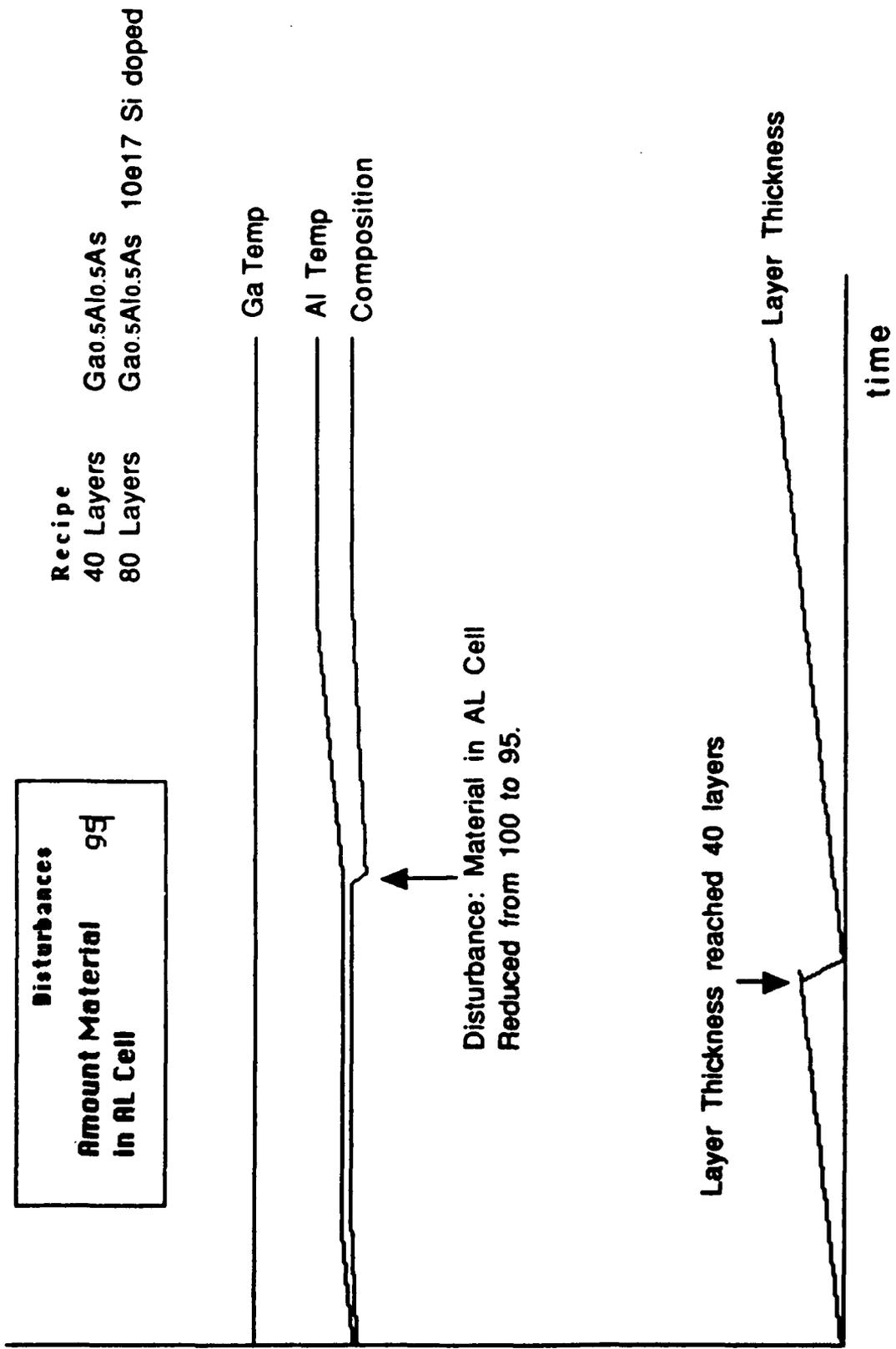


Figure 8: The Self-Directed Controller running an MBE Simulator

With this knowledge, a strategy for minimizing crystalline defects can be formulated and implemented thus improving material quality.

The Ex Situ Loop consists of a neural network model of the process, shown in Figure 9, and a data base preprocessor.[10] Data from each growth run is stored in the database and is selectively used to train the neural network. Once trained the neural network model is used to recommend process inputs, including the recipe, to obtain material outputs desired. The neural network model can also be used to predict the material qualities given a set of process inputs as in the following experiment.

A neural network model was trained with data from a family of 13 growths of bulk, silicon doped, GaAs. The model was used to predict the layer thickness and mobility of 5 other growths of bulk, silicon doped, GaAs. The Mean Absolute Percent Error for layer thickness was 11.79% and the Mean Absolute Percent Error for mobility was 7.52%. A portion of this error is due to the accuracy limitations of the characterization techniques used to compile the training set. For instance, the accuracy of the Photo Hall Measurement which is used to determine the mobility is  $\pm 5\%$ . The size of the training set is very important; a larger training set will reduce the error. Selection of a complete set of inputs is also very important. For example, an input that reflects the quality of the substrate is currently not included. Assuming all substrates are of equal quality may not be sufficient. Also, the temporal variation of the command inputs is not included. A variation due to a power surge cannot be represented by the input set. A lack of significant temporal variation is assumed.

Data collection has been challenging partially due to the sensitive nature of the MBE process. The Ex Situ Loop will be most effective when one MBE machine is used to develop a new material system during a short period of time. Eventually, full implementation of the Ex Situ loop should allow for rapid convergence to appropriate growth conditions for new material systems that have not previously been grown by MBE.

## **5. Other Features**

Together the Inner Loop, Self-Directed Control Loop and Ex Situ Loop form the core of a comprehensive control system for MBE. This System is being developed in Think C on a Macintosh IIfx. The system is extremely user friendly as expected from a Macintosh application. Easy access to PID controller parameters and a complete data logging capability are provided as shown in Figure 10. Windows for configuring setup and for inputting recipes can be called from the menu. A health monitor checks for thermocouple failure, temperature setpoints that are outside the normal operating range, adequate liquid nitrogen flow through the cooling shroud and adequate vacuum. Other checks

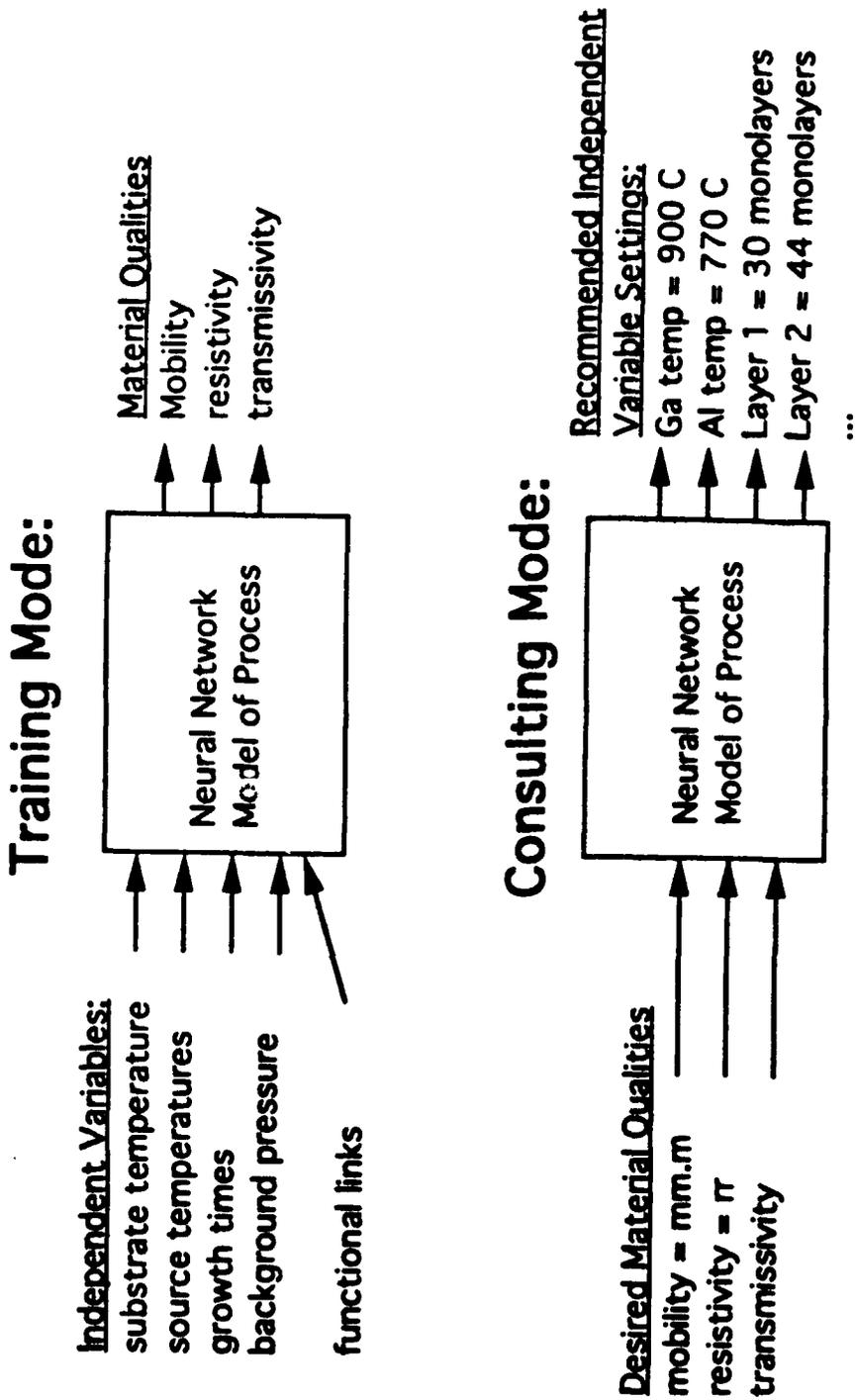


Figure 9: The Neural Network Model of the Process

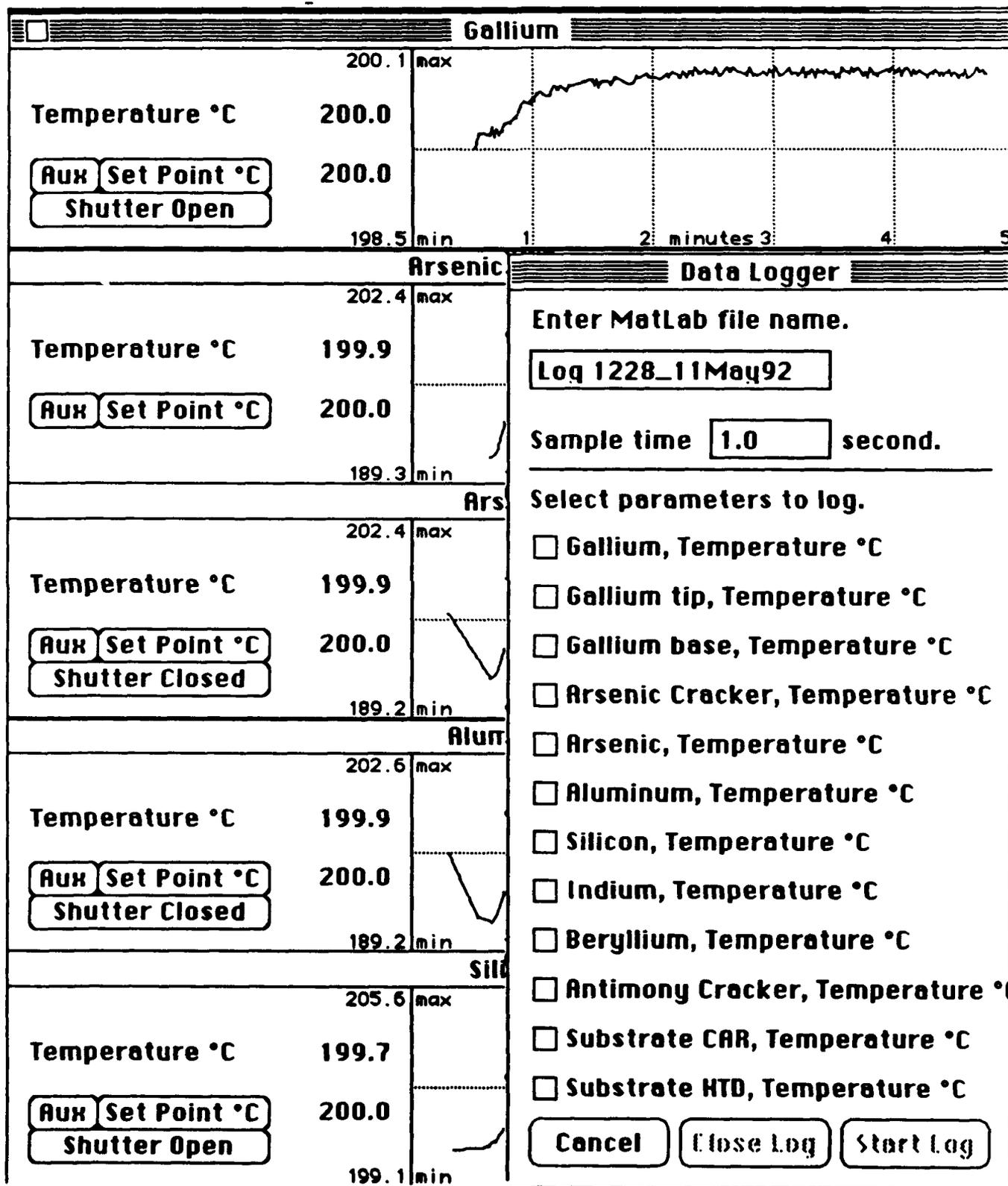


Figure 10: Eurotherm Windows and Data Logger Window

can be added as deemed necessary. Several versions of this system have controlled the Varian MBE machine at the Air Force Materials Directorate over the past year.

## **6. Conclusions**

The capability of the MBE process can be greatly improved through the application of advanced computer control techniques. The Air Force Materials Directorate is developing a unique three level feedback control system. Experimental data has shown that the Inner Loop improves the precision and tracking of the flux and substrate temperature. The robustness of the Inner Loop modules is being developed. The Self-Directed Control Loop enables the quality of the material to direct the process. A knowledge-based expert system uses real time material quality data to choose new command inputs several times per second. This system has the potential to eliminate material variability, limited only by the accuracy of the sensor data. Promising new optical sensor technology is being developed for this control loop. The Ex Situ Loop will speed up development time of new material systems. A continuously evolving neural network model of the process will recommend the recipe and command inputs to obtain desired material qualities. Development of this system is very challenging because gathering data is both difficult and time consuming and the completeness and availability of the inputs has yet to be determined. The components of the control system, interacting in a hierarchical structure, have great promise for improving the consistency and quality of material produced using MBE.

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