Wednesday Morning, November 11, 2009

Vacuum Technology
Room: J1 - Session VT-WeM

Partical and Theoretical Aspects of Gas Dynamics

Moderator: R.E. Ellefson, Consultant

8:00am **VT-WeM1 Gas Dynamics Aspects of Atomic Layer Deposition**, ***S.M. George***, University of Colorado at Boulder **INVITED**

Atomic layer deposition (ALD) is a thin film growth method based on sequential, self-limiting surface reactions. ALD can produce extremely conformal and atomic layer controlled film growth. The rate of ALD film growth is dependent on surface reaction efficiencies and gas dynamics. This talk will review the design of various ALD reactors with emphasis on the role of gas dynamics. The optimum pressure in viscous flow ALD reactors will be shown to be a trade-off between gas entrainment and gas interdiffusion. The most rapid rates of ALD film growth will be achieved using "synchronous modulation of flow and draw" where the reactant exposures occur under near static conditions and viscous flow is only operative during reactant purging. The talk will conclude with a review of new ALD reactors operating at atmospheric pressure.

8:40am **VT-WeM3 Collimated Gas Beam Analysis for Atomic Layer Epitaxy of Cracked Disilane**, *M.P. Nadesalingam*, University of Texas at Dallas, *M. Kanouff*, Sandia National Laboratories, *J. Randall*, Zyvex Labs, *R.M. Wallace*, ***W.P. Kirk***, University of Texas at Dallas

The application of collimated gas beams has enjoyed a central role in many atomic and molecular beam experiments of the past, and is again proving to be important for the development of tip based nanofabrication of new devices such as quantum dots, qubits, NEMS oscillators and biomedical devices. We report the analysis of the molecular flux from micro-capillary array dosers for atomic layer epitaxy experiments of cracked disilane. The spatial distribution as well as the total flux can be important parameters for experiments and fabrication processes. Both analytic and numeric analyses have been performed and show values that differ in some aspects from the early results of Winkler and Yates.1 At high acceptance angles where the target is closer to the source, the flux is found to be greater than the previous results by approximately 10 to 15% for various ratios of source to target diameters. The consequences of our results for atomically precise manufacturing of nanometer scale structures will be discussed.2

References

1. A. Winkler and J. T. Yates, Jr., J. Vac. Sci. Technol. **A 6** (5), 2929 (1988).

2. This material is based upon work supported by the Defense Advanced Research Project Agency (DARPA) and Space and Naval Warfare Center, San Diego (SPAWARSYSCEN-SD) under contract N66001-08-C-2040. It is also supported by a grant from the Emerging Technology Fund of the State of Texas to the Atomically Precise Manufacturing Consortium.

9:00am **VT-WeM4 Decomposition Characteristic of Metal-organic Gases**, ***S. Yamashita***, Tohoku University, Japan, *M. Nagase*, *K. Ikeda*, Fujikin Inc., Japan, *M. Kitano*, *Y. Shirai*, *T. Ohmi*, Tohoku University, Japan

The Film formation process by using Metal-Organic (MO) CVD method is used for various applications such as interlayer dielectric of silicon semiconductor devices, ferroelectric substance film formations and transparent electrode formation. MO gases that are used in MOCVD processes are either in the liquid state or the solid state at room temperature and the vapor pressure of these gases is very low. In order to supply MO gases to the process chamber effectively, MO gases are heated to increase the vapor pressure and are supplied by using various means including the bubbling method. But many MO gases have high reactivity. So there is a possibility that MO gases may decompose during use. Due to this problem, there is the issue that byproduct of MO gas decomposition tend to be deposited in the gas supply system. So we evaluated the thermal decomposition property and the oxidation property of three kinds of MO gases [Tetraethoxysilane (TEOS), Trimethylphosphite (TMP) and Trimethylborate (TMB)] by using the FT-IR method to examine the cause of decomposition in MO gases. When MO gases are heated at an inert gas atmosphere, MO gases can be stably supplied without decomposition occurring until 400℃. This result shows that these gases have high stability regarding heat levels. However, when MO gases are heated at an atmosphere including 50 percent oxygen, decomposition temperature of each gas was significantly reduced and carbon dioxide was produced with the decomposition of MO gases. This result shows that the oxidative decomposition of MO gases occurs during heating in an atmosphere including oxygen. Next, MO gases were heated with a resin material used for the valve seat of the gas supply system. We used polyimide (PI) and Perfluoro-Alkoxy (PFA) as a resin material that can be used for the seat of the valve until 150℃. Firstly, TEOS could be stably supplied through tubing containing resin samples. When TMP and TMB flow through the tubing containing the PI test piece, the TMP and TMB could not be stably supplied even at 50℃ and these gases decomposed. And when we raised the heat temperature, decomposition of these gases furthered the progress. When TMP and TMB flow through the tubing containing PFA test piece, the TMB could be supplied stably at 50℃. Afterwards TMP decomposed and could not stably supplied at 50℃. But when TMP continued to flow for a designated duration of time, TMP could be stably supplied. In this case, when we raised the heat temperature, the decomposition of these gases did not occur. This phenomenon was caused by moisture evaporated from resin materials.

9:20am **VT-WeM5 Numerical Simulation of Rarefied Gas Flows through Short Tubes Driven by a Pressure Drop**, *F. Sharipov*, Unuversidade Federal do Parana, Brazil, ***S. Varoutis***, *D. Valougeorgis*, University of Thessaly, Greece

Rarefied gas flows through short tubes are investigated numerically by the Direct Simulation Monte Carlo method. The flow rate and flow field were calculated as a function of the gas rarefaction, length-to-radius ratio and pressure drop. The gas rarefaction, which is inversely proportional to the Knudsen number, is varied from 0 to 2000, i.e. the free-molecular, transitional and hydrodynamic regimes are embraced. A wide range of the length-to-radius ratio, namely from 0 corresponding to the orifice up to 10 representing a sufficiently long tube, are considered. Several values of the pressure ratio between 0 and 0.7 are regarded. This pressure range covers both gas flow into vacuum and into a back ground gas. It has been found that the rarefaction parameter has the most significant effect on the flowfield characteristics, followed by the pressure drop, while the length-to-radius ratio has a rather modest impact. The effect of gas rarefaction on the choked flow and on the Mach discs at large pressure drops is discussed. A comparison of the present numerical results with available experimental data has shown a good agreement.

9:40am **VT-WeM6 Modelling a 25 Stage Turbomolecular Pump with 6 Orders of Compression with DSMC**, ***R. Versluis***, *R. Dorsman*, TNO Science and Industry, The Netherlands

Last year we presented a new method to model moving surfaces in DSMC. The method was validated by modelling a single rotor of a turbomolecular pump and comparison with experimental results. We have now applied the method to model the gas dynamics inside a 25 stage turbomolecular pump (13 rotors and 12 stators) under various discharge pressures and for various gases and gas mixtures. The turbo pump consists of two sections with different number of blades and different angles. The compression of the turbopump is about 6 orders of magnitude and the flow regime insode the pump goes from free molecular conditions at the inlet side to transitional flow on the discharge side. Interesting phenomena inside the pump are shown, such as a non-linear pressure profile inside he pump, with the non-linearity taking place at a position that would not be expected based on the geometry. Details of the gas flow inside the turbopump are visualized such as the concentration profile of gas mixtures inside the pump, temperature effects and the pressure contours inside the pump. All of these things can also be visualized as a function of time showing the pressure increase at the blade edges ahen a rotor passes a stator and the pressure decrease when the rotor has passed the stator, followed by the backflow of molecules in the wake of the blade.

The method allows a completely new look inside the turbopump and offers possibilities for simulation of new prototypes, optimisation of blade geometry, spacing etc. The current algorithm that calculates the interactions between molecules and rotors is limited to linear blade motions. The rotational motion of the blade is therefore linearized to a straight motion, but the method itself is general. The algorithm can easily be replaced for non-linear velocities although the calculation of collisions between blade and molecules becomes more tedious.

By running the calculations a large cluster of dedicated computers (up to 100 parallel nodes) the calculation time for discharge pressures around 1 Pa is still reasonably small (around 1 day).

The attached document shows an example of the results of a calculation for nitrogen.

10:40am **VT-WeM9 New Spiral Molecular Drag Stage Design for High Compression Ratio, Compact Turbo-Drag Pumps**, ***S. Giors***, *L. Campagna, E. Emelli*, Varian S.p.A, Italy

The current turbo-drag pumps commercially available for high vacuum systems are based on either Gaede or Holweck molecular drag stages technology, used in series downstream axial bladed stages to extend the maximum compression ratio up to the 10 mbar foreline pressure range.

Modern Gaede molecular drag stages use a disk shaped impeller, allowing a very compact design, but their maximum compression ratio is limited by the leakage effect to about 10 per stage.

Holweck stages use a less compact drum-shaped impeller, but are able to supply a higher compression ratio per stage and can easily be designed to supply a higher pumping speed thanks to the presence of many channels in parallel.

In this paper a new spiral molecular drag stage design is presented, with the advantages of both high compression ratio and pumping speed per stage and very compact design: a stage occupying the very tiny axial room of a Gaede, can compress as much as two or three Gaede stages in series, and supply the same compression ratio and pumping speed of a Holweck stage of the same diameter and peripheral speed, in a much smaller axial room.

The new spiral drag stage allows the design of very compact, high compression ratio turbo-drag pumps. The comparison of new design turbo-drag pump in the size of 700 l/s with existing Gaede and Holweck based products of the same size is presented, showing the technology advantages of the new design.

11:00am **VT-WeM10 Numerical Analysis of the Rarefied Gas Flow through a Short Channel into a Vacuum**, ***O. Sazhin***, Ural State University, Russia

A rarefied gas flow through a short channel into a vacuum presents a complex task due to significant non-equilibrium. Therefore, it is possible to find a good number of empirical formulas in open literature for calculating flow rate in this case. Correct approach to solving this problem should be based on the Boltzmann equation [1]. The difficulties of numerical solutions for this equation, caused by a large number of independent variables and a complex structure of a non-linear collision integral, are well-known. In our opinion, direct simulation Monte Carlo (DSMC) method [2], which is customarily viewed as a stochastic solution for Boltzmann equation, is preferable for use in tasks with strong non-equilibrium. DSMC method is an effective tool to solve problems of rarefied gas dynamics from free molecular to viscous regimes. An approach based on using DSMC method allows to take into account several factors, such as strong non-equilibrium, as well as to use various models of the gas-surface scattering and the gas molecule-molecule interactions. Therefore, it is appropriate to use DSMC method to study the rarefied gas flow through a short channel into a vacuum.

Practical application of the results of such research can be in the development and creation of such devices as micro- and nanoseparators, micropumps, microshutters, microgyroscopes, micro- and nanosatellites, and other micro- and nanoelectromechanical systems (MEMS/NEMS) [3]. The flow of gas in MEMS/NEMS, depending on device size and gas pressure, can be viscous, transitional or free molecular.

In this study, the mass flow rate through the channel into a vacuum is calculated over the wide range of gas rarefaction as function of channel's length. To study the gas molecule–molecule interaction influence, we used the variable hard sphere and variable soft sphere models defined for inverse–power–law potential and also the generalized hard sphere model defined for the Lennard–Jones potential. Maxwell, Cercignani–Lampis and Epstein models were used to simulate the gas–surface scattering. This study demonstrates that the gas molecule–molecule interaction and the gas–surface scattering can have a significant influence on the rarefied gas flow through a short channel into a vacuum. The analysis of the flow field, both within the channel as well as in upstream and downstream containers, is presented.

REFERENCES

1. C. Cercignani, *The Boltzmann Equation and its Application*, Springer, New York (1988).

2. G.A. Bird, Molecular Gas Dynamics and the Direct Simulation of Gas Flow, Oxford University Press, Oxford (1994).

3. *Encyclopedia of Microfluidics and Nanofluidics*, ed. by Dongqing Li, Springer, New York (2008).

11:20am **VT-WeM11 Effect of Surface Material and Roughness on Conductance of Channel between Parallel Disks at Molecular Flow**, ***H. Yoshida***, *M. Shiro, K. Arai, M. Hirata, H. Akimichi*, National Metrology Institute of Japan / AIST, Japan

For precise calculations of conductance and pressure distribution in vacuum chamber at molecular flow, it is important to know a degree of realization of diffuse reflection (also called cosine law) at surface. The conductance of an experimental channel changing the surface material and roughness was measured and compared with the results using Monte Carlo calculation assuming diffuse reflection.

The experimental channel consisted of two parallel disks was equipped with the vacuum chamber with an inner volume of 8.42x10-2 m3.The lower disk made from polished stainless steel (SS) has a diameter of 40 mm and a hole of 10 mm in diamter at the center. The upper disk with 51 mm in diameter is located as facing parallel to the lower one. The space between the upper and the lower disks was determined from 0.3 mm to 0.7 mm using gauge blocks as a spacer. After the vacuum chamber was filled with N2, Ar, or He gas at approximately 100 Pa, it was evacuated from the hole of lower disk by turbo molecular pump (0.22 m3/s) through the space between two parallel disks. The conductance of the channel was obtained from the pressure decrease rate in the vacuum chamber.

Eleven upper disks with different material and surface were prepared: polished SS, unpolished SS, quartz, Ti, Cu, Al, alumina with smooth surface, alumina with rough surface, SS with Au coating, SS with Pt coating, and SS with DLC coating. The effect of surface material and roughness on conductance was estimated from the measurement of the conductance of the channel by replacing the upper disk.

The conductance for N2 using polished SS with 0.5 mm in space was 3.68x10-4 m3/s (±2.7%), which was comparable to the calculated value of 3.67x10-4 m3/s (±1.3%). Similarly, the experimental values for N2 and Ar using polished SS, quartz and SS with DLC coating showed good agreement with the calculated ones within the measurement uncertainty. On the other hand, the conductance using SS with Pt coating was about 7% smaller than the calculated one. Their surfaces morphologies were analyzed by optical microscope and atomic force microscope (AFM). The microscopic surfaces of polished SS, quartz and SS with DLC coating were very smooth with the roughness less than 1 nm and the specific area less than 1.01. In the case of SS with Pt coating, however, the microscopic surface was rough with the specific area of 1.10. Judging from the results of all disks, the conductance seemed to be influenced by surface roughness rather than surface material. In the case of He, the experimental value was about 4% larger than the calculated one. This reason should be the influence of the specular reflection and/or the lobular scattering.

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