Modelling graphene sheet growth subjected to plasma containing negatively charged ions

N. Gupta[1], S. C. Sharma[1], and R. Gupta[1]

[1]*Department of Applied Physics, Delhi Technological University (DTU), Shahbad Daulatpur, Bawana Road, Delhi-110042*

Abstract

The paper presents a theoretical model to investigate the effects of negatively charged ions in the reactive plasma on the graphene sheet growth. The present model considers the graphene sheet growth subjected to reactive plasma containing electrons, positively as well as negatively charged ions, and neutrals. The key equations accounted in the present model are charging rate of the graphene sheet, kinetics of all plasma species, the growth rate equation of the graphene sheet. Numerical calculations have been carried out for typical glow discharge plasma parameters and it is found that graphene sheet area decreases with increase in the relative number densities of negatively charged ions in the plasma.

I. Introduction

The plasma species, particularly negatively charged ions in the plasma play a significant role on the growth of the nanostructures in the plasma enhanced chemical vapour deposition. Choi and Kushner [1] have illustrated that negatively charged ions are trapped in the electropositive plasmas and therefore have a long residence time resulting in the growth of critically large clusters. Ostrikov *et al.* [2] have shown that the negative ions in plasma affect the charging and trapping of particulates through the modification of sheath/presheath structure despite of negligible negative ion currents collected by the particles. Levko *et al.* [3] have studied the influence of electronegative gas SF_6 on the plasma stability.

II. Model

In order to investigate the role of negative ions in plasma on the growth of graphene sheet, we consider the embryonic growth of graphene sheet in a plasma consisting of electrons, positively charged ions of carbon source gas i.e., methane (denoted as type A) and neon (denoted as type B), negatively charged ions $\left(SF_6^-\right)$ and neutrals of type A and B. In addition, we assume the positively charged ions to be singly ionised.

A. Charging of the graphene sheet

$$\frac{dq}{d\tau} = j_{iAg} + j_{iBg} - \gamma_e j_{eg}, \tag{1}$$

where q is the charge on the graphene sheet, j_{ikg} is the ion collection current (where *k* refers to A or B type of ion), and j_{eg} is the electron collection current. Equation (1) represents the charged developed on the graphene sheet on account of accretion of ions and electrons on the graphene sheet surface (γ_e is the sticking coefficient of electrons).

B. Kinetic equations of the plasma species

$$\frac{dn_{ik}}{dt} = \lambda_k n_k - \alpha_k n_e n_{ik} - n_g j_{ikg}, \tag{2}$$

$$\frac{dn_k}{dt} = \alpha_k n_e n_{ik} - \lambda_k n_k - n_g \left(1 - \gamma_{ik}\right) j_{ikg} - n_g \gamma_k j_{kg}, \tag{3}$$

$$\frac{dn_{i-}}{d\tau} = \beta_r \frac{dn_s}{d\tau} = \sum_k^{A,B} \lambda_k n_k - \sum_k^{A,B} \alpha_k n_e n_{ik} - \gamma_e n_g j_{eg}, \tag{4}$$

$$\frac{dn_e}{d\tau} = (1 - \beta_r) \frac{dn_s}{d\tau} = \sum_k^{A,B} \lambda_k n_k - \sum_k^{A,B} \alpha_k n_e n_{ik} - \gamma_e n_g j_{eg}, \tag{5}$$

where n_{ik}, n_k, n_{i-}, and n_e are the number densities of ions (of type *k*), neutrals (of type *k*), negatively charged ions and electrons, respectively. $\beta_r = \frac{n_{SF_6^=}}{n_{C^+}}$, is the relative density of negatively charged ions.

Equation (2) represents the growth rate of ions (here, k refers to A or B type of ion) in plasma due to ionisation of neutrals (λ_k is the coefficient of ionization), recombination of electrons and ions (α_k is the coefficient of recombination), and ion collection current at the graphene sheet surface. Equation (3) represents the growth rate of neutrals of type k in plasma on account of recombination of electrons and ions, neutralisation of atoms collected at the graphene sheet surface, account of electron-ion recombination, and neutral collection current (j_{kg}) [4].

Equations (4) and (5) represents the growth rate of negatively charged ions and electrons in plasma, respectively on account of ionization of neutral atoms, electron –ion recombination and electron collection current at the surface of graphene sheet.

C. Growth rate equation of the mass of the graphene sheet

$$\frac{dm_g}{d\tau} = m_A \gamma_A j_{Ag} + m_{iA} \gamma_{iA} j_{iAg}, \tag{6}$$

where $m_g (= \rho_g (l_g \times A_g)), \rho_g$, and A_g are the mass, density and area of the graphene sheet, respectively. Equation (6) represents the increase in mass of the graphene sheet due to accretion of neutrals and ions of type A.

III. Results and Discussion

We have solved Equations (1)-(6) simultaneously for the typical glow discharge parameters with appropriate boundary conditions i.e., $n_{e0} = (1-\beta_r) n_{s0}$, $n_{s0} = 10^{10} cm^{-3}$, $n_{iA0} = n_{iB0} = n_{s0}$, $n_{i-0} = \beta_r n_{s0}$, $n_{A0} = n_{B0} = n_{s0}$, $T_{e0} = T_{-0} = 0.8eV$, $T_{i0} = 2200K$, $T_{n0} = 2000K$, and $\gamma_e = \gamma_{ik} = \gamma_k = 1$. The other parameters of the text are $m_{iA} \approx m_A$ =12 amu (Carbon), $m_{iB} \approx m_B$ =20 amu (Neon), m_{i-}= 146 amu (sulphur hexafluoride), $\alpha_{A0} \approx \alpha_{B0}$ =10^{-7} cm^3/sec.

Figure 1 shows the time variation of the area (A_g) of the graphene sheet for different relative number densities of negatively charged ions (β_r =0.1, 0.2, 0.3, 0.4). It can be seen from Figure 1 that the area of the graphene sheet decreases with increase of the relative number densities of negatively charged ions in the plasma. This is because the neutral atoms available for accretion on the graphene sheet surface decreases as the relative number densities of negatively charged ions increases (cf. Figure 2). Figure 2 shows the time variation of the number density of neutral atoms of type A for different relative number densities of negatively charged ions (β_r =0.1, 0.2, 0.3, 0.4). It can be seen from Figure 2 that on increasing the relative negatively charged ion density, the neutral atom density of type A atoms decays faster. This is because, on increasing the negatively charged ion density in plasma, for a fixed value of positive ion density, more and more neutral atoms ionises to produce ions and electrons. Thus, the neutral atoms available for accretion decreases and as a result the area of the graphene sheet decreases.

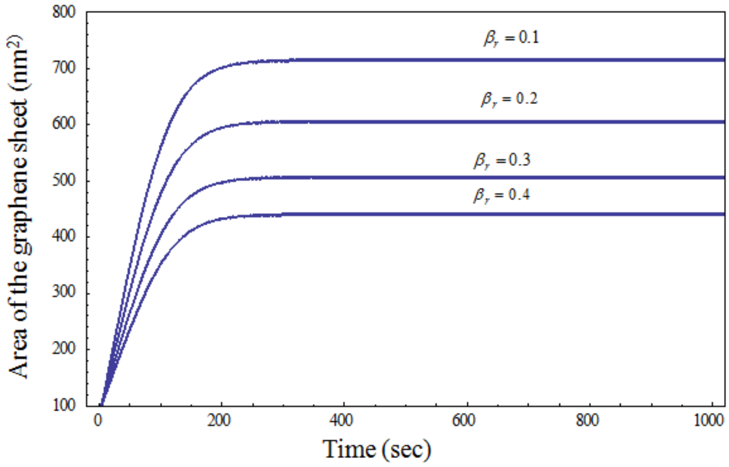

Figure1. Time variation of the area of the graphene sheet for different relative number densities of negatively charged ions (β_r =0.1, 0.2, 0.3, 0.4).

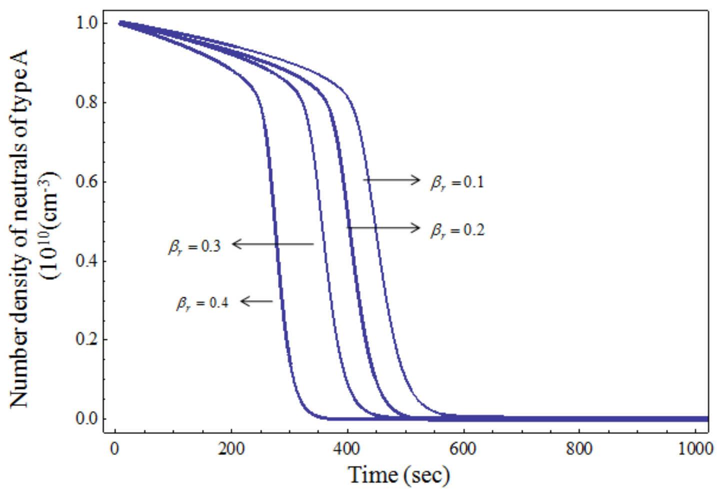

Figure2. Time variation of the number density of neutrals of type A for different relative number densities of negatively charged ions (β_r =0.1, 0.2, 0.3, 0.4).

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