20PA-041

Numerical Simulation on Spatiotemporal Behavior of Charged-Species in Tetrametylsilane Plasmas for Diamond-Like Carbon Coating

DLC成膜用テトラメチルシランプラズマの時間空間構造に関する計算機シミュレーション

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A self-consistent one-dimensional fluid model of tetrametylsilane ($Si(CH_3)_4$, TMS) RF capacitively-coupled plasmas (TMS RF-CCPs) for silicon-containing diamond-like carbon (Si-DLC) has been developed, in order to clarify the fundamental properties in TMS RF-CCPs. The fluid model is composed of the continuity equations for electron and sixteen TMS-derived ion species, the Poisson equation, and the electron energy balance equation. Spatiotemporal variations of charged species density, electron temperature in TMS RF-CCPs were analyzed.

1. Introduction

Diamond-like carbon (DLC) films are the hydrogenated amorphous carbon films, which is composed of a mixture of sp2- and sp3-bonded carbon. Since this films have excellent material properties in high wear resistance, high hardness, low friction, and chemical stability, the films have been widely used for many technological applications, such as automotive, semiconductors, medical devices, and so on [1-3]. Recently, silicon-containing DLC (Si-DLC) films have been investigated, since the friction coefficient of the Si-DLC films is lower than that of DLC films [4]. However, the effect of silicon in Si-DLC films on the plasma and friction properties has not been clearly understood. Therefore, the understanding of fundamental properties in tetrametylsilane ($Si(CH_3)_4$) plasmas, which are ion and radical source of Si-DLC film deposition, is strongly necessitated.

In this paper, the fundamental properties in radio-frequency capacitively-coupled tetrametyl-silane plasmas (TMS RF-CCPs) have been simulated using a one-dimensional (i.e. radially uniform) fluid model. Spatiotemporal variations of charged species density, electron temperature in TMS RF-CCPs, and gas-pressure dependence of fundamental plasma properties were analyzed.

2. Modeling of TMS RF-CCPs

Fig. 1 shows a schematic diagram, considered in this work, of TMS RF-CCPs. The TMS gas with a total pressure of 0.2-2.0 Torr and a gas temperature of 300 K is filled between two parallel-plate metallic electrodes. The TMS RF-CCPs are sustained by applying AC voltage with a driving frequency of 13.56 MHz. The discharge gap length and area of the electrodes are set to be 3.0 cm and 1.0 cm, respectively. The present simulation model is a one-dimensional fluid model on the assumption of quasi-thermal equilibrium. Governing equations

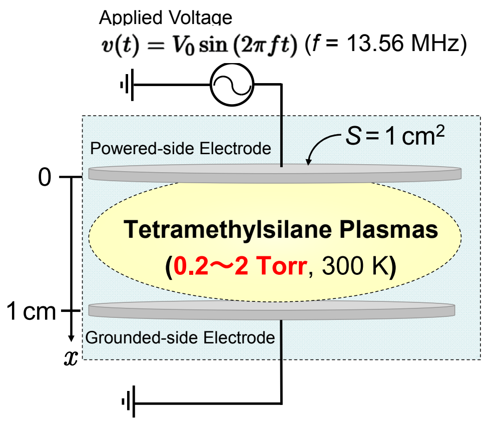

Fig.1: A schematic diagram of the electrode configuration in TMS RF-CCPs.

are composed of the mass balance equations for charged species (electrons and sixteen kinds of ions), the electron energy balance equation, coupled with the Poisson's equation. The particle-species are considered as electrons and sixteen positive ions (e^-, CH_3^+, Si^+, HSi^+, H_3Si^+, $SiCH_2^+$, $SiCH_3^+$, $HSiCH_3^+$, $H_2SiCH_3^+$, SiC_2H^+, $SiC_2H_3^+$, $SiC_2H_5^+$, $Si(CH_3)_2^+$, $HSi(CH_3)_2^+$, $Si(CH_3)_3^+$, $Si(CH_3)_4^+$) and source gas (TMS) in the present model. The spatio-temporal evolutions of the concentration of the charged particles, the electric field strength and mean electron energy (or the electron temperature) can be obtained by solving the above equations until reaching periodic steady-state. The electron transport coefficients, such as diffusion coefficient, drift velocity, and collision rate coefficient, have been calculated using Monte Carlo simulation of electron swarms in TMS gas [5]. As an example, the electron collision rate coefficients in TMS gas as a function of electron temperature are shown in Fig. 2.

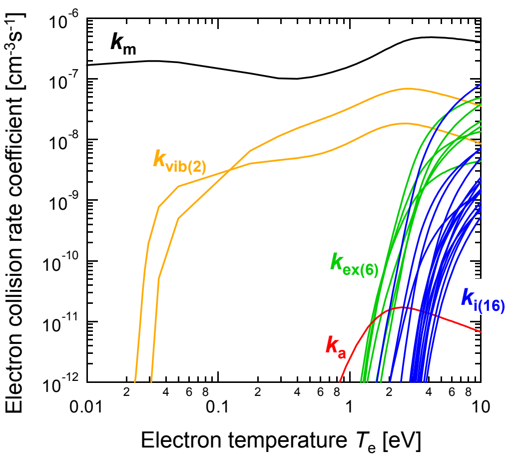

Fig. 2: Electron collision rate coefficients in TMS gas as a function of electron temperature.

3. Results and Discussion

Fig. 3 shows the simulated spatial profiles of (a) the electron and respective ion densities, and (b) the electron temperature and electric field strength in TMS RF-CCPs. In this figure, it is founded that dominant ion species in TMS RF-CCPs are $Si(CH_3)_3^+$, $HSi(CH_3)_3^+$, $Si(CH_3)_4^+$ ions, as shown in Fig. 2(a). In contrast, the other ion species are negligibly low, compared with dominant ion species. In Fig. 2(b), the plasma density and electron temperature in bulk region are about 10^9 cm^{-3} and 0.8 eV, respectively. The electric field strength (2.5 kV/cm) in the vicinity of both electrodes are highly distorted. The other results will be presented at the conference.

Acknowledgments

This work was partly supported by KAKENHI (No.26420247), and a "Grant for Advanced Industrial Technology Development (No. 11B06004d)" in 2011 from the New Energy and Industrial Technology Development Organization (NEDO) of Japan.

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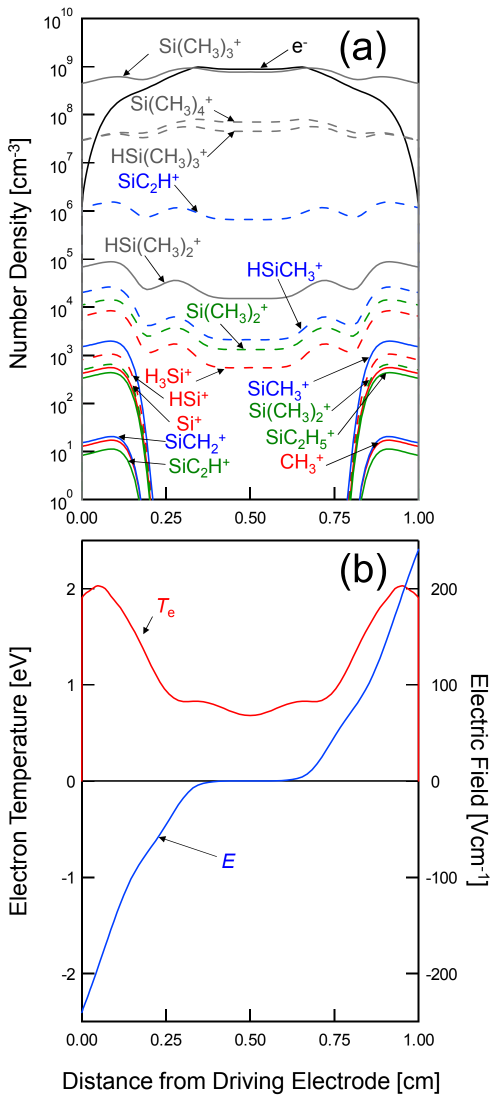

Fig. 3: Spatial profiles of (a) the electron and ion densities, and (b) the electron temperature and electric field strength in TMS RF-CCPs.