A CAD ARCHITECTURE FOR MICROELECTROMECHANICAL SYSTEMS

Fariborz Maseeh[1], Robert M. Harris[2], Stephen D. Senturia[2]

[1]Department of Civil Engineering
[2]Department of Electrical Engineering and Computer Science
Microsystems Technology Laboratories
Massachusetts Institute of Technology
Cambridge, MA 02139

ABSTRACT

A CAD architecture for microelectromechanical systems is presented in which conventional mask layout and process simulation tools are linked to three-dimensional mechanical CAD and finite-element tools for analysis and simulation. The architecture is exercised by an elementary example on the stress-induced curvature of an oxidized silicon wafer. An architecture for an object-oriented material property simulator is also presented in which material properties and their process dependence are stored and are accessed based on the specific process conditions.

I. INTRODUCTION

With the development of increasingly sophisticated microelectromechanical devices, including microsensors, pumps, valves, and micromotors, and with the increasing performance demands being placed on these devices, notably in the precision and accuracy of microsensors, there is a critical need for CAD tools which will permit rational design of these devices. There are two fundamental problems that confront the designer [1,2]: (A) the need to construct a three-dimensional solid model from a description of the mask set and process sequence to be used in fabrication of a micromechanical device; and (B) the need to be able to predict the material properties of each of the constituent components in a device, including possible process dependences of these properties. At the present time, there is no CAD system, either mechanical or microelectronic, which successfully addresses these problems in a coherent way. Koppelman [3] has developed a program called OYSTER which permits construction of a 3-D polyhedral-based solid model from a mask set and primitive process description, but as yet, there is no provision for linking to FEM tools or to standard layout and process modeling tools, and no database for prediction of material properties from the process sequence.

This paper presents an architecture for a microelectromechanical CAD system which addresses these problems, and reports on the first implementation of this architecture. There are two critical functions not presently available in commercial packages: (1) a solid modeling tool (the "Structure Simulator"), which takes mask layout data and a process description and builds a 3-D solid model in a format compatible with the mechanical CAD system; and (2) a "Material Property Simulator", which takes process sequence information from the Structure Simulator, extracts the material property values from a database, and merges the material property information with the 3-D solid model for subsequent mechanical analysis.

The CAD architecture is explained in Section II. In Section III, we illustrate the successful analysis of an example, the thermal-stress-induced curvature of an oxidized silicon wafer, using elementary versions of the Structure Simulator and Material Property Simulator. This example exercises the architecture is some detail. One conclusion of this first attempt is that simple table-lookup for material properties is impossibly cumbersome in the general case due to the process dependence of material properties. Therefore, an object-oriented database approach has been developed for the Material Property Simulator, which is presented in Section IV.

II. CAD ARCHITECTURE

Fig.1 shows the architecture of our CAD system. It consists of three sections outlined by dashed blocks, the Microelectronic CAD section, the Mechanical CAD section, and the Material Property Simulator. The interactions among sections and their various constituents are shown by arrows, the directions of which specify the flow of information. The "User Interfaces" denote the various user's direct access to specific units in each section.

We have implemented this architecture in a Sun-4 host, drawing on existing codes wherever possible. The primary interface for mechanical modeling is through PATRAN [4], a mechanical CAD package which provides for interactive construction of 3-D solid models, graphical display, and interfacing with FEM packages (we are using ABAQUS [5]). The 3-D geometry resides in the PATRAN Neutral File with additional model information in a separate file. Initially, we have used the material-property format of the Neutral File as a first version of the Material Property Simulator while the more elaborate object-oriented version is being developed.

All of the commercially available codes in Fig. 1 are installed and operating. The Structure Simulator has been implemented at an elementary level, and interfaced with the Mechanical CAD. The first entries of material property data (for silicon, silicon dioxide [6], and silicon nitride [7]) have been made in a PATRAN readable file. A simplified example has been successfully tested using this architecture. We now describe the CAD architecture in detail, and then present the example.

A. MICROELECTRONIC CAD

In the Microelectronic CAD section, mask layout is created in CIF [8] format using KIC [9], and the process sequence is created in the MIT-developed Process Flow Representation (PFR) [10] using a standard file editor. SUPREM-III [11] and SAMPLE [12,13] are installed to provide depth and cross-sectional modeling capabilities.

CH2832-4/90/0000-0044$01.00©1990 IEEE

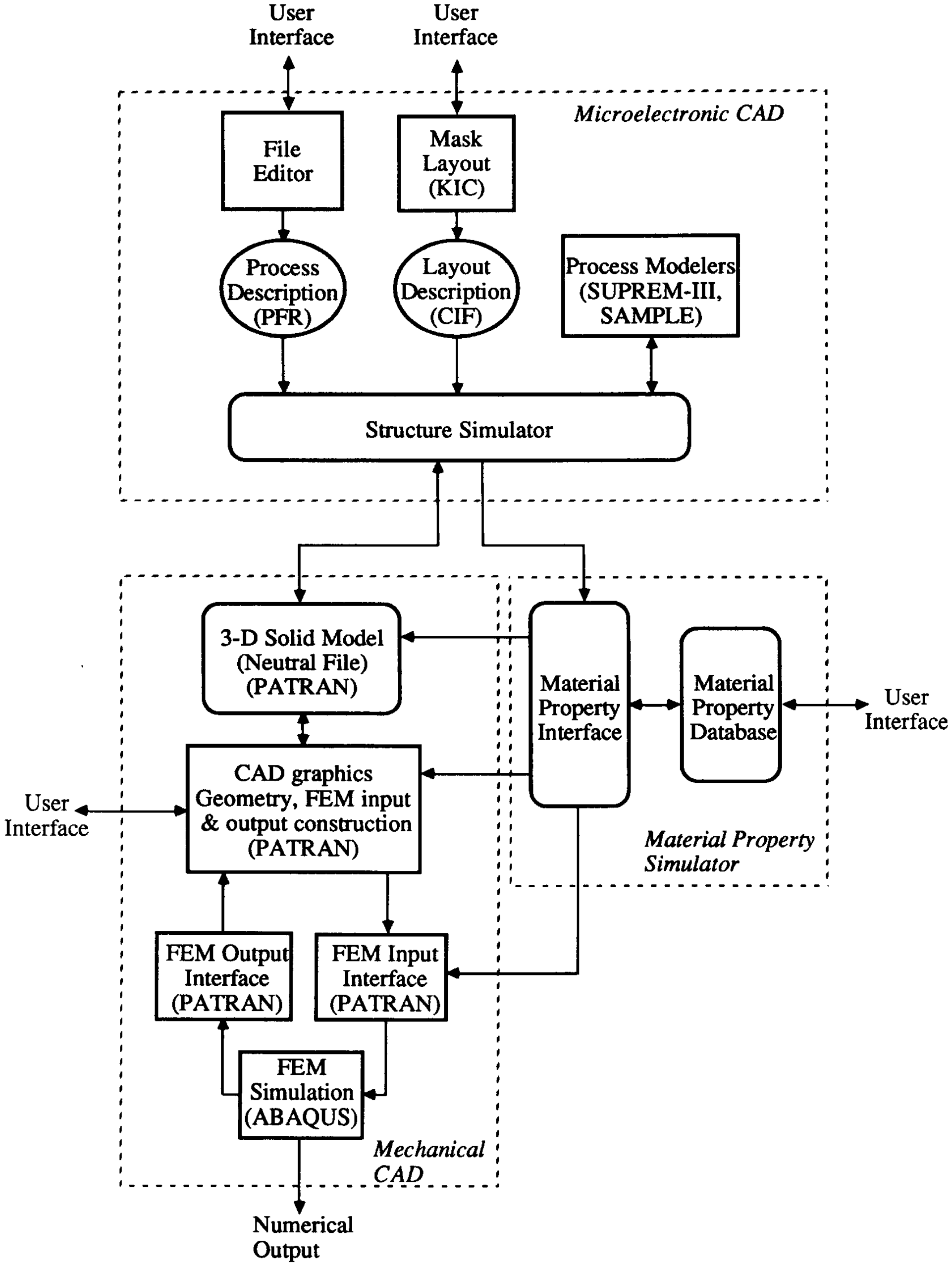

Fig. 1 CAD architecture for microelectromechanical design.
Arrows denote the flow of information.

The critical block in this section is the Structure Simulator, which must merge the mask layout and process information to construct a three-dimensional solid model. Two kinds of information must be tracked, the geometry of the structure (position, shape, and connectivity of each component), and the material type and associated process conditions used to create each component of the structure. The geometry is passed directly to the Mechanical CAD section by creating a PATRAN Neutral File. The material type and associated process conditions for each component are passed to the interface portion of the Material Property Simulator through what we call the Process History File.

Physically, a process step causes a change in the wafer (e.g. diffusion, deposition, etching). The final structure is the result of concatenating a sequence of such changes. This suggests that the Structure Simulator should perform its function in a process-step by process-step basis, making appropriate modifications to the solid model for each process step. The operation of the Structure Simulator is summarized in Table I, and is illustrated in Fig. 2. The current process step is read from the PFR process sequence, and is interpreted as a set of tasks that must be done to create construction operators. When appropriate, the PFR information is passed to the process modelers (SUPREM-III, SAMPLE), and the simulation results from the process modelers are combined with the mask data to create the appropriate construction operators. These are then used to modify the solid model from the previous step, both the geometry portion in the Neutral File, and the material-type information in the Process History File.

The construction operators must be implemented to ensure that the resulting solid model is physically valid (i.e., describing a reasonable approximation to the actual structure). Without careful attention to the robustness of construction algorithms, invalid solid models could result (e.g., an unphysical topology such as a Klein bottle, or two objects occupying the same place). Implementation of robust construction operators is considerably simplified if the operators are required to be a combination of a small set of primitive construction operators. For microelectromechanical design, the following primitive operators constitute a useful minimal set: film deposition and growth, film etching, masking, impurity introduction and diffusion, and wafer joining. For initial implementation, we have selected a restricted subset: conformal deposition, and masked etching. These two primitives provide significant geometric flexibility, and permit the simulation of many interesting microelectromechanical systems.

Table I. STRUCTURE SIMULATOR OPERATIONS

1. • Interpret process step
2. • Determine primitive construction operators
   > Consult layout information and process modelers
3. • Use the primitive operators to modify solid model
4. • Output results
   > Geometric information to Neutral File
   > Material information to Process History File
5. • Repeat steps 1-4 for next process step

B. MATERIAL PROPERTY SIMULATOR

The Material Property Simulator reads the process sequence for each component of the solid model from the Process History File and generates a set of material property data. The material properties are passed to the Mechanical CAD section, either into the PATRAN Neutral File, the PATRAN interactive (graphics) section which creates loads and boundary conditions as it builds the FEM input file, or the FEM input file itself (see Fig. 1). The FEM input file path allows for the use of FEM simulator independent of the PATRAN graphics software; furthermore, it provides for a way to introduce intrinsic stress into the mechanical model. (Note: because of the detailed organization of PATRAN, intrinsic stress must be treated differently than thermal mismatch stress; the latter can be created by thermal loads and dissimilar coefficients of thermal expansion, as in the example to follow.)

Initially, we have elected to use PATRAN-readable file formats to enter material property data (manually) for each type of material, which might become a constituent layer of the device, using dimensions and units compatible with the geometric model in the Neutral File. This zeroth-order approach is used in our example. However, manual construction of data sets for every permutation of process sequences for every material is impractical. An object oriented Material Property Simulator is designed to organize the process dependence of properties in an effective way, and is explained in detail in Section IV.

For simplicity, only thermal stresses are considered in this zeroth-order approach; intrinsic stress is neglected. The object oriented Material Property Simulator, however, will account for both intrinsic stress and thermal stress.

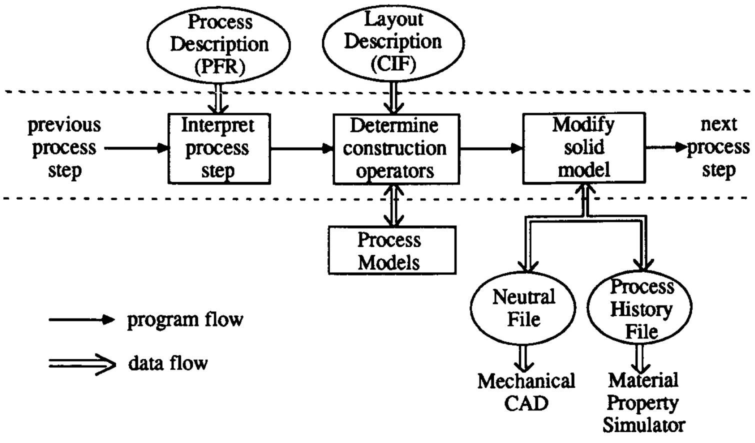

Fig. 2 Single process step operation of Structure Simulator.

C. MECHANICAL CAD

In the Mechanical CAD section, the geometric information from the Microelectronic CAD section is discretized into finite elements, material properties from the Material Property Simulator are associated with their proper geometries, and the appropriate loads and boundary conditions are specified. The solid model geometry and material properties are read and manipulated in PATRAN graphics, and a complete input model suitable for finite element analysis is generated and optimized interactively (see Fig. 1). The FEM model is then translated into an ABAQUS input file for FEM analysis. (Intrinsic stress would also be entered at this point). The results of FEM analysis are then translated back into a form readable by PATRAN graphics for display. PATRAN can then be used to examine the simulated mechanical behavior of the device.

The particular FEM simulator used (ABAQUS in this case) can be replaced by any other for which the PATRAN interfaces exist. Such a replacement would require modification of the details of the Material Property Simulator-to-FEM interface, but no major changes in architecture.

III. EXAMPLE

We next present an elementary example, the wafer curvature technique for thin film stress measurement [14], which exercises our CAD architecture in some detail. This technique, which is based on measuring the pure bending deformation of a supporting substrate due to the residual stress in a deposited film, has been abundantly used in measuring thin film stress. The method works equally well for tensile and compressive films and requires simple setup for measurements. As long as the stiffness of the film is negligible compared with that of the substrate and the out-of-plane deformation of the composite system is smaller than the half of the substrate thickness, this technique can be effectively utilized to measure stress in thin films. Film stress can be related to out-of-plane bending of the substrate via the Stoney equation [14]:

$$\sigma_f = \left(\frac{4}{3}\right)\left(\frac{E_s}{1 - \nu_s}\right)\left(\frac{t_s^2}{t_f}\right)\left(\frac{z}{L^2}\right)$$

where σ_f, E_s, ν_s are film stress, substrate Young's modulus, and substrate Poisson's ratio; t_s and t_f are substrate and film thickness; and z and L are the out-of-plane deflection and length over which the deflection is measured.

The specific process considered in this example is: A 4-inch silicon wafer is thermally oxidized at 1030°C in wet ambient for four hours. The oxide is optionally removed from the back side using a wet etch, which results in wafer bending due to the stress in the front side oxide. This bending can be compared with the Stoney equation.

A menu-driven interface to the Structure Simulator allows the user to create a solid model in PATRAN neutral file format, based on the oxidation process conditions and wafer geometry. (There is no masking in this example.) The user specifies wafer thickness, wafer diameter, oxidation temperature, ambient, and time. The interface calls SUPREM-III, reports the resulting oxide thickness, and incorporates this thickness into the solid-model geometry. Due to the axisymmetric nature of our problem, the resulting model is two dimensional. The model geometry is displayed by the PATRAN graphics, where it is then discretized into finite elements, and appropriate boundary conditions are specified. Material properties are associated with each layer, in this case, by reading from a preconstructed data file readable by PATRAN graphics containing information on silicon, silicon dioxide, and silicon nitride. A thermal cooling load of -1000°C was applied to the entire model to create oxide residual stress due to thermal coefficient mismatch with the silicon substrate. The generated model is optimized and translated to an ABAQUS input file through the PATRAN-to-ABAQUS translator. The resulting input file is then linked to ABAQUS for FEM analysis. The analysis results are translated through the ABAQUS-to-PATRAN translator to files readable in PATRAN graphics, and the final results of the analysis are examined.

In the case of the wafer with double sided oxide, the oxide film is under compressive stress, but there is no out-of-plane deformation due to symmetric loading. When oxide is removed from the backside, the wafer bends to regain equilibrium. Solid models for both double-sided oxide and single-sided oxide were generated in the Structure Simulator as described above, and analyzed under the same thermal load. The wafer bending from the FEM simulation, for the latter case, is in close agreement with the Stoney equation as shown in Fig. 3.

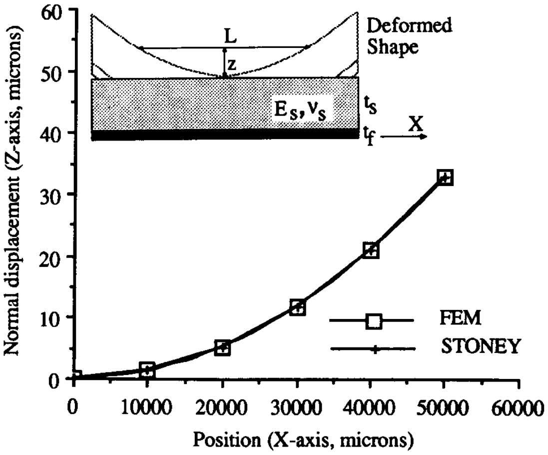

Fig.3 Out-of-plane displacement of an oxidized silicon wafer due to -1000°C thermal load.

IV. OBJECT ORIENTED MATERIAL PROPERTY SIMULATOR

Many of the properties of microelectronic materials, such as stress and density, are process dependent. This necessitates collection and extraction of properties of various materials in an organized way. An object-oriented database environment enables the definition and organization of data sets by their process dependence. This advantage is utilized in the development of the current Material Property Simulator.

Fig. 4 illustrates the Material Property Simulator architecture. It consists of a material property interface unit, and a material property database unit which holds tables of materials properties vs. process conditions. The interface unit consists of an interpolation routine and different interfaces to the mechanical and microelectronic sections, as shown. Process sequence information is read from the Process History File generated by the Structure Simulator. The process information includes the associativity to the corresponding components of the geometry and also a specification of dimensions and units. This information is handed to the interpolation routine, which accesses the material property database to retrieve the required data tables (described below), interpolates (using a multidimensional cubic spline) the resulting information to the values appropriate to the precise process conditions, and converts the dimensions and units to be compatible with the Structure Simulator geometry scale and the applied loads. The neutral file and graphics interface relays the material property information to the PATRAN Neutral File or the graphics unit. The intrinsic stress induced by process is interfaced directly with the FEM simulator input file. This same link can be used to transfer all of the material properties directly to the FEM simulator input file, if it is desired to use the FEM analysis independent of PATRAN graphics.

In the material property database section, the object oriented database environment GESTALT has been selected for storing and retrieving the material properties [15]. GESTALT has several advantages. First, it shields application programs from the many details of the underlying database (currently INGRES, a commercial relational database system [16,17]). It also provides for an environment in which application programs are written in different higher level languages (currently C and LISP). For example, the LISP interface could be used for adding rule-based applications for "intelligent" manipulation of data. GESTALT is flexible enough so that the underlying database can be replaced/upgraded without affecting existing application programs. Furthermore, it is being developed as part of the integrated circuit computer-integrated-manufacturing (IC-CIM) effort at MIT which provides for a natural link to the manufacturing environment. GESTALT can be accessed directly through a user interface for direct input and output of the stored data; it can also be linked to different simulators through the material property interface.

Fig. 5 illustrates the schema of the material property management through the GESTALT interface. The FILM is represented by a name (film_name), its fabrication process (film_process), and the applicable property names (material_property_names). The FILM PROCESS is organized by a name (process_name) and a list of the parameters (process_parameters) used in fabrication. The PROCESS captures the dependency of the material property data with process parameters stored in the relational database INGRES. A material property (material_property_value) versus process parameter (parameter_value) relation can be uniquely retrieved from INGRES by a process_name (with corresponding process_parameter_name) and a film_name (with the corresponding material_property_name). The retrieved values are in the form of a table (or function) for each property vs parameter, and a unique value of the material property can be selected by interpolating in this table for the given process parameter.

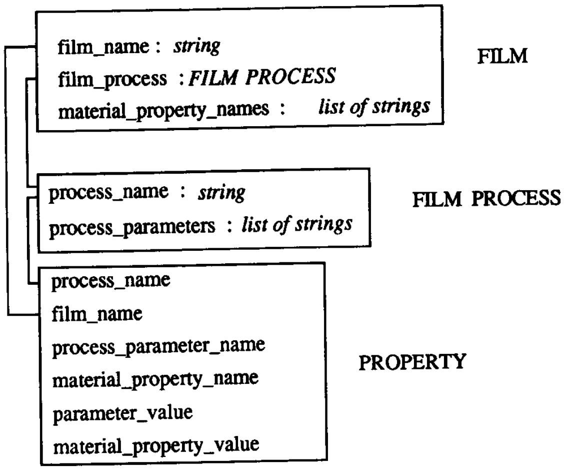

Fig. 5 Architecture of object oriented database organization.

At present, a first version of the Material Property Simulator has been written in C, and initial data for the process dependence of some of the properties of silicon dioxide have been entered into the database. Retrieval and interpolation has been demonstrated, but the interfaces to the rest of the system have not yet been implemented.

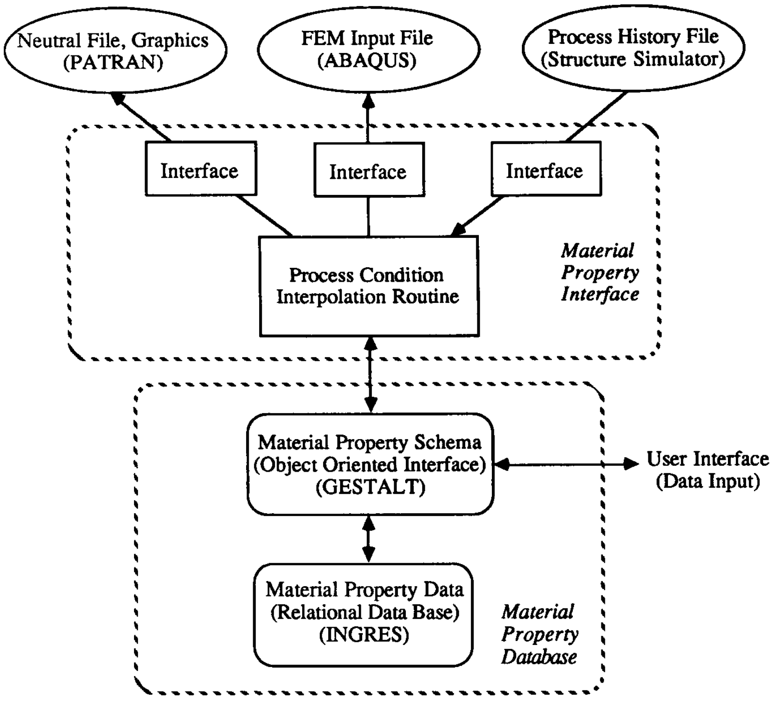

Fig. 4 Material Property Simulator architecture.

V. CONCLUSION

We have presented a CAD architecture for microelectromechanical systems, and have demonstrated the viability of that architecture in an elementary example. An object-oriented approach to the material property database problem is described.

It is anticipated that this architecture, which links the process dependence of material properties with a solid modeling capability, will find broad applications in conventional microelectronic device design, in device packaging, and related fields.

ACKNOWLEDGEMENTS

The authors gratefully acknowledge the helpful discussions and technical assistance of Mr. Michael Heytens, author of GESTALT, in the development of the material property database, Duane Boning for providing the some of the components of the Structure Simulator interface and for his assistance in adapting them to our use, and Prof. Donald Troxel for his many valuable suggestions. We thank Mr. Sean M. Gelston and Mr. Miles Arnone for their help in the literature search of material properties. The microelectromechanical system and material property simulator design is supported in part by DARPA under contract MDA972-88-K-0008, and the Department of Justice under contract J-FBI-88-067. The research is carried out in the Microsystems Technology Laboratories of the Massachusetts Institute of Technology.

REFERENCES

[1] S. D. Senturia, "Microfabricated structures for the measurement of mechanical properties and adhesion of thin films", Transducers '87, Tokyo, 1987, pp. 11-16.

[2] S. D. Senturia, "Can we design microrobotic devices without knowing the mechanical properties of materials?", IEEE MicroRobots and Teleoperators Workshop, Hyannis, 1987.

[3] G. M. Koppelman, "OYSTER : a 3D structural simulator for microelectromechanical design", MEMS '89, Salt Lake City, 1989, pp.88-93.

[4] PDA Engineering, Costa Mesa, CA.

[5] Hibbitt, Karlsson, and Sorensen, Inc., Providence, RI.

[6] F. Maseeh, S. M. Gelston, S. D. Senturia, "Mechanical properties of microelectronics thin films : Silicon Dioxide", MIT VLSI Memo No. 89-575, Oct. 89.

[7] F. Maseeh, M. Arnone, S. D. Senturia, "Mechanical properties of microelectronics thin films: Silicon Nitride", MIT VLSI Memo No. 89-576, Oct. 89.

[8] L. Conway and C. Mead, Introduction to VLSI Systems, Sec. 4.5, Addison-Wesley : Reading, MA, 1980.

[9] G. C. Billingsley, "Program reference for KIC", Memo No. UCB/ERL M83/62, U. C. Berkeley, Oct. 1983.

[10] M. B. McIlrath and D. S. Boning, "Integrated process design and manufacture", presented at SRC workshop on Integrated Factory Management for Integrated Circuits, Nov. 16-17, 1989, College Station, TX.

[11] C. P. Ho, J. D. Plummer, S. E. Hansen, and R. W. Dutton, "VLSI process modeling SUPREM III", IEEE Tran. Elect. Dev., vol. ED-30, no.11, pp.1438-1452, Nov. 1983.

[12] W. G. Oldham, S. N. Nandgaonkar, A. R. Neureurather, and M.M. O'Toole, "A general simulator for VLSI lithography and etching processes: Part I - application to projection lithography", IEEE Trans. Electron Dev., vol. ED-26, no.4, pp.717-722, Apr. 1979.

[13] W. G. Oldham, A. R. Neureurather, C. Sung, J. L. Reynolds, S. N. Nandgaonkar, and M.M. O'Toole, "A general simulator for VLSI lithography and etching processes: Part II - application to deposition and etching", IEEE Trans. Electron Dev., vol. ED-27, no.8, pp.1455-1559, Aug. 1980.

[14] G. G. Stoney, "The tension of metallic films deposited by electrolysis", Proc. R. Soc. London, Ser. A., vol. 82, pp. 172, 1909.

[15] M. L. Heytens and R. S. Nikhil, "GESTALT : An expressive database programming system", ACM SIGMOD Record, vol.18, no.1, pp.54-67, Mar. 1989.

[16] M. Stonebraker, G. Wong, P. Kreps, and G. Held, "The design and implementation of INGRES", ACM Transaction on Database Systems vol.1, no.3,pp.189-222 1976.

[17] INGRES Corp., Alameda, CA.