

76
13
Applying CLIPS to Control of Molecular Beam Epitaxy Processing

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1. Introduction

A key element of U.S. industrial competitiveness in the 1990's will be the exploitation of advanced technologies which involve low-volume, high-profit manufacturing. The demands of such manufacture limit participation to a few major entities in the U.S. and elsewhere, and offset the lower manufacturing costs of other countries which have, for example, captured much of the consumer electronics market.

One such technology is thin-film epitaxy, a technology which encompasses several techniques such as Molecular Beam Epitaxy (MBE), Chemical Beam Epitaxy (CBE), and Vapor-Phase Epitaxy (VPE). Molecular Beam Epitaxy (MBE) is a technology for creating a variety of electronic and electro-optical materials. Compared to standard microelectronic production techniques (including gaseous diffusion, ion implantation, and chemical vapor deposition), MBE is much more exact, though much slower. Although newer than the standard technologies, MBE is the technology of choice for fabrication of ultraprecise materials for cutting-edge microelectronic devices and for research into the properties of new materials.

Investigation of MBE processing science and technology is one of the foremost goals of the Space Vacuum Epitaxy Center (SVEC) at the University of Houston. SVEC, a NASA-sponsored Center for the Commercial Development of Space, is a consortium which includes a number of industrial, academic and government members. Research at the Center includes both study of MBE science at the basic level and investigation into advanced MBE techniques and applications. SVEC's centerpiece project is the Wake Shield Facility (WSF), an orbital MBE laboratory which holds promise for unparalleled quality and volume of MBE processing. The first flight of the WSF is scheduled for April 1992, at which time it will be held at the end of the Shuttle's manipulator arm for an experimental run lasting about two days.

As will be seen below, each individual MBE experiment is a relatively slow process, with a mixture of many straightforward features and some requiring careful attention by an experimenter. Without computer automation, MBE is manpower-intensive to the extent of absorbing a large amount of researchers' time. Fortunately, it is relatively simple to apply automatic control to a typical MBE production system with a PC-class microcomputer. This has been done with the laboratory MBE system at SVEC, using a PC-AT computer to control the sequencing of basic experiment actions. However, the conventional program used to control the experiment is relatively inflexible in any unusual or contingency situation. To remedy this situation and take the place of the experimenter as much as possible, an expert system addition is being developed at SVEC using the CLIPS (C Language Integrated Production System) expert system tool. The applications and implementation of this CLIPS application are described below.

2. Overview of Molecular Beam Epitaxy

The term epitaxy refers to the accumulation of atoms on a surface in an orderly fashion. This means that, if atoms accumulate epitaxially on a crystalline surface, the new atoms will form a crystalline structure that duplicates and extends the lattice of the

original crystal¹. In MBE parlance, the original crystal surface is known as a "substrate" and the deposition-accumulation process is simply called "growth." In the ideal case of epitaxial growth ("two-dimensional" or "layered" growth), hot atoms falling on a hot crystal will have enough kinetic energy when they hit the substrate to migrate to an unoccupied, energetically-favorable spot on the surface where it bonds with neighbor atoms to form flat surface "islands." Thus, the material being deposited will form in ordered layers a single atom thick.

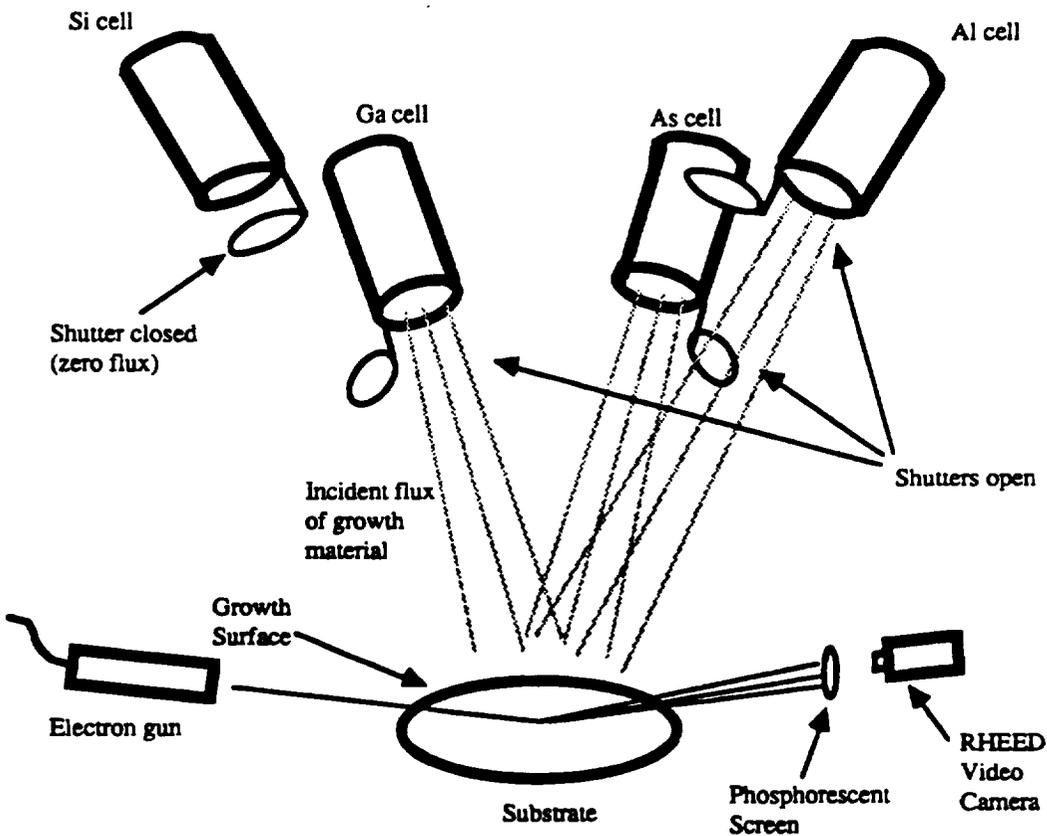


Figure 1. MBE Processing (Growth of AlGaAs film)

MBE growth is achieved by directing a flux of the desired growth materials onto a substrate, which must be in an ultrahigh vacuum (UHV) on the order of 10^{-11} torr to avoid contamination of the growth surface (1 atmosphere = 760 torr). The deposition flux is provided by beams of atoms evaporated from solid ingots heated in cylindrical

crucibles ("cells"). A typical MBE growth process, in which layers of aluminum gallium arsenide (AlGaAs) are deposited on a GaAs substrate, is illustrated in Figure 1. The process and apparatus shown are enclosed, in the laboratory, in a stainless steel vacuum chamber pumped down, baked out at about 200° C for about two days (to drive out contaminants from the chamber walls) and pumped down further to its final operating pressure using ion and turbomolecular pumps.

3. MBE Processing

The basic method of MBE growth is fairly straightforward. As shown in Figure 1, the substrate is placed in front of the deposition sources (effusion cells) which contain ingots of the material to be deposited. The substrate is heated to drive off surface oxides and other impurities and then is adjusted to the proper temperature for favorable surface growth conditions. The cells which are to be used are also heated to drive out impurities, and are then adjusted to the proper growth temperatures, i.e. the temperature for each cell which yields the proper evaporated flux of its deposition material. Care must be taken during this step to avoid thermally stressing the ingots as well as the crucibles themselves. When the proper temperatures have been attained, flat shutters covering the aperture of the appropriate source cells are opened, permitting evaporated atoms from the cells to reach the substrate "target". (It should be noted that even with the sources active, the entire growth chamber is still in a hard vacuum by most standards.) Atoms from the active cells (in this example, aluminum, gallium and arsenic) spray onto the substrate and collect in an ordered manner, forming a lattice on the substrate in a layer-by-layer manner (if the growth parameters are correct and impurities are minimized). A typical growth rate is about one monolayer (single atomic layer) per second, or about a micron per hour. Typical temperatures involved are approximately 150° C for the substrate, 200° for the As cell, 1050° for the Al cell and 950° for the Ga cell.

The principle means for determining the rate and characteristics of the growth is electron diffraction monitoring, also as shown in Figure 1. In this technique, called RHEED (Reflection High Energy Electron Diffraction), 10 keV electrons are fired at a grazing angle onto the substrate as growth occurs. The electrons are diffracted by the top few layers of atoms on the growth surface, and the constructive and destructive interference forms a diffraction pattern on a phosphorescent screen opposite the electron gun. A video camera is used to monitor the pattern, which can indicate whether two-dimensional growth is occurring or not, and what the surface crystal characteristics are. A trained MBE physicist can determine whether or not the growth process is occurring satisfactorily by looking at the screen, and adjust the parameters accordingly. Also, since layered growth produces regular cycles from maximum constructive to maximum destructive interference in the diffracted beams, the physicist can tell how many monolayers have been deposited by simply counting the number of cycles of intensity in the diffraction pattern.

4. Control of MBE - Hardware

There are a variety of devices in an MBE system with a mixture of instrumentation and control interfaces. These are summarized in Table I below. The most important

control devices are those which operate the cells, which are viewed from a control standpoint as the effusion sources and associated shutters taken together. Under optimum circumstances, a particular cell will yield a known flux of its material when its temperature reaches a certain setpoint and its shutter is opened. If all conditions were known and constant, it would be possible to obtain highly reproducible results from run to run without any monitoring.

Table I. MBE Instrumentation and Control Interfaces

Device	Function	Interface
Source Cell	Source effusion	Heater driven by programmable power supply Power supply driven by controller voltage signal Controller driven by serial command link: Setpoint from computer Power signal from controller
	Temperature sensing	Power (voltage, current) from power supply Thermocouple voltage signal to controller Controller reports voltage via serial data link
Shutter	Flux modulation	Shutter motor driven by digital control board Control board driven by computer digital output
Ion Gauge	Pressure sensing	Sensor generates analog reading of pressure Computer A/D reads sensor signal
Mass Spectrometer	Composition analysis	Mass spec generates numeric readings Computer starts/reads via serial comm link
RHEED	Electron gun	Electron gun controlled by voltage signals Computer D/A generates voltage signals

Of course, the conditions of neither the effusion cells nor the other parts of the growth chamber remain the same. A variety of sensors are used to provide feedback from the source cells themselves (controller signal level, thermocouple reading, power supply levels) and from other devices which monitor the flux of the beam and chamber environment (ion gauges, mass spectrometer). Information from these sensors is used not only to monitor the proper progression of an experiment and watch for fault conditions but also to confirm settings of previous growth runs and to calibrate settings against each other when system modifications are made.

The usage of the devices discussed above is illustrated by analyzing the growth process shown in Figure 1 with referral to Table 1. We consider the growth of aluminum gallium arsenide (AlGaAs) on a typical substrate, e.g. gallium arsenide (GaAs). Initially, the substrate and sources are all at standby temperatures (Al: 600° C, Ga: 500° C, As: 100° C, substrate: 100° C) with all shutters closed. The first step is to warm up the

sources and substrate to growth temperature (Al: 1050°C; Ga: 950°C; As: 200°C, substrate: 160°C). This is done by the computer issuing a serial command to the temperature controllers to hold a certain setpoint. In each case, the source or sample must be ramped or "staircased" up in temperature through a certain range in which it is especially vulnerable to undue thermal stress. (The aluminum, for example, is actually molten at growth temperature and must be eased through a phase change.) Also, before reaching their final values, each source/sample is heated above its growth temperature by a small amount to drive off surface contaminants and oxidation. The sequence of warming up the system can take up to about two hours.

When all temperatures have been reached as indicated by the temperature controller readings (measured via thermocouple), the sources are checked for proper flux. This is done by opening the shutter for each cell (by generating a discrete digital signal to the shutter motor controller) and checking the value of its pressure reading with an ionization gauge. (These readings should agree from run to run within about 25 percent.) The desired fluxes are obtained by adjusting the cell temperatures up or down. With all cells properly set, the shutters for (in this case) the aluminum, gallium and arsenic cells are opened and growth begins. At this point, growth is now monitored by using the ionization gauges and mass spectrometer to check the deposition fluxes and the RHEED pattern to verify that epitaxial growth is occurring as planned. When the experiment is finished, the shutters are closed and all temperatures are taken down in reverse sequence to standby temperatures.

5. Control of MBE - Software

Epitaxy process control, as seen above, does not generally require much rapidity of response or analysis on the part of the controlling system, unlike most "real-time" process applications. This fact has enabled us to develop the MBE control software for the SVEC laboratory to satisfy other important requirements, namely: (1) the need to isolate software development from the hardware as much as possible to accommodate changes and transfers to other systems; (2) the need for ease of software development and maintenance in an academic environment with regular personnel changes; and (3) the need for an open architecture to allow additions and other upgrades (such as integration of CLIPS into the software).

Based on these needs, the primary MBE control software at SVEC has been designed to be modular and functionally layered. Modularity, i.e. separation of different software functions into individual units, allows for rapid development of the code by relatively uncoordinated individuals and groups of programmers - again, a desirable feature in an academic setting where regular schedules are difficult to set. Layering allows for a clean separation of the details of the system hardware from the purpose and form of the control software itself. This eases design of the code to make it user-friendly and useful for experimenters who are concentrating on science aspects rather than on esoteric details of programming. In effect, it enhances contact between the highest level of the experiment - the user - with the basic level - the physical processes going on in the MBE growth itself.

The layering begins at the lowest level, that of hardware. Although most MBE chambers and supporting equipment are essentially similar, the control and data-acquisition interfaces vary widely from manufacturer to manufacturer, so the "look" of

the devices to the controlling system can be very different. At the hardware level, then, nothing is assumed other than the basic kind of information the devices collect and accept. The types of parameters which are measured/controlled (e.g., flux of gallium atoms, temperature of the substrate) are known but the manner in which they are changed or monitored is a detail which varies as the laboratory equipment is maintained or upgraded. Thus, these details should be encapsulated as much as possible.

This encapsulation or isolation of system hardware details is achieved by the next level of control, the lowest level of software: the hardware-specific front-end code. This code is composed of drivers and linkages which use and manipulate the machine-specific data on the "bottom" side, i.e. that which couples to the hardware. However, on the "top" side, that which deals with the rest of the software, the view is of process parameters such as those mentioned above. The front-end software thus separates the experimenter's model (physical variables) of the MBE process from the programmer's model (e.g., writing a string to a serial port, reading a D/A signal). The modules which perform this function can be changed relatively easily to accommodate different types of equipment, in a manner similar to changing printer drivers on a word-processing program. Unlike those drivers, however, the front-end modules separate conceptual data levels rather than perform a direct translation.

Above this level is the software that deals with the experiment control itself, which is termed the supervisor level. The supervisor oversees the process by dealing with the process variables on one hand and the commands issued by the experimenter on the other. It performs the timing functions for the experiment, setting temperatures, waiting for setpoints to be reached, opening and closing shutters at predetermined events or intervals, and checking the system for fault conditions. The supervisor software is responsible for suspending operations (closing the shutters, possibly bringing temperatures down to standby) and notifying the experimenter in event of a fault. A fault could be anything from a temperature controller time-out reported by the front-end software to an out-of-range condition on a cell (e.g., measured temperature above high operating limit). Such software, implemented in Turbo Pascal version 5.0, has been in operation at SVEC on a trial basis for about four months and shown acceptable performance running on an AT-class computer. Current capability involves cell temperature and shutter control, with temperature range-checking implemented. Monitoring of flux (pressure) gauge and mass spectrometer data will be added during the summer of 1990. Feedback on the shutter status, requiring some modifications to the MBE hardware, should also become available during this period.

6. Integration of CLIPS into MBE Control Software

Using the MBE process control software described above frees up time for experimenters to a certain extent. However, it is limited to operating by preset parameters alone. If the process does not fit these parameters as it moves along, the supervisor program can only either continue or suspend the process while signalling for operator intervention. This means that there is still a need for an experimenter to be immediately available for responding to computer-generated events. To compensate for this, we seek to add a layer of higher "understanding" above those described above - a layer of knowledge and guidelines for dealing with the exigencies of MBE growth that does not need a human operator present. The layer we are describing, of course, is an

expert system. The system to be applied to the MBE software is being developed and tested, and ultimately integrated, at SVEC using CLIPS version 4.3.

The modular-layered structure of the conventional MBE process control software makes it easy for CLIPS to be added to the system. The block architecture of the epitaxy control system is shown in Figure 2. Again, the lowest level is the instrumentation and control hardware itself, topped by the front-end software. The front end takes in data in raw form using machine-specific codes and converts them to process-variable information. For control, the data flows and conversion occur in the opposite direction as commands from the supervisor are converted into the appropriate groups of control signals. Above this level, the supervisor code stores and monitors the process data, comparing it to prestored configuration data and "scripts" of process commands entered by the experimenter.

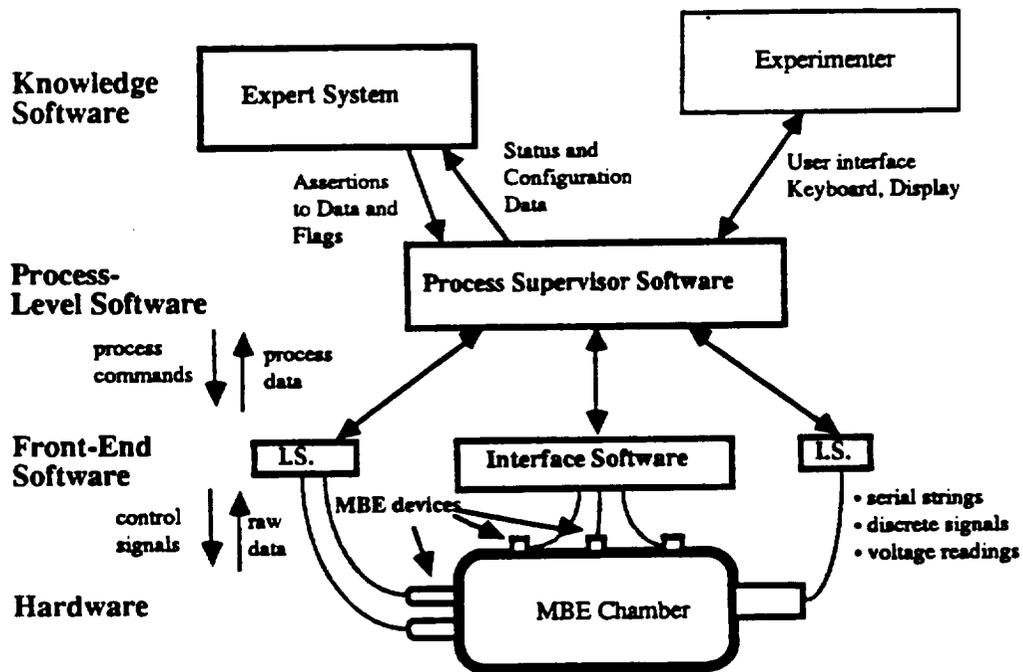


Figure 2. MBE Control Layers

The expert system, as seen in Figure 2 above, fits conceptually into this schematic above the supervisor and "halfway" below the human experimenter. The experimenter, of course, is the final authority on any facet of MBE processing, but when operating unattended, the expert system will have enough of the experimenter's knowledge and experience loaded into it that it will be able to make the same adjustments and decisions an experienced human researcher would make.

The mechanism for implementing this scheme is fairly straightforward. Since the control software discussed in section 5 is written in Turbo Pascal, the code is being rewritten in Turbo C to take advantage of the direct interfacing methods between C and CLIPS². This allows data to be transferred back and forth between CLIPS and the rest of the program. In this program, then, CLIPS is used to "advise" (actually order) the supervisor what to do in a given situation, based on data passed to it from the supervisor, its own rulebase, and data gathered directly by CLIPS.

As an example, consider a typical sequence, wherein the supervisor program obtains a flux reading for the aluminum cell, stores it in a global data area and finds it 50% lower than it should be. The supervisor then pauses the growth (closes the shutters), and then uses the `assert(string)` function to add the facts (flux AI low) and (growth status paused) into the CLIPS knowledge base. The supervisor now uses the `run(iters)` function to call CLIPS and allow forward chaining to proceed. Appearance of the new facts causes rules to fire which retract any previous items about (growth status) and (flux AI). The expert system can now invoke C functions which return data about the cell directly from global storage, such as power and temperature readings. CLIPS then forward-chains with all the data to come to a conclusion about what to do about the misbehaving cell. After reaching a conclusion, CLIPS uses C functions to set flags which tell the supervisor to raise the temperature, notify an operator or any other appropriate action; then control is returned to the supervisor.

Typically, the supervisor would invoke CLIPS after each polling cycle of the MBE devices, i.e. after all the process variables have been refreshed. The supervisor performs the initial checking on the variables as given in the above example; the boundary checks can be performed much faster this way, instead of the expert system individually retrieving and testing each piece of data. When called, CLIPS can be allowed to run to completion if a contingency condition exists, or otherwise can be restricted to run through a small number of rules at a time. Another consideration on invoking the expert is the mode of experiment at the time. For example, during experiments in Atomic Layer Epitaxy (ALE), the experimenter attempts to grow single monolayers of atom, which requires rapid (<1 sec) cycling of the shutters. During this type of experiment, the supervisor will not invoke CLIPS because it is too busy; in fact, all device polling might be suspended during such an experiment. During intermediate-speed runs, CLIPS would definitely be called with a firing limit of just a few rules.

7. Application of CLIPS to MBE Processing

As illustrated in the example above, CLIPS has two basic roles in the MBE processing system. The first is the monitoring and adjustment of growth parameters which are not at their desired points; this is required quite often in MBE work even when there is nothing "wrong" with the MBE apparatus. It is a combination of a number of quite normal factors, which MBE experts have learned to work around - results are simply calibrated for the changed parameters. Naturally, there are also times when an errant parameter is the result of a malfunction in the control or process hardware. The second role of CLIPS, then, in the MBE control software is to guard the process and handle such situations while preserving in order: (1) safety, (2) chamber function and (3) as much as possible in the way of experimental results.

As an example, consider the operation of an aluminum (Al) effusion source cell as depicted in Figure 3. During a growth run, we set the cell (actually, the temperature controller driving the power supply driving the heater filament) to a certain temperature setpoint. At that setpoint, there should be a certain flux ($\pm 25\%$ from run to run), a certain power signal level reported by the temperature controller to maintain the setpoint, and a certain range of voltage/current readings from the power supply itself as it pushes power through the resistive coil of the heater filament. The temperature of the cell is measured by a thermocouple touching the back of the crucible; the voltage generated across the thermocouple is measured and interpreted by the temperature controller, which is calibrated (presumably) for the correct thermocouple type.

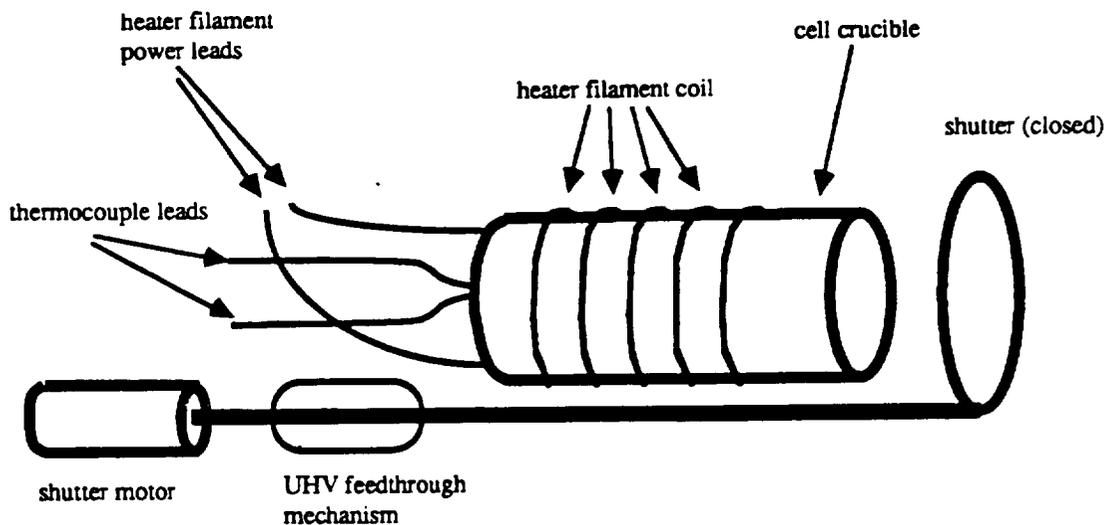


Figure 3. MBE Source Cell

Suppose, for example, that we measured an aluminum flux that was too low - clearly out of the bounds of normal variation - for the current temperature setpoint during a growth of AlGaAs. Can the use of CLIPS help here? It can - especially if the experimenter currently running the machine is relatively inexperienced, and thus not sure of all the system's possible behaviors. This situation is analyzed by an MBE expert in the following manner:

- Is the temperature controller power reading too high for the established setpoint? If so, there is probably a partial break in the filament. This is easily checked by measuring the resistance across the leads to the cell heater filament.
- Is the controller power reading too low? The thermocouple setting on the temperature controller may be wrong. This is also easily checked and corrected by using

the front panel keys on the temperature controller. If this is not the problem, then the thermocouple may have shifted position and be touching or close to the filament. This can only be checked by removing the cell, which exposes a UHV chamber coated with arsenic dust to the air. This means full clean-room gowns and masks for all personnel while the inspection is made, and another lengthy bakeout period to restore the chamber to operation. This is the least desirable option. The optimum action is to attempt to change the cell setpoint until the desired flux is measured, ignoring the temperature measurement, and continue the experiment.

- Is the controller power reading normal? There may be several causes. The shutter may not have moved fully out of the way and is partially blocking the cell aperture. This is easily checked through a chamber inspection port, and is fixed by adjusting the cell motor position. If the shutter position is correct, then the problem may be a cracked cell, caused by thermal stress as discussed previously. When this happens, liquid aluminum flows out of the cell and onto the filament and chamber wall. The determination for this is to look for a filament shorted by the spilled aluminum. This can be detected by looking at the power supply - is the current very high and the voltage correspondingly low? If not, the cell may simply be empty - all the aluminum has been used. Unfortunately, there is no way to tell with the chamber closed. Repairing either of the last two problems, of course, requires opening the chamber, with all the problems mentioned above.

As seen above, the condition we could describe as (flux Al low) can have a number of causes and remedies of widely varying complexity. The value of an expert system here is that this knowledge can be codified quite nicely for entering onto the system, so it can deal with the contingency competently. The system could notify the operator and ask for the results of the non-intrusive checks above, and make a recommendation. If running unattended, the system could halt growth of the AlGaAs sample, cover it with a "buffer layer", and proceed with some other useful material (e.g., GaAs) that did not require use of the aluminum cell.

8. Future Applications of CLIPS to MBE Projects

There are some important uses for CLIPS-using MBE control software waiting in the very near future. One is the use of the expert system to analyze RHEED data. As discussed before, RHEED is the primary analytical "real-time" tool for assuring proper epitaxial growth of a sample. There are two main types of RHEED data: one is the counting of layers deposited during the growth process. This information has been successfully extracted with a computer at SVEC by taking the Fourier transform of the oscillations of diffracted RHEED beam brightness³. The other application, use of the actual diffraction-pattern geometry to determine growth modes, will require the integration of pattern recognition and image analysis tools with the expert system to successfully implement on the computer⁴.

Successful incorporation of these RHEED techniques into a CLIPS-using epitaxy control system will greatly enhance the effectiveness of a much more ambitious project, the Wake Shield Facility (WSF) described in the Introduction. The Wake Shield Facility, currently under construction in Houston, is a circular platform about four meters in

diameter which will be carried in the Shuttle Orbiter payload bay and deployed by the Remote Manipulator Subsystem arm. The platform has a circular shield which faces the direction of orbital motion, pushing aside the incident gas particles which exist at an ambient pressure of about 10^{-8} torr. Since the orbital speed of the platform is greater than the thermal speed of the ambient particles, a low-pressure wake of approximately 10^{-14} torr total pressure is formed behind the shield.

The wake side of the WSF contains the epitaxial growth facility, consisting of a rotating tray ("carousel") of prepared substrate samples, effusion sources (cells) and associated shutters. Monitoring equipment includes, as on the ground-based facilities already discussed, ionization gauges, mass spectrometers, a RHEED system, plus various auxiliary experiments. An 8086-based computer on the Wake Shield will carry out the process sequencing. For the first two flights, all analysis will be done on remote computers via telemetry from the WSF, but the system will then be tested as a free-flying facility which must be able to operate autonomously for days at a time. If successful, this will be the precursor to larger production platforms, operating up to six months at a time while turning out hundreds of ultra-high-quality epitaxial wafers. Such facilities will obviously need a high degree of robust expert control. The use of CLIPS for MBE in the laboratory will provide the development and testing necessary to provide that control.

9. Closing Remarks

We have seen that molecular beam epitaxy is a technology that is well-suited for a control software system using CLIPS as a top-level expert consultant. MBE has a number of well-defined problems which require more expertise than broad knowledge or problem solving to master. Additionally, MBE growth is a slow process which definitely benefits from having a machine take over the task from human researchers, yet has computational loads low enough for CLIPS to be invoked frequently on a 80286-class computer controlling the experiment.

The epitaxial control software at SVEC will integrate CLIPS into a C-language version of a currently-operational Turbo Pascal software package. This will be able to perform standard epitaxial processes in stand-alone mode while dealing flexibly with a fairly broad range of system fluctuations and faults. With the expertise of several MBE researchers at SVEC gradually built up into the system, it will also provide useful training for new personnel at the laboratory, as it has the ability to guide them through the experimental process. The development of CLIPS-using control software at SVEC will eventually lead to use in other facilities, including potentially other MBE research centers as well as the Wake Shield orbital MBE facility.

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AUTHOR INDEX

Al-Mutawa, Souhaila	803	Faul, Ben M.	708
Aldrobi, M.	621	Feagin, Terry	733
Anastasiadis, S.	621	Fenske, T. E.	51
Assal, Hisham	570	Fink, Pamela K.	771
Athavale, N. N.	51	Fischer, Lynn	420
Auburn, Mark	614	Flores, Luis M.	140
			240
Barbee, Diann	881	Frainier, R.	320
Barr, Stanley J.	893	Fritz, Robert H.	347
Barry, Matthew R.	742		
Batra, Sajeev	342	Gathmann, Thomas P.	486
Bensaoula, Abdelhak	926	Geissman, James R.	286
Bhatnagar, Himanshu	554	Geyer, Steve	594
Bhatnagar, R.	320	Glover, John R.	926
Brandt, Larry	881	Goldstein, David G.	603
Braylan, R. C.	375	Gossage, Brett	831
Bretz, R. E.	2	Groleau, N.	320
Brodale, Howard N.	523		
Brooks, William D.	792	Hansen, Roger F.	140
			240
Callegari, Andres C.	698	Heindel, Troy A.	305
Cameron, Barry W.	82	Helbig, H. R.	82
Cary, Judson	420	Hicks, Jaye	218
Cassaro, M. A.	51	Hill, Randall W., Jr.	62
Charnock, Elizabeth	542		479
Chen, Tom	881	Horton, Charles	926
Cheng, Linfu	822	Hua, Grace	69
Chirica, Laurian	426		
Coleman, John	554	Ignatiev, Alex	926
Colombano, S.	320		
Compton, M.	320	Jamison, Keith D.	926
Conway, Tim	765	Johnson, Coe	662
Culp, Donald R.	290	Johnson, Dean	662
Currie, Andrew	420	Johnson, Sally C.	274
		Jones, Don D.	381
De Mori, R.	621		458
Diaz, Aurora C.	581	Jordan, Janice A.	131
Dixit, Vishweshwar V.	118		523
Duque, R. E.	375		
Ebaud, Stephen	174	Kamil, Hasan	642
Eng, Norman	542	Khalife, B.	621
Engel, Bernard A.	381	Kontogiannis, K.	621
	458		

Kosta, Charles P.	534	Nagy, Thomas J.	522
Krolak, Patrick D.	534	Nanney, Van	831
	554	Nivens, Cody R.	902
	893		
Lai, S.	320	O'Donnell, Richard	404
Lam, C.	320	Orchard, Robert A.	581
Landauer, Christopher	493		
Lardas, George D.	247	Parkinson, W. J.	2
Lavery, David B.	792	Patton, Charles R.	470
Leigh, Albert	147	Pauls, Barbara	508
Lin, Min-Jin	131	Pease, J. N.	386
	523	Pickering, Brad	62
			479
Lincoln, David T.	771	Porter, Ken	39
Liu, Jefferey	822		
Loftin, R. Bowen	174	Rabeau, Arthur A.	926
Logie, David S.	642	Ragade, R. K.	51
Lowe, Carlyle M.	742	Rangan, Ravi M.	186
Luger, G. F.	2	Rasmussen, Arthur N.	305
Lund, Chet	784	Read, D. R.	864
		Rewerts, Chris C.	458
Macinnes, Mark A.	342	Reynolds, Joseph	839
Mack, John F.	498	Rhykerd, C. L.	381
Maguire, John	881	Rhykerd, C. L., Jr.	381
Mainardi, Joseph D.	334	Rhykerd, L. M.	381
Manahan, M.	320	Rhykerd, R. L.	381
Marsh, Christopher A.	442	Rogers, James L.	200
Mason, Larry	168	Rogers, Joseph B.	458
Matthews, John	218		
Mayer, Richard J.	131	Saito, Tim	174
	523	Salzman, G. C.	375
McConagha, Patrick	839	Schultz, Roger D.	676
McGee, Brenda J.	554	Sherman, Mark	508
	893	Shewfelt, R. L.	386
McKendrick, John D.	822	Smith, Cathy	550
Mehrotra, Mala	274	Snyder, James	426
Miller, Mark D.	893	Sobkowicz, Clifford	652
Miller, Ross C.	534	Srinivas, Vijay	803
Moon, Young Bai	803	Srinivasan, Raghavan	458
Morris, Keith E.	92	Statler, I.	320
Mueller, Stephen J.	75	Sterle, Mark E.	131
Muratore, John F.	305		523
Murphey, Amy Y.	257	Stewart, C. C.	375
Myers, Leonard	570	Stobie, Iain C.	676
	662	Swanson, David J.	871
	686	Szatkowski, G. P.	334
		Szolovits, P.	320

Taylor, James	686	Wess, Bernard P., Jr.	433
Taylor, Pam	550	White, W. A.	234
Thai, C. N.	386	Whitson, George	550
Tischendorf, Mark	412	Wu, Cathy	540
Vesty, Matt	534	Young, Gary B.	180
 		Young, L.	320
Wannemacher, Tom	155		
Warinner, Andrew	881		