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Computer-aided Design of Plasma Processing Reactors Final Report CRADA No. TC-0339-92

P. Vitello, J. T. Lee, M. Surrendra

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Computer-aided Design of Plasma Processing Reactors

Final Report
CRADA No. TC-0339-92

Date: January 16, 1997 Revision: 1

A. Parties
The project is a relationship between the Lawrence Livermore National Laboratory (LLNL), American Telephone and Telegraph Company (AT&T), and International Business Machines (IBM).

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B. Project Scope
The purpose of this project is to develop and validate a comprehensive computer simulation of plasma processing reactors that will form the basis for a computer-aided design tool that will accelerate the design, selection and use of dry etching equipment by semiconductor manufacturers.

Within the three year period of this agreement, the partners will gather, extend and evaluate the knowledge base and the computer modules required in a computer-aided design tool for plasma etching. They will demonstrate the value of such a simulation tool in the optimization of both the equipment and process for critical etch steps. The project will also provide the foundation for the development of an expert system for use by U.S. semiconductor equipment manufacturers and their customers.

C. Technical
The bulk of the goals of this project were met. Full completion of the SOW was not possible due to a termination of DOE funding two years into the three year planned project. The following is a description of the technical scope of this project and the technical accomplishments.

The computer simulation code developed in this project, INDUCT95, describes absorption of power and plasma formation, the transport of particles to the wafer, the atomic processes occurring in the plasma, the velocity and density distributions of ions reaching the wafer. The code is adaptable to radio-frequency (RF) reactors operating via capacitively coupling or inductively coupling with the plasma.

Working with ORNL, an equivalent circuit model of the inductively coupled power deposition was developed. This model solves the time and space Fourier transformed electromagnetic equations assuming azimuthal symmetry and a single operating frequency. The plasma is treated in the cold dielectric limit, with the circuit current scaled to produce the desired Ohmic heating due to the rf fields in the plasma. Capacitive coupling effects between the coils and the plasma were modeled using a transmission line scheme. The simulation code can be run ignoring coil capacitive effects with only the time averaged rf power being supplied by the inductive coil circuit model, or full coil capacitive effects can be treated by including the time varying voltages on the induction coils in the plasma potential modeling. Comparisons of the equivalent circuit model impedance and experimental data show good agreement for frequencies below the second resonance for a typical cavity design.

For rf substrate bias capacitive power coupling, a separate equivalent circuit model was implemented. This second circuit applied an ac bias to the substrate holder and can be used independently of in conjunction with the rf inductive power deposition model. Comparison by IBM of simulation flux profiles with etch rates in an experimental rf capacitvely coupled reactor were found to be in excellent agreement.

LLNL designed a new, computationally efficient multi-specied electron, ion, neutral fluid transport code to study the transport of ions and neutral molecules and associated fields in generic plasma reactors. The code allows for complex internal structures in cylindrical and Cartesian geometries and is designed to facilitate rapid evaluations of changes in reactor geometry for both high density inductively coupled and RIE capacitively coupled reactors. The fluid code is supplemented by a hybrid kinetic code that can predict detailed velocity distribution functions of ions and electrons, and can check the rates of electronic collision processes.

LLNL has collected and evaluated a database of collision cross sections for argon, nitrogen, and chlorine plasmas with average electron energies 1--20 eV. Cross sections were obtained from the literature and through ab initio calculations of atomic collision processes. Comparisons with swarm and experimental data have been made to validate the accuracy and completeness of the atomic data.

In collaboration with Sandia National Laboratory at Livermore, LLNL has developed a version of the plasma simulation code INDUCT95, which makes use of the chemical kinetics code Chemkin to facilitate the description of chemical reactions in non-equilibrium ionized gases such as plasma reactors.

D. Partner Contribution

Interactions with IBM during the duration of this CRADA were very productive. Key insights into the plasma physics, and techniques of numerical simulation of plasma reactors were gained through the many conversations which took place. The expertise provided by the IBM Principal Investigator, Dr. Surendra, was crucial in developing and benchmarking INDUCT95 for capacitive RIE discharges. IBM has made use of the INDUCT95 simulation code to study a model AME 5000 plasma reactor with Chlorine for front end Si etching and for post-CVD clean applications. In addition IBM contributed much experience in the development of feature scale models of etching and deposition, through the work of Dr. Dalvie and Dr. Hamaguchi. Furthermore, these models were validated against experiment in several key application areas, under the direction of Dr. Rossnagel and Dr. Selwyn.

Through the work of Dr. Lee, AT&T Bell Laboratories provided data on the operation of helicon and helical resonator reactors which was valuable in validating the physics models incorporated in the simulations. The group headed by Dr. Donnelly performed some incisive experiments into the nature of the transient layers which are formed on the edge of the workpiece during etching, through direct studies of the surface and of the molecules that are disorbed into the plasma.

Details of the work by both partners can be found in the references listed below.

No subject inventions were created during this CRADA project.

E. Documents/Reference List

a) Quarterly CRADA reports were submitted through the LLNL Industrial Partnerships Office and an annual project review was conducted by DOE on July 19, 1995

Publications resulting from this project

``Two-Dimensional Fluid Model of High Density Inductively Coupled Plasma Sources," R.A. Stewart, P. Vitello, and D.B. Graves, *J. Vac. Sci. Technol. B.*, **12**, 478 (1994).

``Modeling Inductively Coupled Plasma Tools with Chlorine Chemistry", J.D. Bukowski, R.A. Stewart, D.B. Graves, and P.A. Vitello, *Proc. ElectroChem. Soc. Meeting*, San Francisco, May 1994.

"A Theoretical Study of Low-Energy Electron Collision Processes in Molecular Chlorine," T. N. Rescigno, *Phys. Rev. A* **50**, 1382 (1994).

" Two Dimensional Self-Consistent Fluid Simulation of RF Inductive Sources" , G. DiPeso, V. Vahedi, D.H. Hewett and T.D. Rognlien, *J. Vac. Sci Technol. B, 12*, 461 (1994).

"Comparison of Advanced Plasma Sources for Etching Applications. I. Etching Rate, Uniformity and Profile Control in a Helicon and a Multiple Electron Cyclotron Resonance Source", I. Tepermeister, N. Blayo, F. P. Klemens, D. E. Ibbotson, R. A. Gottscho, J. T. C. Lee and H. H. Sawin, *J. Vac. Sci. Technol.* B, **12**, 2310 (1994).

"Comparison of Advanced Plasma Sources for Etching Applications. II. Langmuir Probe Studies of a Helicon and a Multiple Electron Cyclotron Resonance Source", I. Tepermeister, D. E. Ibbotson, J. T. C. Lee and H. H. Sawin, *J. Vac. Sci. Technol.* B, **12**, 2322 (1994).

"Comparison of Advanced Plasma Sources for Etching Applications III. Ion Energy Distribution Functions for a Helicon and a Multiple Electron Cyclotron Resonance Source", G. W. Gibson, H. H. Sawin, I. Tepermeister, D. E. Ibbotson and J. T. C. Lee, *J. Vac. Sci. Technol.* B, **12**, 2333 (1994).

"Comparison of Advanced Plasma Sources for Etching Applications. I Plasma Induced Damage in a Helicon and a Multiple Electron Cyclotron Resonance Source", N. Blayo, I. Tepermeister, J. L. Benton, G. S. Higashi, T. Boone, A. Onuoha, F. P. Klemens, D. E. Ibbotson, J. T. C. Lee and H. H. Sawin, *J. Vac. Sci. Technol.* B, **12**,1340 (1994).

In Situ Pulsed Laser-Induced Thermal Deposition Studies of the Silicon Chloride Surface Layer during Silicon Etching in High Density Plasma of Cl_2 and Cl_2/O_2 Mixtures," C. C. Cheng, K. V. Guinn, NV. M. Donnelly and I. P. Herman, *J. Vac. Sci. Technol. A* **12**, 2630 (1994).

"Fluorocarbon High Density Plasma VI. Reactive Ion Etching Lag Model for Contact Hole Silicon Dioxide Etching in an Electron Cyclotron Resonance Plasma," O. Joubert, G. S. Oehrlein and M. Surendra, *J. Vac. Sci. Technol. A* **12**, 665 (1994).

"Reactive Ion Etching Lag Investigation of Oxide Etching in Fluorocarbon Electron Cyclotron Resonance Plasmas," O. Joubert, G. S. Oehrlein, M. Surendra and Y. Zhang, *J. Vac. Sci. Technol. A* **12**, 1957 (1994).

"Microprofile Simulations for Plasma Etching with Surface Passivation," S. Hamaguchi and M. Dalvie, *J. Vac. Sci. Technol. A* **12**, 2745 (1994).

"Detection and Modelling of Electrode Topography on Particle Traps," M. Dalvie, M. Surendra, G. S. Selwyn and C. Guarneri, Plasma Sources Sci. Technol. **3**, 442 (1994).

"Neutral Transport in High Plasma-Density Reactors," M. D. Kilgore, H. M. Wu and D. B. Graves, *J. Vac. Sci. Technol. B* **12**, 494 (1994).

``Plasma Uniformity in High Density Inductively Coupled Plasma Tools for Semiconductor Processing," R.A. Stewart, P. Vitello, D.B. Graves, E.F. Jaeger, and L.A. Berry, *Plasma Sources Science and Technology*, **4**, 36 (1995).

``Modeling of Profile Effects for the LLNL Large Area Inductively Coupled Plasma Source," P. Vitello, G.J. Parker, N. Tishchenko, and G. DiPeso, *Proceedings of the Int. Sym. on Plasma Chemistry*, (1995).

"Plasma Processing Uniformity and Control: Experiment and Modeling", M. Surendra and C.R. Guarnieri, *Workshop on Industrial Applications of Plasma Chemistry: ISPC 12*, ed. A. Wendt and J.V Heberlein, 41 (1995).

``Fluid Dynamic Modeling of Plasma Reactors," P. Vitello, *Molecular Physics and Hypersonic Flows*, M. Capitelli, ed., (Kluwer academic publishers), 477 (1995).

"Analytic Model of Power Deposition in Inductively Coupled Plasma Sources", V. Vahedi, M. A. Lieberman, G. DiPeso, T. D. Rognlien and D. Hewett, *J. Appl. Phys.*, **78**, 1446 (1995).

"The Role of the Plasma in the Chemistry of Low Pressure Plasma Etchers", R. E. P. Harvey, W. N. G. Hitchon and G. J. Parker, *IEEE Trans. of Plasma Science*, **23**, 436 (1995).

"Low Energy Electron Collision Processes in NF_3", T. N. Rescigno, *Phys. Rev.* A**52**, 329 (1995).

"A Monte Carlo Collision Model for the Particle-In-Cell Method: Applications to Argon and Oxygen Discharges", V. Vahedi and M. Surendra, Comp. Phys. Commun. **87**, 179 (1995).

"Equilibrium Profiles for RF Plasma Sources with Ponderomotive Forces", G. DiPeso, T.D. Rognlien, V. Vahedi, and D.H. Hewett, *IEEE Trans. on Plasma Science*, **23**, 550 (1995).

"Aspect Ratio Independent Etching: Fact or Fantasy?", A. D. Bailey III and R. A. Gottscho, Jpn. J. Appl. Phys. **34**, 2083 (1995).

"Scaling of Si and GaAs Trench Etch Rates with Aspect Ratio, Feature Width and Substrate Temperature," A. D. Bailey III, M. C. M. van de Sanden, J. A. Gregus and R. A. Gottscho, *J. Vac. Sci. Technol. B* **13**, 92 (1995).

" Competitive Halogenization of Silicon Surfaces in HBr/Cl_2 Plasmas Studied with X-Ray Photoelectron Spectroscopy and In-Situ, Real Time, Pulsed Laser-Induced Thermal Desorption," C. C. Cheng, K. V. Guinn, I. P. Herman and V. M. Donnelly, *J. Vac. Sci. Technol. A* **13**, 1970 (1995).

“Quantitative Chemical Topography of Polycrystalline Si Anisotropically Etched in Cl_2/O_2 High Density Plasmas,” K. V. Guinn, C. C. Cheng and V. M. Donnelly, *J. Vac. Sci. Technol. B* **13**, 214 (1995).

“Radiofrequency Discharge Benchmark Model Comparison,” M. Surendra, *Plasma Sources Sci. Technolog.* **4**, 56 (1995).

“Simulations of Trench-Filling Profiles under Ionized Magnetron Sputter Metal Deposition,” S. Hamaguchi and S. M. Rossnagel, *J. Vac. Sci. Technol. B* **13**, 183 (1995).

“Characterization at Different Aspect Ratios (Radius/Length) of a Radio Frequency Inductively Coupled Plasma Source,”P. N. Wainman, M. A. Lieberman, A. J. Lichtenberg, R. A. Stewart and C. Lee, *J. Vac. Sci. Technol. A* **13**, 2464 (1995).

“"Spatially Averaged (Global) Model of Time Modulated High Density Argon Plasmas,” S. Ashida, C. Lee and M. A. Lieberman, *J. Vac. Sci. Technol. A* **13**, 2498 (1995).

“Global Model of Ar, O_2, Cl_2 and Ar/O_2 High-Density Plasma Discharges,” C. Lee and M. A. Lieberman, *J. Vac. Sci. Technol. A* **13**, 368 (1995).

“Modeling of Non-Local Electron Kinetics in a Low Pressure Inductively-Coupled Plasma,” G. J. Parker, W. N. G. Hitchon and J. E. Lawler, *Phys. Rev. E*, **54**, 6746 (199x).

“Effective Potential Methods in Variational Treatments of Electron-Molecule Collisions., II. Application to HBr.”, T. N. Rescigno, *J. Chem. Phys.*, **104**, 125 (1996).

``Modeling An Inductively Coupled Plasma Reactor with Chlorine Chemistry," P. Vitello, J.N. Bardsley, G. DiPeso, and G.J. Parker, *IEEE Trans. of Plasma Science*, **24**, 123 (1996).

``Experiments and Modeling of a Helicon Source," A.W. Molvik, T.D. Rognlien, J.A. Byers, R.H. Cohen, A.R. Ellingboe, E.B. Hooper, H.S. McLean, B.W. Stallard, and P.A. Vitello, *J. Vac. Sci. Technol.* A, **14**, 984 (1996).

“Electron Kinetics in Radio-Frequency Magnetic Fields of Inductive Plasma Sources”, R. H. Cohen, T. D. Rognlien, *Plasma Sources Science & Tech.*, **5**, 442 (1996)

``Two-dimensional Fluid Model of an Inductively Coupled Plasma with Comparisons to Experimental Spatial Profiles," J.D. Bukowski, D.B. Graves, and P. Vitello, *J. Applied. Phys.*, **80**, 2614 (1996).

“Induced Magnetic-Field Effects in Inductively Coupled Plasmas”, R.H. Cohen and T.D. Rognlien, *Phys. Plasmas*, **3**, 1839 (1996).

“Two-Dimensional Bounded Plasma Simulation Codes”, V. Vahedi and G. DiPeso, *J. Comp. Phys.*, in press (1996).

“High Selectivity Plasma Etching of Silicon Dioxide with a Dual Frequency 27/2 MHz Capacitive Radio Frequency Discharge,” W. Tsai, G. Mueller, R. Lindquist, B. Frazier and V. Vahedi, *J. Vac. Sci. Technol.* B, **14**, 3276 (1996).

“Mass Spectrometric Measurements of Neutral Reactant and Product Densities during Si Etching in a High-Density Helical Resonator Cl_2 Plasma,” V. M. Donnelly, *J. Appl. Phys.* **79**, 9353 (1996).

"A Simple Optical Emission Method for Measuring Percent Dissociations of Feed Gases in Plasmas: Application to Cl_2 in a High-Density Helical Resonator Plasma," V. M. Donnelly, *J. Vac. Sci. Technol.* A, **14**, 1076 (1996).

"Comparison of Advanced Plasma Sources for Etching Applications V. Polysilicon Etching Rate, Uniformity, Profile Control, and Bulk Plasma Properties in a Helical Resonator Plasma Source", J. T. C. Lee, N. Layadi, K. V. Guinn, H. L. Maynard, F. P. Klemens, D. E. Ibbotson and I. Tepermeister, *J. Vac. Sci. Technol.* B, **14**, 2510 (1996).

"Metal Stack Etching using a Helical Resonator Plasma," C. B. Labelle, H. L. Maynard and J. T. C. Lee, *J. Vac. Sci. Technol.* B, **14**, 2574 (1996).

"Plasma Etching Process Development using In Situ Optical Emission and Ellipsometry", J. T. C. Lee, N. Blayo, I. Tepermeister, F. P. Klemens, W. M. Mansfield and D. E. Ibbotson, *J. Vac. Sci. Technol.* B, **14**, 3283 (1996).

"Thin, High Atomic Weight Refractory Film Deposition for Diffusion Barrier, Adhesion Layer and Seed Layer Applications", S. M. Rossnagel, C. Nichols, S. Hamaguchi, D. Ruzic and R. Turkot, *J. Vac. Sci. Technol.* B, **14**, 1819 (1996).

"Liner Conformality in Ionized Magnetron Sputter Metal Deposition Processes", S. Hamaguchi and S. M. Rossnagel, *J. Vac. Sci. Technol.* B, **14**, 2603 (1996).

"Ionization Physical Vapor Deposition of Cu for High-Aspect Ratio Damascene Trench Fill Applications," C. A. Nichols, S. M. Rossnagel and S. Hamaguchi, *J. Vac. Sci. Technol.* B, **14**, 3270 (1996).

"Discharge Equilibrium of a Helicon Plasma," I. D. Sudit and F. F. Chen, *Plasma Sources Sci. Technol.* **5**, 43 (1996).

"Downstream Physics of the Helicon Disharge," F. F. Chen, I. D. Sudit and M. Light, *Plasma Sources Sci. Technol.* **5**, 43 (1996).

"Physics of Helicon Discharges," F. F. Chen, *Physics of Plasmas*, **3**, 1783 (1996)

b) No patent activity or pending applications are associated with this CRADA.
The computer code INDUCT95 has been copyrighted.

c) No subject inventions are associated with this CRADA. No Protected CRADA Information was generated under this CRADA.

d) Background Intellectual Property (BIP) will not be cross-licensed to other parties as a result of this CRADA research, and will remain with its originator.

F. Acknowledgment

Participant's signature of the final report indicates the following:

1) The Participant has reviewed the final report and concurs with the statements made therein.
2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
3) The Participant certifies that all reports either completed or in process are listed and all subject inventions and the associated intellectual property protection measures attributable to the project have been disclosed or are included on a list attached to this report.
4) The Participant certifies that if real property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.

2/13/97

John T. C. Lee Date
American Telephone and Telegraph Company
Bell Laboratories

Attachment I – Final Abstract
Attachment II – Project Accomplishments Summary
Attachment III – Final Quarterly Report

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M. Surendra 9/15/97

M. Surendra Date
International Business Machines Corporation
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2/6/97

J. Norman Bardsley Date
Lawrence Livermore National Laboratory

Attachment I – Final Abstract
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Attachment III – Final Quarterly Report

Computer-aided Design of Plasma Processing Reactors

Final Abstract (Attachment I)
CRADA No. TC-0339-92

Date: January 16, 1997 Revision: 1

A. Parties

The project is a relationship between the Lawrence Livermore National Laboratory (LLNL), American Telephone and Telegraph Company (AT&T), and International Business Machines (IBM).

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A two-dimensional, time-dependent, numerical model of plasma discharges, INDUCT95, was developed based upon a fluid treatment of ions and electrons. For inductively coupled sources, electron heating from external radio frequency coils is calculated self-consistently by solving for the time-averaged power deposited within the plasma. Time dependent biasing of structures can be applied to treat capacitively coupled radio frequency discharges. Complex chemical volume and surface reactions can be treated for neutral gas mixtures. INDUCT95 solves for densities, temperatures, fluxes, and electro-static potential in a plasma discharge. Cylindrically symmetric (r,z) or Cartesian (x,y) coordinates can be used. Both metal and dielectric internal boundaries can be treated for complex structures. Ab initio calculations of cross sections for critical electron molecule collision processes involving etchant gases were completed and published. The theoretical work was accompanied by thorough investigations of processing plasmas and workpiece surface conditions during etching and deposition of semiconductor materials, using capacitively and inductively coupled RF, electron cyclotron resonance, helicon and helical resonator reactors. Comparison of theory and experiment demonstrates the role of the plasma conditions in controlling both the geometric and chemical evolution of the semiconductor wafer surface.

Computer-aided Design of Plasma Processing Reactors

Project Accomplishments Summary (Attachment II)
CRADA No. TC-0339-92

Date: January 16, 1997 Revision: 1

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B. Background

Before the development of the INDUCT95 code there was no integrated time-dependent, two-dimensional numerical plasma discharge code capable of efficiently treating both inductively coupled and capacitively coupled discharges. Prior simulations of plasma reactors were either done in one-dimension, which ignored many of the important issues needed to be addressed for reactor optimization, or were done with simulation codes which were not well integrated, and hence were difficult to use and modify.

The expertise supplied to this project by LLNL was through its experience in developing efficient, accurate, and stable simulation codes for plasma discharges. This complemented the partner's capabilities which were hands-on experience with the plasma reactors being modeled, and both experimental and theoretical tools to study surface phenomena..

C. Description

The purpose/objective of the project was to develop a comprehensive computer simulation of plasma processing reactors that would form the basis for a computer-aided design tool. Such a design tool would be used to accelerate the design, selection and use of dry etching equipment by semiconductor manufacturers.

The roles of LLNL was to develop the basis numerical simulation model and to gather and evaluate the atomic data needed to model realistic plasma reactors. The role of the partners was to provide data concerning commercial reactors, and to do comparative testing of the simulation model with experimental data.

Working with ORNL, an equivalent circuit model of the inductively coupled power deposition was developed. This model solves the time and space Fourier transformed electromagnetic equations assuming azimuthal symmetry and a single operating frequency. The plasma is treated in the cold dielectric limit, with the circuit current scaled to produce the desired Ohmic heating due to the rf fields in the plasma. Capacitive coupling effects between the coils and the plasma were modeled using a transmission line scheme. The simulation code can be run ignoring coil capacitive effects with only the time averaged rf power being supplied by the inductive coil circuit model, or full coil capacitive effects can be treated by including the time varying voltages on the induction coils in the plasma potential modeling. Comparisons of the equivalent circuit model impedance and experimental data show good agreement for frequencies below the second resonance for a typical cavity design.

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In collaboration with Sandia National Laboratory at Livermore, LLNL has developed a version of the plasma simulation code INDUCT95, which makes use of the chemical kinetics code Chemkin to facilitate the description of chemical reactions in non-equilibrium ionized gases such as plasma reactors.

D. Expected Economic Impact

INDUCT95 has been used by IBM to optimize the operation of its semiconductor fabrication facility in Burlington, Vermont, and will be able to continue to use the code in this manner. Semiconductor equipment manufacturers such as Applied Materials and Lam Research are benefiting in improved design of etching tools either through direct use of INDUCT95 or through development of the physical models developed under this CRADA. The code has been used in the development of the large area etching tool for flat panel displays under a contract to the US Display Consortium. The cross sections for Cl_2 and NF_3 were used in the development of downstream etching reactors by Sandia National Laboratories and its own CRADA partners.

These benefits to industry will accrue not only through use of the simulation code and physics models, but also through the employment of post-doctoral scientists who were trained under this CRADA project.

The results of the INDUCT simulations of plasma uniformity and comparisons with experimental results will assist in the transition from 200mm to 300mm semiconductor wafers and from second to third generation (550mmx650mm) substrates for flat panel displays. In addition the sheath and feature profile models will help in the analysis and solution of problems such as charge-induced damage and aspect-ratio dependent etching that are becoming more serious as feature sizes are reduced and aspect ratios increased.

The introduction of computer simulations and computer-aided design into the design and use of semiconductor manufacturing equipment is a new phenomenon and it is difficult at this stage to quantify the number of jobs created and resulting benefits.

The reinvigoration of the U. S. semiconductor fabrication industry and of the semiconductor manufacturing equipment industry has contributed significantly to job creation, to the U. S. balance of payments and to the availability of more powerful microelectronic products, such as personal computers. Government-industry cooperation through Sematech and CRADAs has played a significant part in this renewal. The continued health of the semiconductor industry infrastructure is essential to the provision of the information technology on which the Department of Defense will rely in the 21st century.

Commercial development of the INDUCT code will be considered. IBM and AT&T have indicated that they are not planning to apply their options for commercial development. If they decide not to follow up on their option, discussions will be undertaken with specialized software houses to ensure that the progress made in this CRADA is incorporated in future semiconductor equipment Computer-Aided Design software.

E. Benefits to DOE

Current plans at LLNL are to use INDUCT95 as a basis for further development of plasma discharge models. These models will be used to aid in the design of classified experiments supporting DOE Defense Program objectives for Stockpile Stewardship.

Portions of INDUCT94 were integrated into the Sandia National Laboratory code AURORA and INDUCT95 has been made available for their use. With the reorientation of the Industrial Partnership Program at LLNL, no further development of INDUCT95 is anticipated either for the semiconductor or display industries.

F. Industry Area

As indicated above, the two industries that are benefiting from this CRADA are semiconductor manufacturing and semiconductor equipment manufacturing.

G. LLNL Point of Contact for Project Information

Peter Vitello
P.O. Box 808, L-014
Lawrence Livermore National Laboratory
Livermore, CA 94551
(510) 422-0079
(510) 424-4320 FAX

H. Company Size and Point(s) of Contact

IBM is a large multinational corporation with many thousands of employees involved in many lines of business. The appropriate technical contact is

Dr M. Surendra
Tel: 914-945-2410

American Telephone and Telegraph Company (AT&T) was also a large multinational corporation with many thousands of employees involved in communications and computer industries. Following the recent break-up of AT&T, the semiconductor manufacturing operations and all the staff associated with this project became part of Lucent Technologies. The appropriate technical contact is

Dr. John T. C. Lee,
Tel: 908-582-3706

I. Release of Information

I have reviewed the attached Project Accomplishment Summary prepared by Lawrence Livermore National Laboratory and agree that the information about our CRADA may be released for external distribution.

Tsing-Chung Lee

John T. C. Lee Date
American Telephone and Telegraph Company
Bell Laboratories

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M. Surendra Date
International Business Machines Corporation
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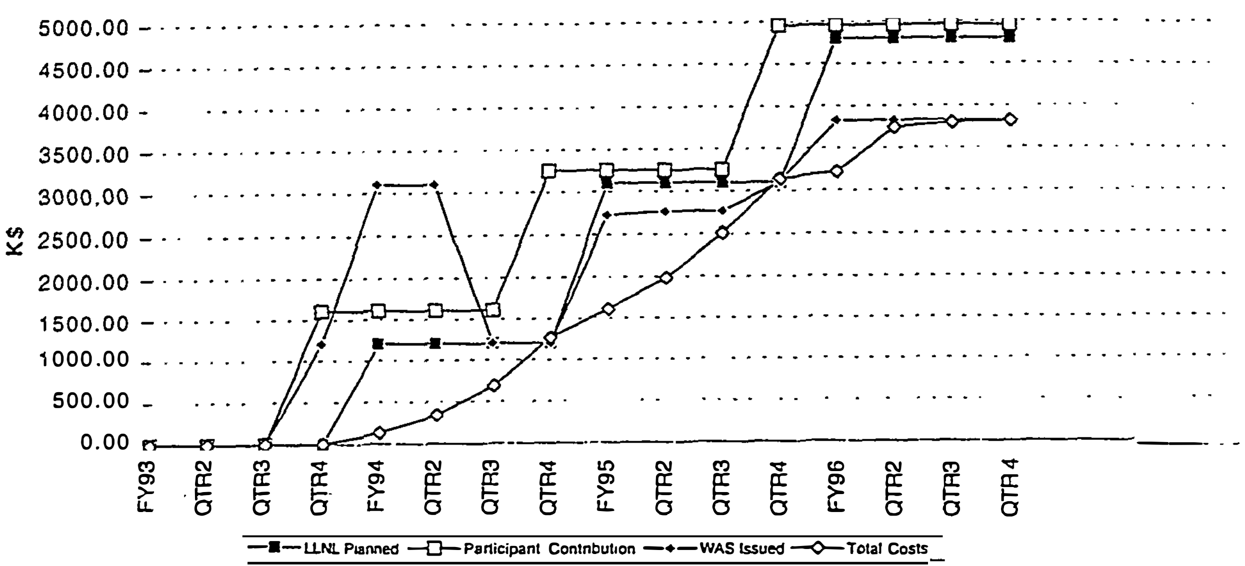
Lawrence Livermore National Laboratory
Final Quarterly Report (Attachment III)

Title:	Computer-Aided Design of Plama Processing Reactors	Reporting Period:	07/01/95 - 09/30/96
Participant:	AT&T Bell Labs & IBM	Date CRADA Executed:	10/26/93
DOE TTI No.:	93-LLNL-099-C1	DOE Approval Date:	9/14/93
CRADA No.:	TC-0339-92	Scheduled Ending Date:	10/25/96
TACT:	M&P	Project Completion Date:	9/30/96
Account Numbers	4775-13 to 17	B & R Code (S):	DP030101 35DP0301
Accounts Closed:	9/30/96		

Approved Funding Profile ($K)

	FY93	FY94	FY95	FY96	FY97	Total
LLNL Planned	0	1200	1900	1700	0	4800
Participant In-Kind	1604	1653	1701	0	0	4958
Participant Funds-In	0	0	0	0	0	0
WAS DP030101	1200	0	1852	736	0	3788
WAS 35DP030101	0	0	48	-5	0	43
Total Costs	0	1264	1876	680	0	3821



DP030101	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD
FY93	0	0	0	0	0	0	0	0	0	0	0	0	0
FY94	0	68	66	45	97	65	108	123	117	105	169	302	1264
FY95	77	157	108	126	119	129	144	173	209	145	120	365	1873
FY96	14	7	19	443	25	56	10	34	7	-3	30	0	641
FY97	0	0	0	0	0	0	0	0	0	0	0	0	0

3778

35DP0301	Oct	Nov	Dec	Jan	Feb	Mar	Apr	May	Jun	July	Aug	Sep	FYTD
FY93	0	0	0	0	0	0	0	0	0	0	0	0	0
FY94	0	0	0	0	0	0	0	0	0	0	0	0	0
FY95	0	0	0	0	0	2	0	0	0	0	0	0	3
FY96	39	0	0	0	0	0	0	0	0	0	0	0	39
FY97	0	0	0	0	0	0	0	0	0	0	0	0	0

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STAFF w/phone:

Lab PI:	J. Norman Bardsley (510) 422-6008	Participant:	AT&T – Dr. John T. C. Lee (908) 582-3706
Resource Manager:	Vicki Evans (510 423-0158		IBM – Dr. M. Surendra (914) 945-2410
DOE OAK:	Jerry Scheinberg (510) 637-1653	DOE HQ:	C. Fowler (202) 586-5834

Lawrence Livermore National Laboratory
Final Quarterly Report (Attachment III)

Reporting Period: 07/01/95 - 09/30/96
DOE TTI No.: 93-LLNL-099-C1
CRADA No.: TC-0339-92

Milestones and Deliverables:

List the complete set of milestones for all phases of the CRADA. Continue on separate pages if necessary.
Report any changes from the original CRADA or previous quarterly report on the CRADA Change Form.

	Completion Date: Scheduled	Actual
1 Plasma Chemistry Data	03/94	03/94
2 Capacitive Coupling	05/94	05/94
3 Transport code	04/94	02/94
4 RF problem definition	05/94	05/94
5 Surface chemistry data	04/94	04/94
6 Helicon/ECR diagnostics	05/94	02/94
7 Model tests	08/94	08/94
8 Power absorption analysis	11/94	10/94
9 Bias frequency study	11/94	09/94
10 Aspect ratio model	11/94	08/94
11 Membrane transport study	11/94	11/94
12 Complex chemistry base	11/94	11/94
13 Cluster tool measurements	11/94	10/94
14 RIE code development	05/95	03/95
15 Code assembly	08/95	08/95
16 High priority data update	11/95	
17 Code verification	11/95	
18 Diagnostic comparisons	11/95	
19 Data update	08/96	
20 Etching data validation	08/96	
21 Code completion	10/96	

Verification of participants' in-kind contribution was made in accordance with LLNL policy. Explain basis of verification: Please initial: YES JNB NO ______

AT&T: Visit to LLNL by D. Ibbotson; visit to AT&T by J. N. Bardsley, and V. Vahedi.

IBM: Visits to IBM by J. N. Bardsley and V. Vahedi.

List any subject inventions by either party (include IL# for LLNL inventions), additional background intellectual property, patents applied for, software copyrights, publications, awards, licenses granted or reportable economic impacts

The intellectual property produced under this CRADA consists of the numerical plasma reactor simulation code INDUCT95. The Regents of the University of California Copyright notice has been included in the INDUCT95 source code to inform users that the materials are copyright-protected.

No subject inventions have been applied for be either the industrial partner nor LLNL.

Collaborative licenses have been granted for the purposes of testing and collaborative development of INDUCT95.

Verification that all equipment and proprietary information has been returned to the initial owner or permanently transferred Please initial: YES X NO ______

Reporting Period: 07/01/95- 09/30/96
DOE TTI No.: 93-LLNL-099-C1
CRADA No.: TC-0339-92

Accomplishments

Describe Technical/Non-Technical lessons learned and other observations.
Summarize causes/justification of deviations from original scope of work.

The project has laid the foundations for the development of effective Computer-Aided Design Software, through the coding and validation of relatively simple models of the physics and chemistry of processing plasmas and the surface of the semiconductor surface. At the beginning of the project, it was estimated that the development of 3-D, multicomponent simulations with accurate representations of plasma and surface chemistry that will run efficiently and speedily on work stations would take 10-15 years. It is possible that this time schedule can now be shortened, if this work is continued by collaboration between academia, research laboratories, the semiconductor and equipment industries and software companies.

The severe reduction in the funds available for the third year of the project had two major effects. The first was that the development of physics models for magnetized plasmas was not completed. The second was that the excellent work on surface profile models and surface chemistry performed by the Industrial Partners was not fully integrated into the INDUCT code. Hopefully, both of these opportunities will be taken up elsewhere.

Reviewed by CRADA project Program Manager: ____________ Date: ____________

Reviewed by Karena McKinley, APL Partnering, IP&C: ____________ Date: ____________

Direct questions regarding this Report to IP&C Resource Manager, Susan Springer, at (510) 422-5507