

Vol.3 Issue.4

Stopping and Range of Ions in Matter data of polymeric materials simulating the process of ion implantation in plasma immersion

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Abstract

This work introduces the physico-chemical surface properties of three commercial polymers: white polyvinyl chloride (PVC), polyethylene terephthalate (PET) from two- liter bottles, and low-density polyethylene (LDPE) as results of plasma immersion ion implantation (PIII) using SF6 and N2 plasmas at low-pressure vacuum system. The experiments were conducted in the Technological Plasmas Laboratory (LapTec) between 2011 and 2013. For comparison, SRIM/TRIM calculations/Monte Carlo code were used to access the following output data: ion range and distribution (screening a Gaussian histogram); number of backscattered ions nB; and vacancies produced nVaccording to Kinchin–Pease formalism. In both approaches (experimental and simulated), it was used as inputting data: the main ion implantation parameter: -1000 Vof high-voltage negative pulses in PIII experiments which are matched to 1 keV of inputenergy data in the virtual SRIM environment using F+ and N+ as projectiles ions, and rigid PVC, PET mylar and LDPE marlex as targets. The purpose was to link the surfaceproperties of the polymeric samples obtained in laboratory by PIII technique: Θ ; Θ (t); R(z); T(λ) and B (by WVTR) with the output data about ion ranges and distribution, provided by the SRIM simulation. In addition, parameters of energy loss (eV/ångstrom) by ionization, vacancy and phonons were collected. In the first approach (laboratory or experimental outcomes), contact angle measurements, Θ , presented high values for Fluorine PIII (> 110o) and low values for Nitrogen PIII (< 50o), both, stables by Θ (t) in until 30 days. The roughness, R(z), had a soft increase to few tenths of nanometers in all cases (Rz < 20 nm) for PVC and PET, and (Rz < 50nm) for LDPE. Optical transmittance at visible range, T (λ), presented either increase, from ${\sim}82\%$ to ${\sim}84$ % for PET, for both (SF6 and N2) plasmas or reduction of T (λ) from 80 to 70%, depending on the conditions. In addition, Barriers properties (B) were considerably increased, by observing the reduction of vapor transmission rate (WVTR) from 6.12 \pm 0.33 to 1.05 \pm 0.17 g/m2 day for PET, and 6.4 \pm 0.41 to 0.81 \pm 0.12 g/m2 day for LDPE. The chemical analysis (by XPS and FTIR) pointed for three polymeric samples, an unsaturated structure containing high proportion of fluorine and C-F bonds using SF6 plasmas and; high proportion of O containing groups for treatment using N2 plasmas by PIII. SRIM results pointed: a low random scattering or penetration of ions in low fluency distributed in the polymeric matrix, owing to inelastic collisions, which the ranged from 0 to 350 nm of utmost depth, h. It was fitted then, a quite symmetric Gaussian curve. The mean values were also analysed. N+ ions had higher penetrations than F+. The -dE/dx were attributed, in major, to phonons yield (60 to 70 %) compared to ionization (10 to

20 %) or vacancies (< 4%). The use of computational tools, in our case, Stopping and Range of Ions in Matter: SRIM/TRIM calculations in conjunction with Monte Carlo Code were useful tools to compare experimental data and simulated data for all conditions, attending to the ion implantation process. Analogously, for 1 keV (equivalent to -1000V high voltage negative pulses) of input energy resulted in mean values from 45 to 70 Å of modified layer for F+, and from 60 to 70 Å of modified layer for N+. PET is more resistant to irradiation than PVC and LDPE. Considering the input of 99.999 incident ions, the numbers of backscattered ions were, in general much lower (0.018 %) than the ions penetrated and recoiled. The energy loss was mainly owing to the phonons, in most % generated by recoils atoms than generated by the incident ions. The outcome is that, those values of modified layer are enough to modify the surface of those polymers.

Keywords

Plasma immersion ion implantation, SRIM (Stopping and Range of lons in Matter), Irradiated polymers.

INTRODUCTION

lon implantation is a major application of plasma processing in a variety of applications in which the surfaces of materials are to be treated. The implantation process requires a source of ions and a means to accelerate them toward the surface. Two general methods are in use today: *ion beam* implantation, in which a beam of ions is directed toward a substrate, and *plasma* implantation, in which the ions produced in a plasma discharge surrounding or near the object to be implanted are extracted from the plasma and accelerated into the object.

lon implantation is designed to modify the surface properties of materials without changing their bulk properties. The implantation process may offer improvements in their properties or may actually be used to degrade the surface, depending on the application. It is becoming economically attractive in Japan, Europe, and the United States and can be done on metals and alloys, as well as on semiconductors, ceramics, insulators, and polymers. Some of the surface properties that can be modified by this process are hardness, fatigue, toughness, adhesion, wear, friction, corrosion oxidation, dielectric properties, magnetic properties, superconductivity, resistivity, and catalysis.

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