Modelling and Control of $Si_{1-x}Ge_x$ Thin Film CVD

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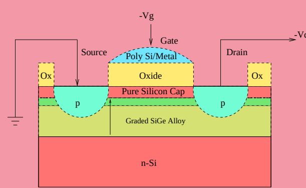
Research Objectives

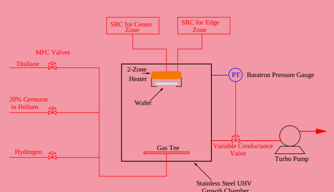
- Develop manufacturing process to produce integrated circuit structures with precise characteristics.
- Integrate optical sensors with physical models for on-line film composition and thickness measurement and feedback control.
- Demonstrate the manufacturing process by growing structures with specified composition and thickness uniformity in a ultra-high vacuum chemical vapor deposition reactor.

Germanium profile engineering



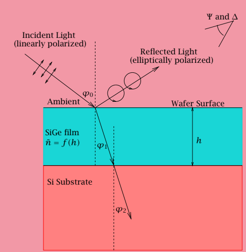
- In recent years, strained Si_{1-x} Ge_x films have attracted substantial attention as heterostructure materials for column IV bandgap-engineered devices.
- SiGe combines the integration and cost benefits of silicon with the speed of more esoteric and expensive technologies such as gallium-arsenide with applications to wireless communication.
- Enhancement of device properties such as lower threshold voltages, increased mobility, and larger drive current are determined by the germanium fraction in the alloy.
- Precise compositional and thickness control allow epitaxial heterostructures to be fabricated with tailored band structures and, consequently, tailored electronic and optical properties.

Ultra-High Vacuum Chemical Vapor Deposition Reactor

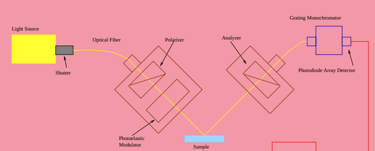


- The gas flow rates, the wafer temperature, and the reactor pressure are the systems' manipulated variables.
- The base level data acquisition and control platform is LabView running on a 500 MHz Pentium.
- A physical model that accounts for major effects has been developed.
- The optical sensor under development has been installed on the reactor for real time estimation of film composition and thickness.

On-line ellipsometric composition measurement

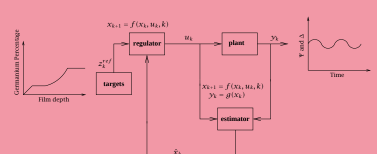


- Sensor must be non-invasive and provide composition measurements in real time.
- Ellipsometry is an experimental method that measures the polarization transformation that occurs when a beam of polarized light is reflected from a surface.
- The state of polarization is related to the properties of the reflecting material, such as the composition of |Ge| and film growth rate.
- The ellipsometer measures the ratio of the complex reflectance of light polarized parallel to (p) or perpendicular to (s) the plane of incidence.



- The ellipsometer reports Ψ and Δ for various wavelengths, λ.

Regulation and estimation functions of the controller



State estimation

- Find the most likely value of the state given measured outputs
- Process model

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{f}(\mathbf{x}_k, \mathbf{u}_k, k) + \omega_k \\ \mathbf{y}_k &= \mathbf{g}(\mathbf{x}_k) + \nu_k. \end{aligned}$$

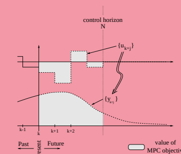
- Inputs, $\mathbf{u}$: MFC flows for disilane and germane, reactor pressure, substrate temperature
- States, $\mathbf{x}$: Gas phase concentrations, substrate surface concentrations, production rates, and optical admittance
- Outputs, $\mathbf{y}$: Ellipsometric data (Ψ and Δ) for various wavelengths
- Optimal estimate of the state

$$\hat{\mathbf{x}}_{k|k} = \hat{\mathbf{x}}_{k|k-1} + \mathbf{K}_k(\mathbf{y}_k - \mathbf{g}(\hat{\mathbf{x}}_{k|k-1}, k))$$

- $\mathbf{K}_k$ is the Extended Kalman Filter (EKF) gain

$$\mathbf{K}_k = \hat{\mathbf{P}}_{k|k-1}\mathbf{G}_k^T \left(\mathbf{G}_k \hat{\mathbf{P}}_{k|k-1}\mathbf{G}_k^T + \mathbf{R}_\nu\right)^{-1}$$

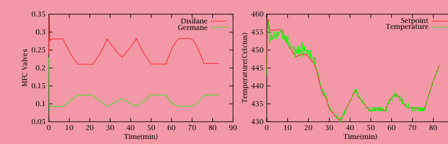
Model predictive control



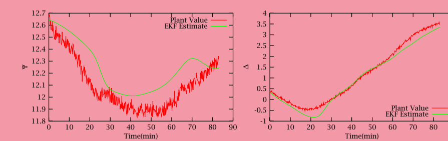
- The essence of MPC is to optimize, over the manipulatable inputs, forecasts of process behavior
- Forecasting is accomplished with a process model
- The model is the essential element of an MPC controller
- Updating the problem based on the measurement and re-solving the optimization introduces feedback into the controller
- Features
  1. Incomplete state measurement
  2. State and sensor noise
  3. Nonzero disturbances and offset free control
  4. Non-square systems
  5. Constraints on inputs and states

Closed-loop experiment showing rejection of a 10° temperature error

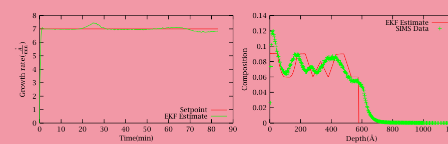
Manipulated variables



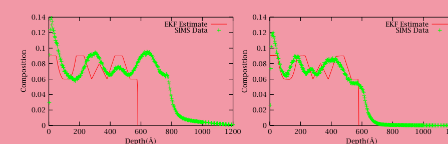
Measured outputs



Resulting film



Comparison of films grown open-loop and closed-loop



Accomplishments

- Developed first principles kinetics, reactor and optical sensor models. Demonstrated model-based recipe growth of graded films with complex as well as simple alloy profiles.
- Developed a time-varying state estimator based on the dynamic sensor model and ellipsometer's measured outputs. The state estimator is a novel applications of systems theory in this industry and provides the framework for addressing the multi-sensor fusion problem.
- Designed a controller utilizing the feedback of the best estimate of the film and reactor state based on the dynamic model and ellipsometric measurements.
- Successfully rejected a large unmeasured temperature disturbance. Ellipsometer detected error, state estimator correctly identified temperature disturbance, and controller compensated.
- First demonstration of feedback control using online optical film measurements to grow aggressive alloy composition profiles in which flowrates of several component gases and reactor temperature must be varied simultaneously in order to achieve the profile of interest.