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Particle-in-cell Modelling of a Neutral Beam Source for Material Processing in Nanoscale Structures Fabrication

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Abstract. Neutral beam processing has evolved into one of the most promising methods for overcoming plasma process induced damage. Surface treatment by neutrals avoids problems with surface charging effects, frequently encountered when using common ion treatment, especially for low k-materials. In this paper, the influence of various parameters on the neutralization of ion beams in Ar-CF_4 mixture based on a Particle in Cell with Monte Carlo collisions (PIC/MCC) simulation is studied. The efficiency of neutralization has been treated by considering both surface neutralization of ions and collisions of ions in the gas.

Introduction

Plasma etching is an essential technology for the manufacture of integrated circuits, treatment of materials (such as implantation) and especially for achieving massively parallel production of well organized and designed nanostructures [1,2]. Plasma etching requires high etching rate, anisotropy, uniformity across the wafer and process reproducibility. Therefore, plasma etching processes that use charged particles can cause plasma induced damage (PID), especially as the size of the structures and the aspect ratio (depth to width ratio) decrease. In the nanoscale range, plasma induced damage may result in unacceptably high defect rates [3,4], so replacement of some plasma processing steps with neutral beams might be necessary. It was shown recently by Samukawa [5] that reproducible 8 nm structures may be produced by plasma etching provided that Various types of fast neutral beams were considered including hyperthermal neutrals produced by accelerating ions across the sheath from a plasma onto a surface [6], a neutral beam produced by ion-neutral scattering [7], neutral beam produced by ion-electron recombination [8] and fast neutrals created in charge transfer collisions [9]. Of all these sources of fast neutrals only the very energetic fast neutrals produced in charge exchange meet the requirements for etching of dielectrics such as SiO_2 [9-12] which requires very high energy particles. The first functional fast neutral etching was realized based mainly on surface neutralization of fast ion beams [13,14] in narrow tubes. In principle however this technique is a combination of the earlier surface neutralization [6] and depending on the operating pressure the charge transfer production of the very high energy neutrals. In development of very high energy neutral beams the most important feature is the ion energy distribution function (IEDF) which gives rise to fast neutrals. In this paper we compare IEDFs for several species of ions found in standard processing plasmas and how those may be converted to fast neutrals.

The first observation of plasma charging damage has been reported by Yoshida in 1983 [15]. Hashimoto has tried to explain the origin of the plasma process induced damage (PPID) by using the electron shading mechanism [16]. As the feature size shrinks toward the nanoscale, the effect of PPID on the device characteristics becomes a more serious problem [16-19]. The kinetics of surface neutralization as required by the current sources of fast neutral beams was studied by Stojković et al. [20]. On the other hand, the importance of the gas phase neutralization for the realistic devices as proposed in the literature was first pointed out in the same paper [20] and applied to the system proposed by Samukawa and coworkers [13,21].

In this paper, surface neutralization of ions and gas phase neutralization in Ar-CF_4 mixture have been studied separately by means of computer simulations. Particle-in-cell (PIC) and particle-in-cell/Monte Carlo (PIC-MC) code [22] combined with the Monte Carlo code [23] have been extensively used to evaluate neutralization of Ar^+ and CF_3^+ ions in Ar-CF_4 mixture.

Simulation technique

Plasma simulation codes [22,23] have achieved a high level of sophistication and are routinely used for modeling plasma etching reactors, for predicting the etch rates, evolving profiles of the micron-scale features fabricated in plasma-assisted processes, or for determining the influence of various plasma parameters on the ion-surface collisions. Furthermore, the difficulty in achieving well-defined experimental conditions and the limited diagnostic techniques available for small scale discharges, favor the investigation of nanoscale systems by simulation tools. The system that was studied is made of the gas layer and a tube. The system for neutralization consists of thin tubes (diameter 1.4 mm and length 10 mm - 100 mm) which are parallel to the axis of the field. The tubes are made of reflecting walls and for the sake of simplicity we assumed 100% reflectivity. The initial beam of ions is gradually converted to fast neutrals in gas phase and ion-tube wall collisions at a grazing incidence. The initial beam consists of ions which are gradually converted to fast neutrals in gas phase and ion-tube wall collisions at a grazing incidence. The probability of neutralization in ion-wall collision is 100% [20] while the overall efficiency is less than 100% since all ions do not collide with walls or molecules.

In order to determine the ion energy and angular distribution functions for Ar-CF_4, we have modified the code to take into account cross sections data required for proper description of kinetics in gas mixtures. PIC/MCC calculations were performed for Ar-CF_4 plasmas at 13.56 MHz, for three different values of the gas pressure of 50 mTorr, 100 mTorr and 200 mTorr and the interelectrode separation of 2 cm. The obtained ion energy distribution functions (IEDFs) and ion angle distribution functions (IADFs) for Ar^+ and CF_3^+ ions were applied as an input to the Monte Carlo codes based on the null collision technique and a complete set of scattering cross sections that accurately represents collisions in argon and fluorocarbon mixture [24]. The Monte Carlo codes that were used have been developed to follow ion and fast neutral transport in parallel plate geometries with complex boundary conditions. An electric field was applied to bring the slow ions out of the system without giving them any significant energy.

The neutralization efficiency as a result of collisions of ions with the aperture walls was determined by using code that takes into account geometrical properties of the system. Overall neutralization efficiency can be obtained by multiplying probabilities for neutralization in the gas phase collisions and on the walls. We were especially interested in the influence of various parameters, such as, the gas pressure, the aperture length and the diameter of the tube on collisions of ions with the walls and overall probability of neutralization.

Results and Discussion

Ion surface collisions. The positive Ar^+ and CF_3^+ ions created in RF Ar-CF_4 plasma were accelerated by the sheath voltage and bombard the surface exposed to the plasma with energies typically of the order of tens to hundreds of eV. Due to the ion surface collisions inside the apertures, some ions are neutralized. This process can be described by the efficiency of neutralization defined as the number of neutrals that leave the tube normalized to the flux of the incident ions. Neutralization efficiency due to ion surface collisions and for geometry of the neutral beam source from [12,20] were calculated for three different values of the pressure of 50 mTorr, 100 mTorr and 200 mTorr. The results are shown in Figure 1.

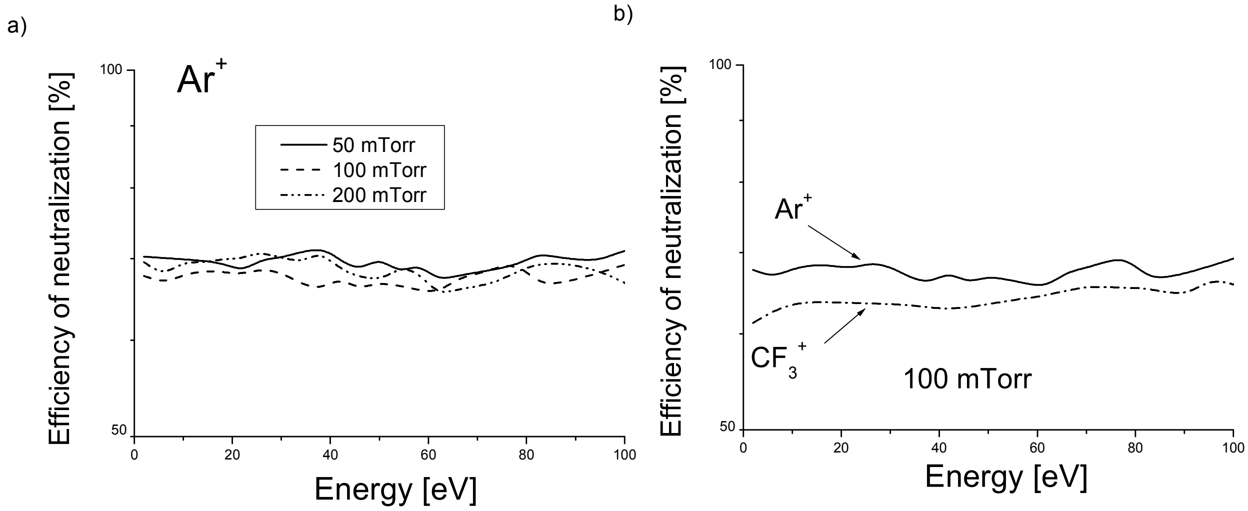

Fig. 1 The energy dependence of the efficiency of neutralization due to ion surface collisions for: a) Ar^+ ions at the three different pressures and b) Ar^+ and CF_3^+ ions at the pressure of 100 mTorr.

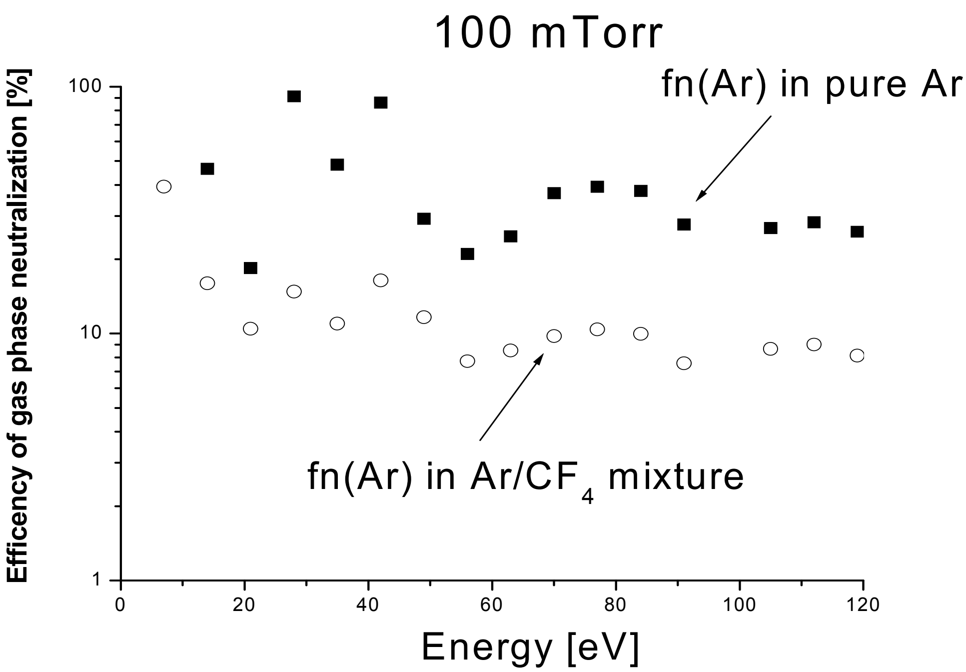

Fig. 2 Efficiency of gas phase neutralization in pure argon (solid symbols) and in the mixture (open symbols) (the mixture consists of 20% CF_4 and 80% Ar); at the pressure of 100 mTorr. Label *fn* denotes fast neutrals.

As can be seen from Fig. 1a, the pressure has very little effect on the neutralization efficiency in the tube. In principle that means that the angular distribution did not change much in the pressure range that was covered. On the other hand, from Fig. 1b, we may conclude that efficiency of neutralization that corresponds to Ar^+ ions is somewhat larger than that for CF_3^+ ions. The analysis of the results presented in Figure 1 shows that at the pressure of 100 mTorr, neutralization efficiency of Ar^+ reaches 70%, while for CF_3^+ is around 60%. This is merely due to the shape of the ion energy distribution function and its associated angular distributions.

a)

b)

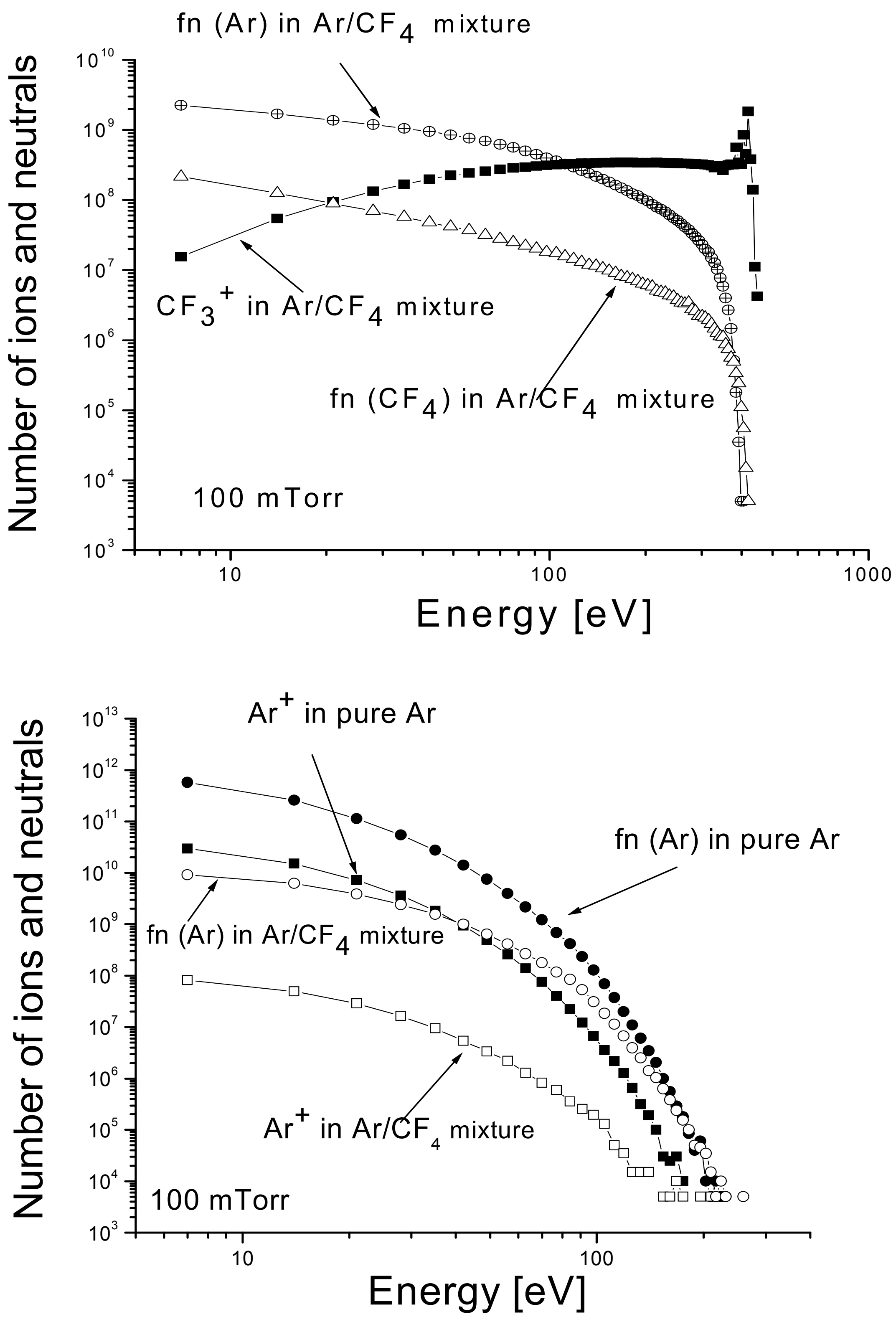

Fig. 3 Number of particles (ions and neutrals) versus the particle energy for: a) CF_3^+ ions and fast neutrals originating from ion Ar molecule collisions in the mixture (the mixture consists of 20% CF_4 and 80% Ar); b) fast neutrals originating from Ar^+ ions in pure argon and in the mixture. Calculations were performed at the pressure of 100 mTorr. Label *fn* denotes fast neutrals. Results were obtained for the reduced field of E/N =4.5 kTd.

Gas phase collisions. The process of neutralization and creation of fast neutrals due to ion neutral collisions (resonant charge transfer) in the gas phase has been considered by using the set of the Monte Carlo codes with parameters as previously specified. Gas phase collisions may occur within the tubes. After leaving the tubes the residual ions can also suffer further collisions and produce fast neutrals. In Fig 2 we show the efficiency of neutralization of Ar^+ ions in pure Ar and in the mixture. As expected the neutralization in pure argon is more efficient due to the effect of the resonant charge transfer. Fast neutral energy distribution has a similar shape to the ion energy distribution.

DC Townsend source of fast neutrals RF discharges were used for processing of integrated circuits because of their ability to produce high density plasmas, to have control of the IEDF and ability to achieve high ion energies by separate application of a bias voltage. However, application of a mesh or a plate with cylindrical channels allows a separate control of ion and fat neutral beam properties and even application of DC discharges such as hollow cathode discharges which are used as very efficient ion beam sources. To support such a possibility we have calculated ion and fast neutral energy distributions from a Townsend regime DC discharge operating at E/N= 4.5 kTd. The results are shown in Fig. 3. While Townsend discharges cannot be used in practical applications because of their low density the results indicate a large degree of control of the properties of the energy distribution functions and efficiency of gas phase neutralization into high energy neutral beams. This approach is in line with the original proposal [23] that a Townsend regime discharge with a mesh to separate ions from neutrals could be used as an efficient source of very high energy neutral beams.

Conclusion

Plasma processing is indeed one of the crucial modern technologies that have made a significant impact on fabrication of integrated circuits (IC) and consequently in electronics and consumer goods in general. The challenges that remain to be solved include the ability to deposit and pattern new materials at nanometer scales that are needed in new generations of microlectronics fabrication. Damage to ICs during manufacturing as a result of charging of the dielectrics during finalization of interconnects is both reducing the profitability and reducing the ability to reach large sizes of microchips and make complete integration of a computer or digital TV on a single chip. The damage includes both the processing problems such as etch stop which were associated with charging [18], but also breakdown of the FET dielectric which may occur due to smaller and smaller deposited charge as the dimensions are reduced.

Simulation results presented here were obtained for realistic geometries and realistic energy distributions obtained from a plasma. In that sense they are the extension of the previous results that were obtained for a monoenergetic beam. We have shown previously that geometrical properties of the tube, such as the length and diameter ratio are very important in determining the efficiency, but gas phase collisions also give a significant contribution to the ion beam neutralization even under relatively low pressure conditions as used by Samukawa and coworkers [13]. The PIC code used here with the added interface of Monte Carlo codes and calculations of geometrical factors are sufficiently detailed description to analyze the realistic processes in plasma tools.

In this paper we have in particular analyzed the ion energy distribution functions and the resulting fast neutral energy distribution functions. In general fast neutrals have a very similar distribution to the initial ions and therefore the same optimizations of the IEDFs will apply to high energy neutral sources. One may conclude that operation of the plasma sources at around 50 mTorr will lead to a large degree of neutralization. At the same time we discuss a possibility to use dc discharges, in particular Townsend discharge with a mesh to produce very high energy neutral beams [23].

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