Journal of Aerosol Science 44 (2012) 1–10

Contents lists available at SciVerse ScienceDirect

Journal of Aerosol Science

journal homepage: www.elsevier.com/locate/jaerosci

Statistical Lagrangian particle tracking approach to investigate the effect of thermophoresis on particle deposition onto a face-up flat surface in a parallel airflow

Sang-Hee Woo, Sang-Chul Lee, Se-Jin Yook*

School of Mechanical Engineering, Hanyang University, Seoul 133-791, Republic of Korea

ARTICLE INFO

Article history:
Received 8 May 2011
Received in revised form
16 September 2011
Accepted 8 October 2011
Available online 15 October 2011

Keywords:
Thermophoresis
Deposition velocity
Wafer
Photomask
Parallel flow

ABSTRACT

Thermophoresis can affect the particulate contamination of wafers and photomasks. Thermophoretic effect on particle deposition velocity in the cleanroom environment has been intensively investigated for the free-standing wafer situated perpendicular to the top-down airflow, but it has been examined by few studies for the wafers or photomasks in the parallel airflow. In this study, the particle deposition velocity onto a face-up flat surface under the influence of thermophoresis was numerically investigated, when the face-up flat surface was exposed to the parallel airflow. Statistical Lagrangian Particle Tracking (SLPT) model with the aid of commercial codes, i.e. FLUENT and DPM, was employed. The SLPT model was validated by comparing the numerically obtained particle deposition velocities with the theoretically predicted data, with and without considering the thermophoresis, and found to produce correct results. The effects of temperature difference (between the face-up flat surface and the ambient air), parallel airflow velocity, and particle density on the particle deposition velocity onto the face-up flat surface in the parallel airflow were investigated using the SLPT model, when the temperature of the face-up flat surface was either higher or lower than the ambient temperature.

1. Introduction

Particulate contamination is one of the main factors affecting the product yield in semiconductor manufacturing. The feature size is anticipated to decrease to 27 nm by 2014, according to the International Technology Roadmap for Semiconductors (ITRS 2010). If the 1/2 rule is applied, particles larger than the half of the critical dimension (CD) are thought of as contaminants. With decreasing CD, therefore, the lower limit of particle size for contamination control is getting smaller. It is expected that the product yield will deteriorate due to the increase of die size with the use of 450-mm-wafers. Moreover, photomasks used for the Extreme Ultraviolet Lithography (EUVL) are vulnerable to contamination by particles due to the impossibility of the use of pellicles (Asbach et al., 2006; Yook et al., 2007a). As a result, the control of particulate contamination in semiconductor manufacturing is of great importance.

Particle deposition velocity can be used to assess the degree of particulate contamination. A lot of studies have been conducted to investigate the particle deposition velocity onto a free-standing wafer situated perpendicular to

---

* Corresponding author. Tel.: +82 2 2220 0422; fax: +82 2 2220 2299.
E-mail address: ysjnuri@hanyang.ac.kr (S.-J. Yook).

0021-8502/$ - see front matter © 2011 Elsevier Ltd. All rights reserved.
doi:10.1016/j.jaerosci.2011.10.003

a unidirectional airflow coming down from the cleanroom ceiling. Brownian diffusion and gravitation settling were considered as the main mechanisms for particle deposition (Liu & Ahn, 1987; Otani et al., 1989; Pui et al., 1990; Bae et al., 1994). In addition to these two particle deposition mechanisms, the effect of thermophoresis and/or electrophoresis on the particle deposition velocity was examined (Peterson et al., 1989; Ye et al., 1991; Opiolka et al., 1994; Bae et al., 1995; Tsai et al., 1998; Yoo & Oh, 2005; Yook et al., 2007b). In these studies, however, the airflows were assumed to be perpendicular to the face-up surfaces of the free-standing wafers.

Not only the wafers but also the photomasks can be exposed to a parallel airflow, when they are transported by robot arms. Liu & Ahn (1987) suggested an equation for calculating the particle deposition velocity onto a face-up wafer surface in a parallel flow. Yook & Ahn (2009) developed the Gaussian Diffusion Sphere Model (GDSM) for predicting the diffusional particle deposition on a flat surface in a parallel flow. Yook et al. (2010a) suggested correlations for estimating the mean mass transfer coefficient onto a flat surface of various areal shapes like square, rectangle, circle, ellipse, or rhombus in a parallel flow. In addition to Brownian diffusion, the effect of gravity on the particle deposition velocity onto a wafer or a photomask in a parallel flow was taken into account, assuming a face-down or a face-up critical surface (Choi & Yook, 2010; Yook et al., 2010b; Lee & Yook, 2011; Lee et al., 2011). The effect of thermophoresis or electrophoresis on the protection of EUVL photomasks against a horizontal aerosol flow was investigated (Engelke et al., 2007; Yook et al., 2007c). In the studies of Engelke et al. (2007) and Yook et al. (2007c), however, the flow pattern was quite different from that of the uniform parallel flow due to the injection of aerosol particles from a circular tube into the quiescent air, and the particle deposition velocity was not obtained. In other words, few studies have reported the particle deposition velocity onto the flat surface situated parallel to the airflow under the influence of thermophoresis or electrophoresis.

The objective of this study, therefore, is to investigate the particle deposition velocity onto the face-up flat surface in the parallel flow, when thermophoresis either enhances or suppresses the particle deposition on the face-up critical surface. A numerical model based on the Lagrangian particle tracking simulation is employed to calculate the particle deposition velocity. The simulated particle deposition velocities, first, are compared with the predicted values by the theory of Liu & Ahn (1987) and the GDSM of Yook et al. (2010b), assuming the face-up flat surface in the parallel flow, in order to validate the accuracy of the present model in terms of Brownian diffusion, gravitational settling, and inertia. Second, the present model is verified in terms of thermophoresis in addition to diffusion, settling, and inertia, by comparing the simulated particle deposition velocities onto the heated face-up wafer situated perpendicular to the top-down airflow, with the experimental data of Ye et al. (1991) and the particle deposition velocities predicted by the theory of Bae et al. (1995). Then, the effect of thermophoresis on the particle deposition velocity onto the face-up flat surface exposed to the parallel flow is numerically investigated.

2. Numerical

2.1. Simulation of airflow

The FLUENT, a commercially available Computational Fluid Dynamics (CFD) software, was employed to simulate the airflow around a flat surface. Fig. 1a shows a two-dimensional calculation domain for obtaining the flow field around a flat plate situated parallel to the airflow. The size of the calculation domain was 1452.4 mm $\times$ 1004.05 mm. The plate length was $L_p = 152.4$ mm, which was equal to the size of the EUVL photomask. The plate thickness was 0.05 mm, in order for the effect of the plate thickness on the particle deposition velocity to be negligible. A uniform airflow with the velocity of U_{in} was established in the direction parallel to the plate surface. Fig. 1b illustrates a two-dimensional axisymmetric calculation domain for simulating the flow field around a horizontal wafer situated perpendicular to the top-down airflow. The size of the simulation domain was 1075 mm $\times$ 1701 mm. The radius of the wafer was $R_w = D_w/2 = 75$ mm. The wafer thickness was assumed to be 1 mm. The top-down airflow with the velocity of U_{in} was assumed in the direction normal to the wafer surface.

Rectangular grids were used to establish the computational mesh. The grids in the near-wall region were very fine in order to simulate the boundary layer flow accurately. After the grid test was performed, the number of grids for the calculation domain shown in Fig. 1a was determined to be about 285,000 with the smallest grid size of 5 μm and that for the simulation domain illustrated in Fig. 1b was approximately 568,000 with the smallest grid size of 50 μm. Continuity, momentum, and energy equations were solved. The ambient temperature and pressure were set to be $T_a = 20\,^{\circ}$C and $P_a = 1$ atm, respectively. The temperature of the plate or the wafer, i.e. T_p or T_w, was varied to investigate the effect of thermophoresis on the particle deposition velocity. The flow was assumed to be steady, incompressible, and laminar. The boundary conditions were imposed as inscribed in Fig. 1. No-slip condition on either the flat plate or the wafer surface was assumed. The SIMPLE algorithm was used to couple the velocity and pressure. The direction of gravity was set to be downward. The gravitational acceleration was $g = 9.81$ m/s^2. The criterion for convergence was 10^{-6} for the continuity, momentum, and energy equations.

2.2. Calculation of particle deposition velocity

Statistical Lagrangian Particle Tracking (SLPT) model, developed by Yook et al. (2007a), was employed and adjusted to calculate the particle deposition velocity. Particle motion was analyzed using the Discrete Phase Models (DPM), incorporated in the FLUENT. The DPM was based on the Lagrangian approach. The effects of Brownian diffusion, Stokes