

行政院國家科學委員會專題研究計畫 期中進度報告

電子迴旋共振化學汽相沉積反應腔體中電漿製程模擬

計畫類別：整合型計畫

計畫編號：NSC92-2120-M-009-002-

執行期間：92 年 08 月 01 日至 93 年 07 月 31 日

執行單位：國立交通大學機械工程研究所

計畫主持人：吳宗信

計畫參與人員：周欣宜 許國賢

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中 華 民 國 93 年 5 月 31 日

行政院國家科學委員會補助專題研究計畫 **成果報告**
x 期中進度報告

電子迴旋共振化學汽相沉積反應腔體中電漿製程模擬 (1/3)
Plasma flow simulation for nanostructure formation in
ECR-CVD chamber (1/3)

計畫類別： ☐ 個別型計畫 ☒ 整合型計畫

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共同主持人：

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中 華 民 國 93 年 5 月 25 日

行政院國家科學委員會專題研究計畫成果報告

奈米解析度記錄媒體及其他應用之包覆合金碳奈米結構陣列，其製造、機械/熱性質及製程特徵之研究子計畫三(1/3)-電子迴旋共振化學汽相沉積反應腔體中電漿製程模擬 (Plasma flow simulation for nanostructure formation in ECR-CVD chamber)

計畫編號：NSC 92-2120-M-009-002

執行期限：2003 年 8 月 1 日至 2004 年 7 月 31 日

主持人：吳宗信 國立交通大學機械工程學系

中文摘要

在本研究計畫，吾人將以數值方法，模擬用來製造奈米碳管等相關製程的電子迴旋共振化學氣相沈積電漿源腔體，內部中甲烷/氫氣混合氣體電漿流場。在第一年，硬體方面，吾人已成功建立及測試 23 節點、linux 作業系統的電腦叢集，以提供電漿數值模擬使用。程式碼方面，電漿流場模擬中，許多重要部分的程式碼也已陸續完成測試，如下列所示：1.模擬靜電場分佈所用的平行有限元素法 Poisson 方程式程式碼 2.模擬靜磁場分佈所用的平行有限元素法向量 Poisson 方程式程式碼 3.平行帶電粒子運動及電磁場與電荷權重(PIC)程式碼。在未來第二年，吾人將對現正進行的平行帶電粒子與中性原子間蒙地卡羅碰撞法，和馬克思威爾方程程式碼，做進一步的報告與說明。

關鍵詞：奈米碳管、迴旋共振化學氣相沈積、Poisson 方程式、向量 Poisson 方程式、馬克思威爾方程程式、PIC

Abstract

In this project, we intend to simulate the plasma flow using methane/hydrogen gases as the precursors in an ECR-CVD (electron cyclotron resonance) chamber, which is used to manufacture nanotube-like structure in other related projects. In the first year, we have successfully built and tested a 23-node PC-cluster system in our laboratory, which runs Linux OS. This PC-cluster system shall be used for simulating plasma flow in the project as time continues. Several important

components of the proposed simulation code have also been developed and verified. These include a parallel Poisson equation solver using finite-element method (FEM) for simulating electrostatic distribution, a parallel Poisson vector potential solver using FEM for simulating magnetostatic distribution, a particle tracing module for moving charged particles under the influence of Lorentz force and a particle-in-cell (PIC) method for interpolating the force field (E and B) and charge between particles and grid points. Development of the Monte Carlo collisions (MCC), considering the collisions of charged particles and neutrals, and the Maxwell equation solver using FEM is currently in progress and shall be reported in the second year.

Keywords: plasma flow, finite element, Poisson equation, Maxwell equation, particle in cell, Monte Carlo collision.

1. INTRODUCTION

In the other related project [1], ECR-CVD chamber has been used to manufacture nanostructures that can be potentially applied in higher-area-density magnetic recording media. The success of the materials processing forming nanostructures in this direction more or less depends upon trials-and-errors method. No systematic theoretical or modeling study has been conducted. To optimize the materials processing in forming nanostructures, fundamental understanding of the plasma flow inside the ECR-CVD chamber is inevitable, although it is very complicated in

essence.

Materials processing plasmas have been modeled numerically using either the fluid model [2] or the particle model [3]. The fluid model is computationally much more efficient if mobility and diffusion coefficients are provided in advance. The fluid model is valid when the electron density distribution is close to the Maxwellian. If the deviation cannot be neglected, the particle method has to be used for simulating the plasma. The particle method is a solution method for solving the Boltzmann equation. The particle method is a realization of this stochastic process using uniform random numbers (Monte Carlo simulation).

Advantages of the particle method include the justified application to low-pressure plasma as in the ECR-CVD chamber, energy distribution functions of electrons and ions as part of the solution, and unnecessary evaluation of mobilities, diffusion coefficients, and relaxation times for various values of reduced electric field, driving frequency and magnetic field.

The study was planned to be able to model the full-scale methane/hydrogen plasma flow inside the ECR-CVD chamber at the end of the three-year project. In this report, we describe briefly the preliminary results developed in this direction. In the following, numerical method

2. NUMERICAL METHOD

In this section, we will describe respectively the numerical methods employed for solving related governing equations.

2.1 Poisson Equation Solver

Poisson equation describing the electrostatic distribution can be written as

$$\nabla^2 \phi = -\frac{\rho}{\varepsilon_0} \quad (1).$$

where ϕ ($\vec{E} = -\nabla \phi$) is the electric potential, is ε_0 the permittivity and ρ is the net volumetric charge. In this research, we have applied Galerkin residual finite-element method to discretize equation (1). Resulting discretized equation can be written as

follows,

$$\sum_{i=1}^4 \sum_{j=1}^4 \left[\iiint \left(\frac{\partial N_i^{(e)}}{\partial x} \frac{\partial N_j^{(e)}}{\partial x} + \frac{\partial N_i^{(e)}}{\partial y} \frac{\partial N_j^{(e)}}{\partial y} + \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial N_j^{(e)}}{\partial z} \right) dx dy dz \right] a_{ij} \\ = \iiint \left(\frac{\rho}{\varepsilon} \right) N_i^{(e)} dx dy dz + \iiint N_i^{(e)} \tau_n d\Omega$$

(2), where $N_i^{(e)}$ is the shape function in node i . We have employed tetrahedral mesh in three-dimension for the flexibility of adapting to complicated geometry. Resulting algebraic equation from equation (2) is then solved using preconditioned conjugate gradient method (PCG).

2.2 Vector Potential Poisson Equation Solver

Vector Poisson equation describing the magnetostatic distribution can be written as follows,

$$\nabla^2 \vec{A} = -\mu_0 \vec{J} \quad (3)$$

in which the gauge condition has been enforced, $\vec{B} = \nabla \times \vec{A}$ and $\vec{J} = \nabla \times \vec{M}$. Similarly, we have applied Galerkin residual finite-element method to discretize equation (3). Resulting discretized equation can be written as follows,

$$-\frac{1}{\mu} \sum_{i=1}^4 \sum_{j=1}^4 \left[\iiint \left(\frac{\partial N_i^{(e)}}{\partial x} \frac{\partial N_j^{(e)}}{\partial x} + \frac{\partial N_i^{(e)}}{\partial y} \frac{\partial N_j^{(e)}}{\partial y} + \frac{\partial N_i^{(e)}}{\partial z} \frac{\partial N_j^{(e)}}{\partial z} \right) dx dy dz \right] a_{ij} \\ = \iiint N_i^{(e)} (\vec{M} \times \vec{n})_x d\Omega - \iiint (\vec{M} \times \nabla N_i^{(e)})_x dx dy dz + \frac{1}{\mu_0} \iiint N_i^{(e)} \tau_n d\Omega$$

(4). Similarly, 3D tetrahedral mesh is used throughout the study unless otherwise specified. Resulting algebraic equation from equation (4) is then solved using preconditioned conjugate gradient method (PCG).

2.3 PIC/MCC method

The PIC method [4] was originally designed for collisionless charged particle simulations. It models the movement of charged particles under the influence of Lorentz force ($F = q(E + v \times B)$, q : particle charge, E : electric field, B : magnetic field) and solves the field equations (Maxwell or Poisson equation) due to redistribution of charge density (ρ) and charge current (J) at each time step. A mesh is introduced to sample the space charge and current distributions that enter the field equation. The sampling is performed by appropriate *charge assignment* from the particle

locations to the grid points. Afterwards, the computed fields (E & B) from field equations at grid points are *interpolated* back to the charge-particle positions. Then, charged particles are moved to their new positions using the concept of *Boris rotation* [3] without actually computing the forces explicitly. This process repeats itself to obtain the self-consistent solution during the simulation. This is the so-called particle-in-cell (PIC) method.

In order to reproduce plasmas, one has to inevitably resolve the *smallest* time scale, i.e., electron time scale. It is estimated that electrons are the fastest particle in the plasma, with their velocities in the range of 10^5 - 10^6 m/s. Thus, this requires an electron time step of 10^{-10} - 10^{-9} s to properly model the electron trajectories in the presence of magnetic field. Thus, the time steps of ion and electron would be very much different to obtain the correct physics.

In addition, the so-called PIC/MCC method is to include the MC collisions, in the PIC method, between charged particles, and neutral particles and charged particles under the circumstances of weakly ionized plasma. This concept can be clearly shown in **Fig. 1**. The collisions between charged particles (or Coulomb collisions) are often neglected if low plasma density is concerned, as is the case in the bulk plasma region in DC-magnetron sputtering chamber. Only the collisions between charged particle and neutral particle will be taken into account in the current proposed study. In dealing with these collisions using Monte Carlo method, reliable cross section data are required.

2.4 Parallel Processing

Due to the expected high computational cost for PIC/MCC method and the necessity of solving the electrostatic/Maxwell equation at each electron/ion time step, parallel processing is strongly required for the practical purpose. We will present the proposed parallel processing, considering PIC/MCC method and field equation solver, in the following in turn.

2.4.1 Parallel PIC/MCC method

Since the MCC method is

fundamentally a particle method that possesses high parallelism as the DSMC method, we will apply the similar parallel implementation using dynamic domain decomposition we have developed in our group [5]. Details can be found in this reference and references cited therein. We will only briefly describe the method here. In this parallel technique, Stop at rise (SAR) scheme is used, based on a degradation function, to detect the necessity of repartitioning of the computational domain that uses multilevel graph-partitioning technique. In addition, the PIC method is only a way of interpolation of between nearby charged particles and nodal points; thus, it should pose no problem in parallelizing it.

2.4.2 Parallel field equation solvers

For parallel processing field equation (Poisson equation/vector potential Poisson equation/Maxwell equation), we need to formulate the system of equations in parallel format by storing the coefficient matrix in a distributed manner. As a first step, we will use the same grid distribution used by the PIC/MCC method since we expect the computational overhead in PIC/MCC would be much higher than that of solving field equation. We will solve equations using parallel version of preconditioned conjugate gradient method [6] using compressed-sparse-row (CSR) concept. In this method, we need to update the data at the interface nodes between sub-domains by communication using MPI.

3. RESULTS AND DISCUSSIONS

3.1 PC-Cluster System

We have built a 23-node PC-cluster system in our laboratory that were assembled and tested by ourselves. Main specifications include 2.4GHz processor each (AMD), 0.5GB RAM each and 1 Gbps Ethernet switch. We have been using Linux for all OSs since it is free and robust. System is now being used intensively for parallel processing. Pictures of these two systems are shown in Fig. 2 (<http://www.me.nctu.edu.tw/~MuST>).

3.2 Parallel Poisson Equation Solver

Completed parallel Poisson equation solver is verified by comparing the simulated data with analytical solution for a simplified one-dimensional parallel plate case. Test conditions include: 1000V at top plate, grounded at lower plate. Multilevel graph partitioning technique is used to partition the computational domain. Typical surface domain decomposition is illustrated in Fig. 3 for 20 processors using the number of nodes as the weighting criterion. Simulated electrostatic potential distribution is shown in Fig. 4, which agrees with the analytical solution very well. Code has also been verified for other benchmark test cases, including concentric cylindrical shells (inner: high voltage, outer: grounded) and charged sphere under constant electric field. Results are compared excellently with analytical solutions. Study of parallel performance is currently in progress and will be reported in the future.

3.3 Parallel Vector Potential Poisson Equation Solver

Permanent magnets arranged in octupole-shape (Fig. 5) are used to verify the completed parallel vector potential Poisson equation solver. 22 processors are also used for this simulation. Results of simulated magnetic flux vector are shown in Fig. 6 with 0.82 Tesla (upward) in the central airgap and are compared very well with the simulated data using commercial code such as *Ansoft*, which is often used in the magnetic society. Capability of simulating magnetostatic field having highly varying permeability is demonstrated using the test case of a permanent magnet (magnetization=1M Tesla upward), attached to a yoke ($\mu_r=1000\mu_0$), as sketched in Fig. 7. Simulated magnetic flux vector is illustrated in Fig. 8, which clearly shows the excellent capability of this solver.

3.3 Coupled PIC and Poisson Equation solver

Completed parallel PIC method coupled with previous described Poisson equation solver is verified by computing a simplified 1-D parallel plate with both plates grounded

and uniform ion distribution between the plates (Fig. 9). Ions collide with plates are absorbed (removed). 20 processors are used throughout the simulation. 10 particles per cell initially are used. Results of computed potential distribution are illustrated in Fig. 10 at various time steps. Results at $t=0$ compares very well with the exact solution.

4. CONCLUSIONS

In the first year of the current project, we have developed and verified a parallel PIC method for charge/field interpolation coupled with a parallel Poisson equation solver for electrostatic potential. Several works planned in the very near future are briefly summarized as follows:

1. To include the MCC collision into the parallel PIC-Poisson equation solver, which is currently in progress.
2. To develop a parallel Maxwell equation solver based on the previous experience in parallel Poisson equation solver.
3. To include the Maxwell equation solver into the parallel PIC/MCC module.
4. To apply the above completed code to compute the methane/hydrogen plasma approximately beginning at the end of second year of the project.

References

1. 郭正次 : Fabrication and characterizations of the alloy-encapsulated carbon nanostructures for applications in nano-resolution storage media and others. NSC 92-2120-M-009-001.
2. T. Makabe, Research Report 2000-2001, Lab. Plasma Electronics, Keio University.
3. K. Nanbu, IEEE Plasma Science, Vol. 28 (2000), pp. 971-990.
4. Birdsall, C.K. and Langdon, A.B., Plasma Physics via Computer Simulation, McGraw-Hill, New York, NY, USA, 1985.

5. Wu, J.-S. and Tseng, K.-C., "Parallel DSMC method using dynamic domain decomposition," 23rd Internal Symposium on Rarefied Gas Dynamics, British Columbia, Canada, July, 2002. Also, AIP Conference Proceedings, Editors: Ketsdever, A.D. and Muntz, E.P., Vol. 663, pp.406-413, 2003.
6. Saad, Yousef, Iterative Methods for Sparse Linear Systems, PWS Publishing Company, International Edition, 1996.

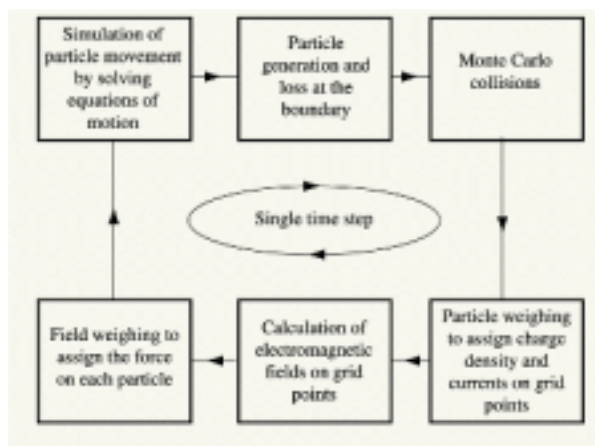


Fig. 1 Typical computational procedures during a single time step for a PIC/MCC simulation



Fig. 2 23-node PC-Cluster system at MuST

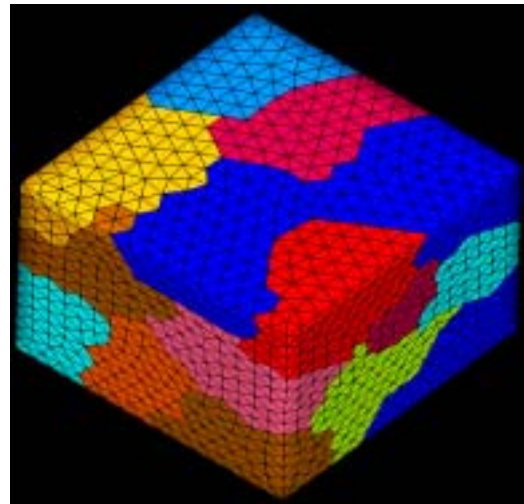


Fig. 3 Surface domain decomposition for parallel Poisson solver (20 processors)

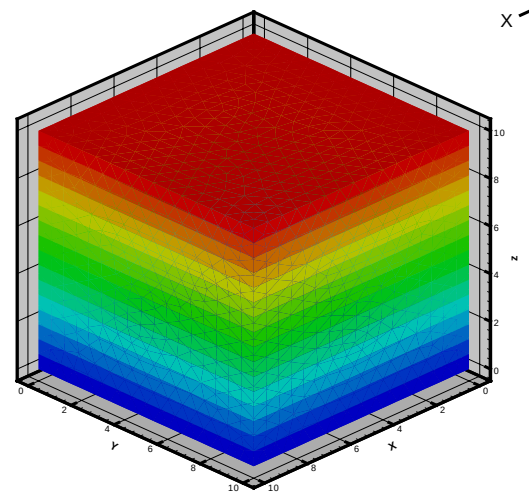


Fig. 4 Electrostatic potential distribution (colors are graded evenly in volts) (top plate: 1000 V, lower plate: 0 V)

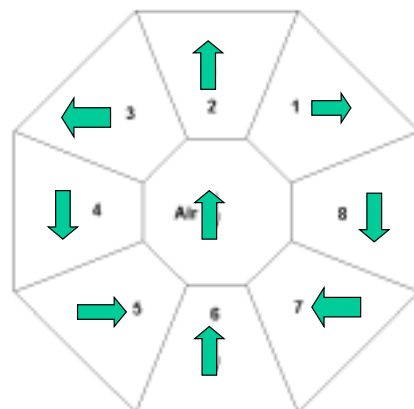


Fig. 5 Permanent magnets arranged in an octopus-shape

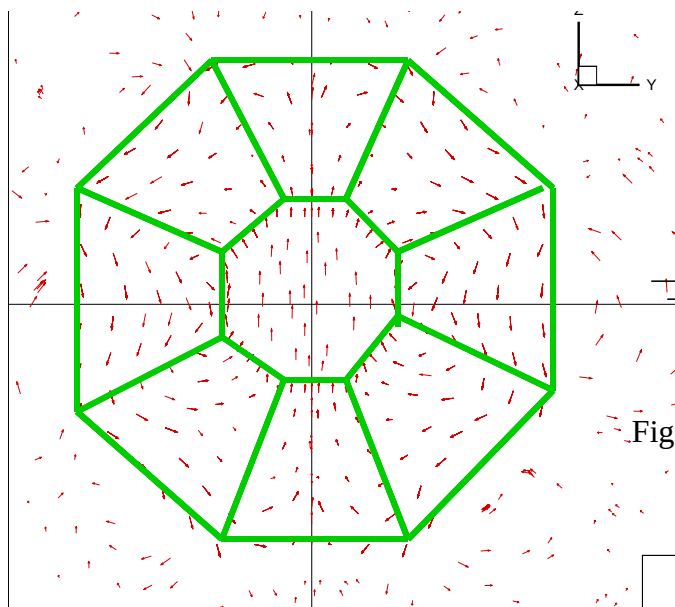


Fig. 6 Computed magnetic flux

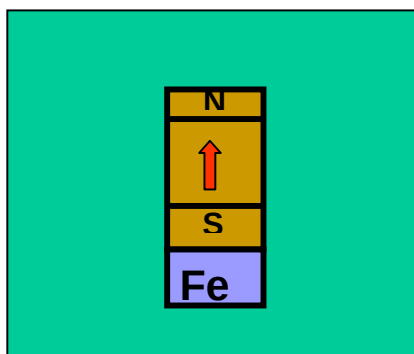


Fig. 7 Permanent magnet connected with a yoke ($M=1$ Tesla, $\mu_r=1000\mu_0$)

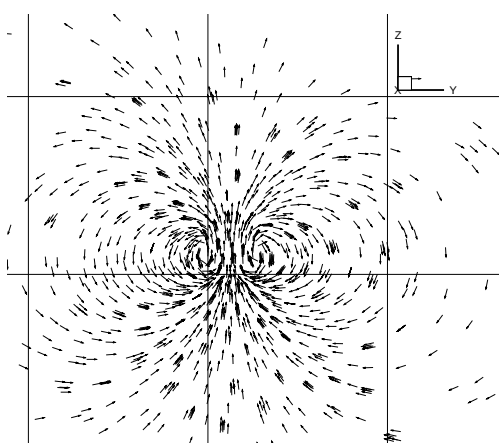


Fig. 8 Distribution of magnetic flux vector

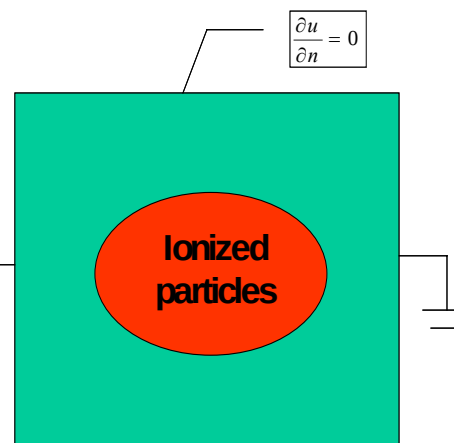


Fig. 9 Sketch of the ionized particles between parallel plate with both ends grounded

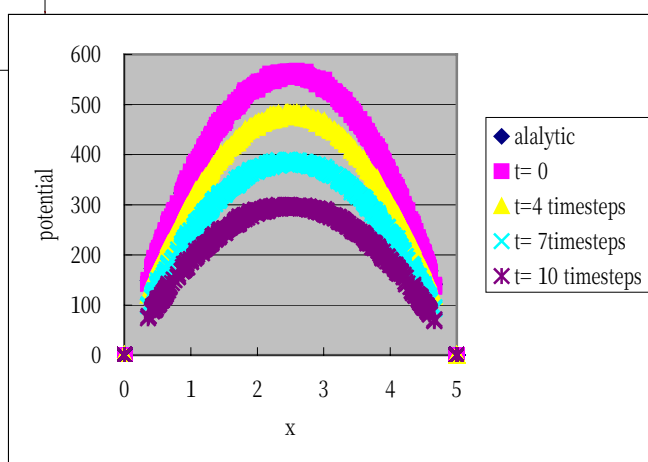


Fig. 10 Potential distribution between the parallel plates at different time steps with initially uniform ion distribution

