RESEARCH

Study on characteristics of microchannel jet for showerhead in diferent fuid regimes based on hybrid NS‑DSMC methodology

Wansuo Liu1 · Xiangji Yue1 · Zeng Lin1

Received: 12 July 2023 / Accepted: 18 December 2023 / Published online: 15 February 2024 © The Author(s), under exclusive licence to Springer-Verlag GmbH Germany, part of Springer Nature 2024

Abstract

The uniformity of the deposition in the plasma-enhanced chemical vapor deposition (PECVD) process is greatly infuenced by the uniform efect of the microchannels in the showerhead. Most of the previous studies on showerheads have primarily focused on the axial-direction of microchannels. However, there is a lack of comparative studies on the infuence of radial changes and diferent fow regimes on the fow characteristics of microchannels. In this paper, we utilized the coupling of the Navier–Stokes and Direct Simulation Monte Carlo (NS-DSMC) methods to compare the diferences between expansion type microchannels and equal-diameter type microchannels in the slip and transition regimes. The results indicate that in the slip fow regime, the microchannel of equal diameter exhibits a stronger jet compared to the expansion type. However, this situation reverses as the slip fow regime transitions to the transition regime. This refects the infuence of the fow regime on the characteristics of the microchannel and the potential of the combined type to enhance deposition uniformity.

Keywords NS-DSMC method · Transition regime · Showerhead · Microchannel fow · PECVD uniformity

1 Introduction

Plasma-enhanced chemical vapor deposition (PECVD) is a manufacturing process used in flm production. Its characteristic is to conduct the plasma combination reaction by ionizing the reaction gas in a rarefed environment and then depositing the product on the surface. Therefore, the uniformity of the gas will directly afect the uniformity of the fnal deposition on the surface.

To enhance the uniformity of the gas, a showerhead structure is typically incorporated into the reaction chamber. This structure is typically a circular baffle that improves the gas uniformity through the microchannels on it. Lee et al. ([2019\)](#page-10-0) studied the distribution of holes in the showerhead, specifcally focusing on the infuence of the hole open area ratio in the showerhead structure on the flm thickness distribution within the wafer. The results indicated that the shape of flm deposition could be controlled, and the uniformity of flm thickness was improved by optimizing the hole open area ratio of the showerhead structure. In addition, there are

 \boxtimes Zeng Lin zlin@mail.neu.edu.cn other researchers who are focused on studying the structure of holes. Wi et al. (2012) present the characteristics of hydrogenated microcrystalline silicon thin flms deposited from a $SiH₄/H₂$ in the PECVD system equipped with a showerhead. The results show that a higher deposition rate is found in the deep and dense hole region when the shape and density of the holes on the electrode are varied. Xiang et al. ([2019\)](#page-10-2) investigated the deposition of a large-area silicon–nitride flm using silane and ammonia by PECVD in a 300 mm apparatus with a vertical showerhead. The inherent non-uniformity of flms could be improved by utilizing showerheads with holes of diferent depths. These studies not only demonstrate the infuence of hole structure on the uniformity of the showerhead but also examine two types of hole structures: the equal-diameter type and the expansion type. It can be observed that the distribution and structure of holes directly afect the uniformity of the showerhead.

Not only does the structure of the showerhead itself afect uniformity but also the fuid environment can also impact its performance by affecting the flow through the holes. Guensuk et al. studied the Amorphous Carbon Layer (ACL) deposition rate at 733 Pa and 550 ℃, the Knudsen number (*Kn*) is around 0.02181. Moreover, Sung-Suk et al. studied the PECVD reactor at a pressure of 8 torr and a temperature of 200 ℃, and the *Kn* is approximately 0.00132.

 1 School of Mechanical Engineering and Automation, Northeastern University, Shenyang 110819, China

Fig. 1 System of PECVD reaction

Furthermore, Kim and Lee ([2017\)](#page-10-3) investigated the structure of a showerhead in a capacitively coupled plasma (CCP) reactor, which utilized an axisymmetric fuid mode in the regime of transition fow. The fow regimes in the above articles are between the slip fow regime and the transition flow regime. From the information in microchannel research (Weng et al. [1999\)](#page-10-4), it is believed that the flow regime would afect the pressure distribution in the microchannel of the showerhead. Therefore, it is necessary to study the infuence of rarefed characteristics of the microchannel on the uniformity of the showerhead.

The research on microchannels in rarefed fuids mainly focuses on the distribution of gas pressure, velocity, and temperature within the channel. However, there is a lack of relevant research on jet uniformity. This article focuses on microchannel research and investigates the impact of various microchannel structures and fow regimes on showerhead jet uniformity, by integrating microchannel flow with showerhead uniformity. On one hand, it can enhance research on the fow characteristics of radial structural variations in the microchannel. On the other hand, it can be benefcial in improving the fow uniformity of the showerhead.

2 Experimental procedure

To validate the simulation method used for transition regimes, we conducted experiments to detect plasma using Langmuir probes. The experimental device is shown in Fig. [1.](#page-1-0) The inner diameter of the vacuum chamber was 340 mm, and the spacing between the upper and lower plates was 60 mm. The gas was injected into the vacuum chamber through the showerhead, and the fow is controlled by the mass fow controller. The upper plate was connected to a radio frequency power source (13.56 MHz) and generated plasma through capacitive coupling. The experimental parameters were set based on the optimal parameters for the oxidation process. The working vacuum was 6.5 Pa, and the radio frequency power was 200 W. The ratio of gas mass flow rate between Ar and O_2 was 1:1, with both gases flowing at a rate of 5 sccm. The Langmuir probe utilized a conventional tungsten probe that was adjusted in position by the drive system. It sweeps the sawtooth waveform with $a \pm 110$ V output. By using the Langmuir probe, the plasma density can be measured. In this paper, the cross-section of the probe above plate 20 mm was selected for analysis.

3 Numerical method and verifcation

There are various possibilities for the flow regime in the microchannels of the PECVD chamber. Normally, it will be in the slip flow or transition flow regime. There are significant diferences in the calculation methods used for the two flow regimes (Yuan et al. [2020\)](#page-10-5). The continuum flow method that incorporates a slip boundary correction is appropriate for the slip fow regime, but it is not suitable for the transition fow regime. In this paper, a coupled Navier–Stokes and Direct Simulation Monte Carlo (NS-DSMC) method was used to calculate the transition regime. The regions where the continuum flow method is not applicable were determined by calculating the *Kn*. The region would be appropriately expanded and solved using a DSMC method. Thermal radiation is not considered in the calculation, and the heat transfer mechanism between the gas fowing inside the microchannel and the wall is only through molecular interaction. This is because diatomic molecules do not participate in radiant heat exchange under the current rarefed conditions (Huang and Lai [2012\)](#page-10-6).

3.1 The NS method

A three-dimensional model was used for the simulation. The calculation grid adopted a tetrahedral mesh with better adaptability over a wide range, while locally using a hexahedral mesh for higher accuracy. The fundamental governing equations, which include the continuity equation, momentum equation, and energy equation, were discretized using the fnite volume method. The inlet pressure was 800 Pa, and the outlet pressure was 667 Pa. The *Kn* was 0.0091–0.0109, and a slip boundary correction was adopted. The tangential momentum accommodation coefficient σ was properly chosen, and the NS solution became in agreement with the experiment when the fnite slip velocity was introduced along the microchannel surfaces (Arkilic et al. [1997a](#page-10-7); Beskok et al. [1996\)](#page-10-8) given by

$$
u_s = u_w + \left(\frac{2-\sigma}{\sigma}\right) \left(\frac{Kn}{1-bKn}\right) \left(\frac{du}{dn}\right)_{wall}
$$
 (1)

where u_s is the dimensionless slip wall velocity, u_w is the dimensionless no-slip wall velocity, σ is the tangential momentum accommodation coefficient, and $\left(\frac{du}{dn}\right)$ *wall* denotes the normal velocity gradient at the surfaces. The accommodation coefficients $\sigma = 1$ are invoked to model diffuse reflection walls (Rafi et al. [2019](#page-10-9)). The density-based com-pressible flow (Gad-el-Hak [1999\)](#page-10-10) and SST turbulence model were adopted. The calculation convergence accuracy is 10^{-4} . The maximum velocity and average pressure were monitored, and the monitoring data reached a stable value before the calculation was completed. The NS method is based on the continuity assumption. However, as the non-continuum efect increases, kinetic theory suggests that the NS equations would become invalid (Fan and Shen [2001](#page-10-11)).

3.2 The DSMC method

Bird proposed the DSMC method, which is based on statistical methods instead of solving the continuity assumption equation (Bird [1976\)](#page-10-12). The DSMC method describes the state of the system by tracking the positions and velocities of a large number of particles. Each calculated particle in DSMC represents a specifc number of real particles. Through grid division, the motion state of particles in each grid area can be calculated to represent the fow state of the grid area.

Based on the open-source OpenFOAM software, the rarefed fuid was simulated using the dsmcFoam module with the DSMC method (Palharini et al. [2015](#page-10-13)). The molecular free path (*λ*) was calculated as

$$
\lambda = \left(\frac{2(5-2\omega)(7-2\omega)}{15}\right) \left(\frac{\mu}{\rho}\right) \left(\frac{m}{2\pi kT}\right)^{1/2} \tag{2}
$$

where ω is the temperature coefficient of viscosity, m is the atomic mass, k is the Boltzmann constant, *T* is the temperature, μ is the gas dynamic viscosity, and ρ is the gas density. Ensuring that the mesh size was a fraction of the free path (Cai et al. [2022\)](#page-10-14), the time-step size was a fraction of the average collision time, and the average number of particles per cell was 25 (Ghazanfari et al. [2022;](#page-10-15) Scanlon et al. [2010](#page-10-16)). A variable hard sphere (VHS) collision model was used (Rafi et al. [2019;](#page-10-9) Moss and Price [1997\)](#page-10-17). The Maxwell wall condition, which is suitable for rarefied flow interaction, was used (Virgile et al. [2022](#page-10-18)). The computational efficiency of the DSMC method depends on the number of particles, which in turn is related to the free path. Therefore, the DSMC method is mostly used to solve the non-continuum regime of the fow feld.

3.3 The slip fow method verifcation

In the slip flow simulation, the FLUENT calculation module in ANSYS software was used for the simulation. The accuracy of the microchannel jet calculation is verifed by comparing it with other scholars' research.

Beskok et al. ([1996](#page-10-8)) studied the combined effects of compressibility and rarefaction in gas microfuidics in slip fow structures with *Kn* less than 0.3. Arkilic et al. [\(1997b](#page-10-19)) proposed an analytical solution for the pressure distribution in microchannels based on a frst-order slip boundary condition model. The models of ARKILIC et al. and BESKOK et al. demonstrate that compressibility can lead to non-linear pres-sure distributions. In previous studies (Huang and Lai [2012](#page-10-6); Jang and Wereley [2004](#page-10-20); Ko and Gau [2011;](#page-10-21) Pong et al. [1994](#page-10-22); Zohar et al. [2002\)](#page-10-23), it was shown that the pressure distribution in microchannels exhibits non-linear behavior, which is expressed as $S_{\text{non-linear}}$. The formula for calculating the dimensionless non-linearity is defned as:

$$
non-linearity = \frac{S_{non-linear}}{S_{base}}
$$
 (3)

w h e r e $S_{non-linear} = \int_0^L (P(x) - P_{linear}(x)) dx$ $,S_{base} = (P_{in} - P_{out})L/2$. Considering the fluid's thinness, Gao et al. [\(2018\)](#page-10-24) modifed formula ([3\)](#page-2-0) to:

non-linearity_(Kn=0)=
$$
\frac{1}{3} - \frac{2}{3\left(\sqrt{1 + \frac{32Lc^2Ma^2}{TRr_0Re}} + 1\right)}
$$
 (4)

where *L* is the pipe length, *c* is the pipe fow velocity, *Ma* is the Mach number, *T* is the temperature, *R* and r_0 are the viscosity coefficients, and *Re* is the Reynolds number. It is shown that for a given gas type and microchannel, the nonlinearity in the continuum fow region depends on *Ma* and *Re*. In order to study the characteristics of microtube flow more succinctly, the pressure ratio (η) is utilized to simplify formula [\(4](#page-2-1)). Because *η* has considered the infuence of *Ma* and *Re* on non-linearity. Gao et al. provided a simplifed formula as follows:

$$
non-linearity_{(Kn=0)} = \frac{1}{3} - \frac{2}{3(n+1)}
$$
 (5)

Formula ([5](#page-2-2)) shows that non-linearity is the only effect of pressure ratio in the continuum fow regime. The nonlinearity increases with the increase of *η*. When *η* approaches infnity, it can reach the maximum limit of non-linearity (33%). When η approaches 1, the non-linearity becomes 0, and the compressibility of the fuid disappears.

Weng et al. ([1999](#page-10-4)) normalized the fow feld values in their study of microchannel fow, as shown in Fig. [2](#page-3-0)a. In this figure, D_0 represents the inverse Knudsen number $(D_0 = \frac{2r}{\sqrt{\pi} \lambda})$. Figure [2a](#page-3-0) shows the non-linear characteristics under diferent pressure ratios and rarefaction. It demonstrates that the non-linearity decreases as the pressure ratio decreases. Comparing our simulation data with Fig. [2b](#page-3-0), it can be seen that the non-linear characteristics of our simulation results are consistent with the research fndings of WENG et al.

The analysis results of Gao et al. [\(2018\)](#page-10-24), Huang and Lai ([2012](#page-10-6)), Jang and Wereley [\(2004](#page-10-20)), and Pong et al. [\(1994\)](#page-10-22) are compared, as shown in Fig. [3.](#page-3-1) The range of *Kn* studied includes slip flows. GAO et al. studied a range of 0.02–6.6, Huang et al. studied a range of 0.0015–0.014, Jang et al. studied a range of 0–0.104, and PONG et al. studied a range of 0–0.155. The analysis results of Huang et al., Jang et al., and Pong et al. are very consistent with the formula ([5\)](#page-2-2) provided by Gao et al. In $\eta = 1.2$, the non-linear result of formula ([5](#page-2-2)) is 3%, while our simulation result is 4.53%. The simulation result is consistent with the previous fndings.

Fig. 2 Relative outlet pressure distribution curves, **a** Pressure curves of different inverse Knudsen numbers and pressure ratios (Weng et al. 1999), **b** Pressure ratio 1.2 pressure curves

3.4 The transition fow simulation method and verifcation

In the case of an inlet pressure of 8.35 Pa and an outlet pressure of 6.5 Pa, the *Kn* value ranged from 0.0025 to 1.12. The flow field in the PECVD chamber was primarily in the laminar continuum fow regime, whereas the gas in the 0.8 mm diameter microchannel was in the transition fow regime (Aktas et al. [2001](#page-9-0)). We adopt the NS-DSMC coupling algorithm to solve this multi-fow regime problem. The NS-DSMC coupling method is based on the open-source OpenFOAM software. A steady-state solver called rhoSimpleFoam was used in the continuum fow regime. Rarefed regimes in the microchannel fow feld were solved using the DSMC procedure in the dsmcFoam module.

The DSMC method has a high computational accuracy (Wagner [1992\)](#page-10-25), but the disadvantage is that it requires a large number of computational resources in the continuum regime. The NS method also exhibits high reliability specifcally for the continuum domain. Therefore, we established the coupling of NS and DSMC methods to solve diferent regions. Our coupling method did not modify the two modules; instead, it facilitated interaction between two excellent algorithms at an appropriate position. We believe that the key issue to be solved by the coupling method is not computational accuracy, but computational efficiency. Therefore, we compared the results of the NS-DSMC method with those of the DSMC method in order to achieve the same level of accuracy but with higher computational efficiency.

First of all, the statistical scatter calculated by DSMC will only cause numerical fuctuations of the boundary grids but will have little effect on the internal grids. Therefore, the overlapping grid method can be used to transfer internal data for coupling (Schwartzentruber and Boyd [2006\)](#page-10-26). The DSMC region was extended into the NS region to create an overlapping region. The coupling process must be carried

Fig. 3 Comparison of calculation and experimental results

out in the continuum domain in order to smoothly transition the program from the particle domain simulation to the continuum domain (Eggers and Beylich [1994](#page-10-27)). The size of the overlapping grid has little efect on the results (Aktas and Aluru [2002\)](#page-9-1), and its purpose is to transfer the internally stable solution of DSMC and ensure the validity of the NS method in the coupled region. Therefore, we extend the DSMC area to the NS area, as shown in Fig. [4.](#page-4-0)

Second, a state-based coupling approach is adopted (Roveda et al. [1998,](#page-10-28) [2000;](#page-10-29) Farber et al. [2016](#page-10-30)). Boundary conditions are imposed on rarefed gas molecular simulations using Chapman-Enskog velocity distributions (Aktas and Aluru [2002](#page-9-1)). Compared to the boundary conditions of the Maxwellian distribution, the Chapman-Enskog distribution is better suited for boundary conditions that are close to the equilibrium region (Schwartzentruber and Boyd [2006](#page-10-26)). The flow velocities of simulated molecules into DSMC boundary cells are obtained from the Chapman-Enskog velocity distribution function, which is based on macroscopic flow variables.

Furthermore, by adopting the sub-relaxation technique, the statistical errors in DSMC can be efectively reduced (Sun and Boyd [2005\)](#page-10-31). Both the sub-relaxation technique and the overlapping grid are used to transfer the stable results of the DSMC domain to the NS domain. The overlapping grid and the Chapman-Enskog distribution are used to exchange boundary conditions between continuum domains and molecular domains (John and Damodaran [2009](#page-10-32)).

Also, we adopted a two-way coupling method instead of the traditional one-way coupling method (Rafi et al. [2019](#page-10-9); Virgile et al. [2022](#page-10-18)). Normally, the NS-DSMC method is calculated using the NS method and then handing over the larger *Kn* domain to the DSMC method. The data is oneway from NS to DSMC. We applied the two-way method to feed the DSMC method data back to the NS method, both of which would evolve simultaneously. The comparison results between one-way and two-way coupling are shown in Fig. [5,](#page-4-1)

Fig. 4 Schematic diagram of calculation area division

which indicate that the two-way coupling method achieved higher efficiency and accuracy.

Finally, the time decoupling of the steady-state coupling process is achieved by employing the Schwarz alternation method. By adopting the serial Schwarz alternation method, the exchange of subdomain steady-state solutions is realized, allowing for the evolution of the entire fow feld. Using the Schwarz alternation method and Dirichlet-Dirichlet boundary conditions, the location of the solver interface for the two domains is pre-specifed to facilitate data exchange. This method is suitable for coupled low-speed steady-state problems, and the implicit iterative coupling method is used to avoid the issue of explicit integration to the global steadystate (Aktas and Aluru [2002](#page-9-1)).

In Fig. [6](#page-5-0), NS-DSMC (NS) represents the calculation result of the NS subdomain in the coupling method, and similarly NS-DSMC (DSMC) is the result of the DSMC subdomain. The results showed that the NS-DSMC results were

Fig. 5 Comparison of 10,000–60000 calculation step result curves between one-way coupling and two-way coupling at the inlet position of the microchannel, **a** one-way coupling method, **b** two-way coupling method

highly consistent with the DSMC results which illustrate that the coupling method has been completed. The electron density obtained from Langmuir probe detection equipment and the fow feld velocity calculated using the NS-DSMC method are shown in Fig. [7](#page-5-1). The cross-sectional position is situated in the middle of the chamber. The position of 0.00 m represents the center of the chamber, and the position of -0.10 m indicates the edge of the chamber. It can be seen that the results of the NS-DSMC method are consistent with the experimental results, which aligns with the fndings of Yambe et al. (Yambe et al. [2014](#page-10-33)).

4 Results and discussion

The microchannel and chamber geometry studied in this article are shown in Fig. [8](#page-6-0). The coordinate system uses the vertical direction (gas fow direction) as the z-axis and the horizontal direction (radial direction) as the x and y axes. The coordinate origin is the center of the outlet of the microchannel, situated at the center of the chamber.

In the slip flow regime situation, as shown in Fig. [9](#page-7-0)a, b, the equal-diameter type had a stronger jet, and the axial velocity of the equal-diameter type was higher than that of the expansion type. The results in Fig. [9b](#page-7-0) is in the middle line of the microchannels in Fig. [9a](#page-7-0). In the transition regime situation, the characteristics of the jet were inverted for the two types of microchannels. As shown in Fig. [9](#page-7-0)c, the line out of the microchannel labeled as "z 0.0015" indicates a distance of 0.0015 m from the outlet. The equal-diameter type had a higher velocity than the expansion type, but the situation changed at "z 0.004" where the expansion type had a higher velocity. The velocity distribution exhibits a signifcant disparity between the slip fow regime and the transi-tion flow regime. Figure [9a](#page-7-0) and c have different velocity

channel flow field

Fig. 7 Comparison of electron density and velocity calculated by NS-DSMC method

magnitudes, mainly due to calculations performed under two different pressures. This does not affect the conclusion. Although (a) and (c) have diferent pressures and velocities, we are comparing the performance of the equal-diameter type and expansion type under the same conditions, i.e., (a) or (c). It needs to be explained here that the reason why the pressure is not adjusted to make the fow rate level consistent is because the pressure environment used is the continuum pressure and transition fow pressure that will appear in actual production.

First, the difference between transition flow and slip flow can be analyzed by examining the pressure in the microchannel. As shown in Fig. [10](#page-8-0), the pressure evolution was smoother for the transition regime in the microchannel. The pressure in the slip fow regime signifcantly decreased at the outlet. This means that the fuid consumed more energy to expand in the outlet, resulting in the formation of a highvelocity jet of the equal-diameter type. In addition, the area around the outlet would form vortices to stabilize the jet, which resulted in the equal-diameter type producing a stronger jet than the expansion type in the slip flow regime.

The difference in jet behavior between slip flow and transition flow for equal-diameter types is analyzed above. After that, the diference between the equal-diameter type and expansion type in the transition regime is shown in Fig. [11.](#page-8-1) The fgure illustrates the velocity distribution in the horizontal direction. The equal-diameter type has a high horizontal velocity, indicating that the fow energy is expended in the horizontal direction. The fuid expanded diferently for the expansion type and equal-diameter type microchannels. For the expansion type, the fuid would expand within the conical cavity. The direction of fuid energy difusion was primarily focused on the vertical direction due to the constraints imposed by the walls. By comparison, the difusion **Fig. ⁶**Comparison of NS-DSMC and DSMC result curves of micro-

Fig. 8 Schematic diagram of simulation structure

direction for the equal-diameter type would be in all directions from the outlet.

To eliminate the diferences caused by the fow rates of the two types of microchannels, we also analyzed the efect of fow resistance. The velocity of the equal-diameter type is used as the base. By decreasing the diameter of the expansion type, the fow resistance was increased. The 100% increase in fow resistance shown in Fig. [12](#page-8-2) indicates that the expansion type got the same flow resistance as the equaldiameter type. It shows that the expansion type got a higher flow velocity, even when the flow resistance increased to 1.7 times that of the equal-diameter type.

Last but not least, it is important to ensure that the composite structure exhibits the same characteristics as the microchannel in diferent fow regimes. The microchannel composite structure is shown in Fig. [13.](#page-9-2) The flow in the chamber was simulated in both slip fow and transition fow regimes using the same structure. In the center of the chamber, the velocity in the slip fow regime was higher than that in the transition regime, and the velocity was higher in the transition fow regime at the edge of the chamber. This

phenomenon was observed in the slip flow regime, where the equal-diameter type exhibited a stronger jet compared to the expansion type. However, this situation would reverse in the transition regime. The result is consistent with the fow characteristics of the single microchannel.

From the above, it can be seen that in PECVD production, when attempting to control the deposition distribution of the flm using various types of microchannel combinations, it is essential to have a thorough understanding of the fuid regime. Under various flow regimes, the flow velocity varied signifcantly among diferent microchannels. The expected flm thickness distribution can only be obtained through the correct microchannel distribution. Otherwise, a signifcantly diferent distribution might result.

The expansion type microchannel exhibited a signifcantly higher velocity than the equal-diameter types in the transition regime. The expansion type should be placed in the center of the PECVD chamber, while the equal-diameter type should be placed at the edge. In this way, the velocity diference between the central area and the edge can

Fig. 9 Microchannel jet velocity contours and curves, **a** slip fow region contours, **b** slip flow region axial velocity curves, **c** transition fow region contour and curves

 $\left(\mathbf{c}\right)$

Fig. 10 Pressure distributions of slip fow and transition fow in equal-diameter type microchannels

be reduced, thereby improving the uniformity of the flm thickness.

5 Conclusion

In this paper, the NS-DSMC method, which is commonly used for return capsule and micro-thruster plume analysis in near-Earth space, is applied to calculate the fow feld in PECVD. Different from other PECVD flow field calculations that use continuum flow methods, the NS-DSMC method can accurately obtain the gas fow characteristics in the transition regime or molecular state within the microchannel on

Fig. 12 Comparison of the velocity distribution of the expansion type and the equal-diameter type under diferent fow resistances

the showerhead, as well as its jet characteristics. This is of great signifcance for PECVD processes that are sensitive to flow field effects.

We also adopted a two-way coupling approach in our study. Diferent from the conventional one-way coupling method, the data in the two-way coupling method will be transmitted bidirectionally between the NS and DSMC modules. This allows for simultaneous updates of the two calculation domains, resulting in improved calculation efficiency. The NS-DSMC coupling method matches the results of the DSMC method and is consistent with the experimental fndings.

Fig. 11 Horizontal distribution of jet velocity

Fig. 13 Velocity distribution curves in slip fow and transition fow regimes with the same microchannel distribution at 1 mm above the wafer

By comparing the microchannel jet data under diferent fow regimes, we found that the fuid regime infuences the pressure distribution in the microchannel, which in turn afects the jet characteristics of the microchannel. The equaldiameter type exhibits a higher jet velocity in the continuum regime. In the transition regime, the expansion type microchannel has a higher velocity. Therefore, the design of the showerhead microchannel needs to be compatible with the process environment. Diferent fuid regimes can result in variations in velocity distribution and cause changes in the thickness of the deposited flm.

In addition, when using a combination of various microchannels, it is recommended to place the type with higher velocity in the central area and the type with lower velocity on the edge. This arrangement helps to minimize the difference in flow velocity between the center and the edge, resulting in improved deposition uniformity. Diferent from other methods of altering the length of the microchannel, the fow rate can be adjusted by enlarging the size of the outlet. This could potentially be a new approach for improving showerhead functionality.

The NS-DSMC method used in this paper is not a stateof-the-art adaptive boundary method. The adaptive boundary method can automatically determine the coupling position based on the distribution of the fow feld, instead of using a pre-specifed position as adopted in this paper. In this paper, the method of pre-specifed coupling position serves two purposes. One purpose is to facilitate the establishment of two-way coupling, while the other purpose is to serve as the foundation for establishing a unifed coupling method in the future. Using the two-way coupling and unifed coupling methods can greatly improve the calculation efficiency of the showerhead fow feld.

Author contributions Wansuo Liu (First Author): Conceptualization, Data Curation, Formal Analysis, Investigation, Resources, Methodology, Software, Validation, Writing - Original Draft; Xiangji Yue: Methodology, Project Administration, Software, Validation; Zeng Lin (Corresponding Author): Conceptualization, Funding Acquisition, Resources, Supervision, Writing - Review & Editing.

Funding This work was supported by National Natural Science Foundation of China [grant numbers 51775096]; Chinese Academy of Sciences WEGO Research Development Plan [grant numbers [2007]006]; and Fundamental Research Funds for the Central Universities, China [grant numbers N2003009].

Data availability The authors confrm that the data supporting the fndings of this study are available within the article. Raw data that support the fndings of this study are available from the corresponding author, upon reasonable request.

Declarations

Conflict of interest The authors declare no competing interests.

References

- Aktas O, Aluru NR (2002) A combined continuum/DSMC technique for multiscale analysis of microfuidic flters. J Comput Phys 178(2):342–372. <https://doi.org/10.1006/jcph.2002.7030>
- Aktas O, Aluru NR, Ravaioli U (2001) Application of a parallel DSMC technique to predict fow characteristics in microfuidic flters. J

Microelectromech Syst 10(4):538–549. [https://doi.org/10.1109/](https://doi.org/10.1109/84.967377) [84.967377](https://doi.org/10.1109/84.967377)

- Arkilic EB, Schmidt MA, Bruer KS (1997a) Measurements of the TMAC in silicon microchannels. Rarefed gas dynamics. Peking University Press, p 983
- Arkilic EB, Schmidt MA, Breuer KS (1997b) Gaseous slip flow in long microchannels. J Microelectromech Syst 6(2):167–178. [https://](https://doi.org/10.1109/84.585795) doi.org/10.1109/84.585795
- Beskok A, Karniadakis GE, Trimmer W (1996) Rarefaction and compressibility effects in gas microflows. Fluids Eng 118(3):448-456. <https://doi.org/10.1115/1.2817779>
- Bird GA (1976) Molecular gas dynamics. NASA STI/Recon Tech Rep A 76:40225
- Cai G, Liu L, He B et al (2022) A review of research on the vacuum plume. Aerospace 9(11):706. [https://doi.org/10.3390/aerospace9](https://doi.org/10.3390/aerospace9110706) [110706](https://doi.org/10.3390/aerospace9110706)
- Eggers J, Beylich AE (1994) New algorithms for application in the direct simulation Monte Carlo method. Rarefed Gas Dyn Theory Simul 19:166–173
- Fan J, Shen C (2001) Statistical simulation of low-speed rarefed gas fows. J Comput Phys 167(2):393–412. [https://doi.org/10.1006/](https://doi.org/10.1006/jcph.2000.6681) [jcph.2000.6681](https://doi.org/10.1006/jcph.2000.6681)
- Farber K, Farber P, Gräbel J et al (2016) Development and validation of a coupled Navier–Stokes/DSMC simulation for rarefed gas flow in the production process for OLEDs. Appl Math Comput 272:648–656. <https://doi.org/10.1016/j.amc.2015.05.040>
- Gad-el-Hak M (1999) The fuid mechanics of microdevices—the Freeman scholar lecture. J Fluids Eng 121(1):5–33. [https://doi.org/10.](https://doi.org/10.1115/1.2822013) [1115/1.2822013](https://doi.org/10.1115/1.2822013)
- Gao R, O'Byrne S, Liow JL et al (2018) An experimental study of pressure distribution nonlinearity in a circular micro-tube. Exp Thermal Fluid Sci 97:468–483. [https://doi.org/10.1016/j.expth](https://doi.org/10.1016/j.expthermflusci.2018.05.020) [ermfusci.2018.05.020](https://doi.org/10.1016/j.expthermflusci.2018.05.020)
- Ghazanfari V, Shademan MM, Mansourzadeh F (2022) Investigation of feed flow effect using CFD-DSMC method in a gas centrifuge. J Nucl Res Appl 2(4):7–14.<https://doi.org/10.24200/jon.2022.1027>
- Huang CY, Lai CM (2012) Pressure measurements with moleculebased pressure sensors in straight and constricted PDMS microchannels. J Micromech Microeng 22(6):065021. [https://doi.org/](https://doi.org/10.1088/0960-1317/22/6/065021) [10.1088/0960-1317/22/6/065021](https://doi.org/10.1088/0960-1317/22/6/065021)
- Jang J, Wereley ST (2004) Pressure distributions of gaseous slip fow in straight and uniform rectangular microchannels. Microfuid Nanofuid 1(1):41–51. <https://doi.org/10.1007/s10404-004-0005-8>
- John B, Damodaran M (2009) Hybrid continuum–direct simulation Monte Carlo and particle-laden fow modeling in the head-disk interface gap. IEEE Trans Magn 45(11):4929–4932. [https://doi.](https://doi.org/10.1109/TMAG.2009.2029390) [org/10.1109/TMAG.2009.2029390](https://doi.org/10.1109/TMAG.2009.2029390)
- Kim HJ, Lee HJ (2017) Efects of the wall boundary conditions of a showerhead plasma reactor on the uniformity control of RF plasma deposition. J Appl Phys 122(5):053301. [https://doi.org/](https://doi.org/10.1063/1.4996998) [10.1063/1.4996998](https://doi.org/10.1063/1.4996998)
- Ko HS, Gau C (2011) Local heat transfer process and pressure drop in a micro-channel integrated with arrays of temperature and pressure sensors. Microfluid Nanofluid 10(3):563-577. [https://doi.org/10.](https://doi.org/10.1007/s10404-010-0690-4) [1007/s10404-010-0690-4](https://doi.org/10.1007/s10404-010-0690-4)
- Lee G, Sohn DK, Seok SH et al (2019) The efect of hole density variation in the PECVD reactor showerhead on the deposition of amorphous carbon layer. Vacuum 163:37–44. [https://doi.org/10.](https://doi.org/10.1016/j.vacuum.2019.02.009) [1016/j.vacuum.2019.02.009](https://doi.org/10.1016/j.vacuum.2019.02.009)
- Moss JN, Price JM (1997) Survey of blunt body fows including wakes at hypersonic low-density conditions. J Thermophys Heat Transfer 11(3):321–329.<https://doi.org/10.2514/2.6252>
- Palharini RC, White C, Scanlon TJ et al (2015) Benchmark numerical simulations of rarefied non-reacting gas flows using an

open-source DSMC code. Comput Fluids 120:140–157. [https://](https://doi.org/10.1016/j.compfluid.2015.07.021) doi.org/10.1016/j.compfluid.2015.07.021

- Pong KC, Ho CM, Liu J et al (1994) Non-linear pressure distribution in uniform microchannels. ASME-Publications-FED 197:51–51
- Rafi KMM, Deepu M, Rajesh G (2019) Effect of heat transfer and geometry on micro-thruster performance. Int J Therm Sci 146:106063.<https://doi.org/10.1016/j.ijthermalsci.2019.106063>
- Roveda R, Goldstein DB, Varghese PL (1998) Hybrid Euler/particle approach for continuum/rarefied flows. J Spacecr Rocket 35(3):258–265.<https://doi.org/10.2514/2.3349>
- Roveda R, Goldstein DB, Varghese PL (2000) Hybrid Euler/direct simulation Monte Carlo calculation of unsteady slit fow. J Spacecr Rocket 37(6):753–760.<https://doi.org/10.2514/2.3647>
- Scanlon TJ, Roohi E, White C et al (2010) An open source, parallel DSMC code for rarefed gas fows in arbitrary geometries. Comput Fluids 39(10):2078–2089. [https://doi.org/10.1016/j.compfluid.](https://doi.org/10.1016/j.compfluid.2010.07.014) [2010.07.014](https://doi.org/10.1016/j.compfluid.2010.07.014)
- Schwartzentruber TE, Boyd ID (2006) A hybrid particle-continuum method applied to shock waves. J Comput Phys 215(2):402–416. <https://doi.org/10.1016/j.jcp.2005.10.023>
- Sun Q, Boyd ID (2005) Evaluation of macroscopic properties in the direct simulation Monte Carlo method. J Thermophys Heat Transfer 19(3):329–335. <https://doi.org/10.2514/1.12542>
- Virgile C, Albert A, Julien L (2022) Optimisation of a hybrid NS– DSMC methodology for continuous–rarefied jet flows. Acta Astronaut 195:295–308. [https://doi.org/10.1016/j.actaastro.2022.](https://doi.org/10.1016/j.actaastro.2022.03.012) [03.012](https://doi.org/10.1016/j.actaastro.2022.03.012)
- Wagner W (1992) A convergence proof for Bird's direct simulation Monte Carlo method for the Boltzmann equation. J Stat Phys 66:1011–1044.<https://doi.org/10.1007/BF01055714>
- Weng CI, Li WL, Hwang CC (1999) Gaseous flow in microtubes at arbitrary Knudsen numbers. Nanotechnology 10(4):373. [https://](https://doi.org/10.1088/0957-4484/10/4/302) doi.org/10.1088/0957-4484/10/4/302
- Wi SS, Kim YG, Lee HJ et al (2012) Effects of showerhead hole structure on the deposition of hydrogenated microcrystalline silicon thin flms by vhf PECVD. J Vac Sci Technol A 30(4):04D113. <https://doi.org/10.1116/1.4721287>
- Xiang D, Xia H, Yang W et al (2019) Parametric study and residual gas analysis of large-area silicon-nitride thin-flm deposition by plasma-enhanced chemical vapor deposition. Vacuum 165:172– 178.<https://doi.org/10.1016/j.vacuum.2019.04.017>
- Yambe K, Taka S, Ogura K (2014) Relation between plasma plume density and gas fow velocity in atmospheric pressure plasma. Phys Plasmas 21(4):043511. <https://doi.org/10.1063/1.4873384>
- Yuan Z, Zhao W, Jiang Z et al (2020) Modifed nonlinear coupled constitutive relations model for hypersonic nonequilibrium fows. J Thermophys Heat Transfer 34(4):848–859. [https://doi.org/10.](https://doi.org/10.2514/1.T5761) [2514/1.T5761](https://doi.org/10.2514/1.T5761)
- Zohar Y, Lee SYK, Lee WY et al (2002) Subsonic gas flow in a straight and uniform microchannel. J Fluid Mech 472:125–151. [https://doi.](https://doi.org/10.1017/S0022112002002203) [org/10.1017/S0022112002002203](https://doi.org/10.1017/S0022112002002203)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional afliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.