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Analysis of microscopic parameters of surface charging in polymer caused by defocused electron beam irradiation

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ABSTRACT

The relationship between microscopic parameters and polymer charging caused by defocused electron beam irradiation is investigated using a dynamic scattering-transport model. The dynamic charging process of an irradiated polymer using a defocused 30 keV electron beam is conducted. In this study, the space charge distribution with a 30 keV non-penetrating e-beam is negative and supported by some existing experimental data. The internal potential is negative, but relatively high near the surface, and it decreases to a maximum negative value at $z = 6\,\mu m$ and finally tend to 0 at the bottom of film. The leakage current and the surface potential behave similarly, and the secondary electron and leakage currents follow the charging equilibrium condition. The surface potential decreases with increasing beam current density, trap concentration, capture cross section, film thickness and electron–hole recombination rate, but with decreasing electron mobility and electron energy. The total charge density increases with increasing beam current density, trap concentration, capture cross section, film thickness and electron–hole recombination rate, but with decreasing electron mobility and electron energy. This study shows a comprehensive analysis of microscopic factors of surface charging characteristics in an electron-based surface microscopy and analysis.

1. Introduction

Charging characteristics and space charge of various polymer microscopic factors caused by defocused electron beam irradiation have always been an interesting aspect in scanning electron microscopy (SEM) (Cazaux, 2012; Cazaux et al., 2013; Maekawa et al., 2007; Pawley, 1992; Reimer, 1993; Touzin et al., 2006; Ura, 2001), electron beam microanalysis, lithography (Bai et al., 2003; Bolorizadeh and Joy, 2007; Ciappa et al., 2010; Ko and Joy, 2001), and space application since 1960s (Oatley et al., 1966). Various microscopic parameters may influence the surface charging characteristics and distort the accuracy of the electron beam microanalysis. Moreover, polymer charging may cause the breakdown of the polymer of microelectronic devices, but it may also lead to undesirable image effects induced by emitted electrons from the polymer surface (Joy and Joy, 1996; Li and Zhang, 2010; Ura, 1998). Therefore, more efforts are needed to understand the relationship between various microscopic parameters and surface charging characteristics for predicting and diminishing the charging effect.

Polymers are widely used to protect, resist, and assist materials in various fields, and the related microscopic parameters of their surface charging characteristics have already been preliminarily investigated (Belkorissat et al., 2005; Cazaux, 2005; Fakhfakh et al., 2012; Jbara et al., 2008). Based on low electron mobility (Sessler et al., 2004) and resistivity (Vila et al., 2005), the charging characteristics and charging equilibrium are jointly influenced by the primary electron current, secondary electron current, leakage current, and physical parameters of the electron mobility, electron energy, film thickness, trap concentration, capture cross section and recombination rate. Several approaches that address the issue have been developed and proposed in a number of theoretical analyses. The radiation-induced conductivity model (Berraissoul et al., 1986; Cornet et al., 2008; Tyutnev et al., 2007; Yang and Sessler, 1992; Yasuda et al., 2008) is an empirical model that predicts experimental results. The generation-recombination model (Sessler et al., 2004) considers the generation of a carrier pair by incident electrons and the microscopic transport mechanisms of both electrons and holes, respectively. More recently, SEM-based analysis of the charging characteristics and surface charging of various parameters has attracted much attention (Dapor et al., 2010; Fakhfakh et al., 2012; Jbara et al., 2008; Kechaou et al., 2008; Mahapatra et al., 2006). However, only a few studies have

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been conducted to determine the influence of complex microscopic parameters on surface charging because of the difficulty in measurement. Moreover, insufficient microanalysis had been conducted on the surface potential of the charge transport condition corresponding to a defocused electron beam.

We have recently proposed a comprehensive model for defocused electron beam charging of grounded polymer films, and simulated transients of negative charging by considering electron scattering, transport, and trapping (Cao et al., 2012; Feng et al., 2013; Li and Zhang, 2010). Thus, this study was designed to reveal the microscopic parameters of surface potential characteristics of polymers using a defocused electron beam using our newly developed model for self-consistent simulation of surface charging characteristics. The trapping process of an electron and hole is considered by the Poole–Frenkel effect and accordingly clarified the negative charging effect of polymer (Cornet et al., 2008; Touzin et al., 2006). In this paper, we report the relationship between complex microscopic factors with space charge, space potential and total charge densities as well as surface potential. These results regarding polymer characteristics are considered as examples in our simulation, but the general results are applicable to other polymers.

2. Numerical model

2.1. Electron scattering

The scattering of atoms and electrons entering the film is simulated using the Monte Carlo method (Czyzewski et al., 1990; Joy, 1995) and the elastic scattering is computed using the Rutherford scattering cross-section (>10 keV electrons) (Cao et al., 2012; Feng et al., 2013).

$$\sigma = 5.21 \times 10^{-21} \frac{z^2}{E^2} \frac{4\pi}{\alpha(1+\alpha)} \left(\frac{E+511}{E+1022} \right)^2, \tag{1}$$

where σ, E, z, α denote the Rutherford scattering cross section, the incident electron energy, the mean atomic number, the shielding factor, respectively.

The average rate of energy loss during inelastic scattering is calculated using the modified Bethe equation (Joy, 1995). The fast secondary model is used in our simulation to deal with the secondary electrons (SEs) (Joy, 1995). SE is generated for each inelastic scattering event after gaining the lost energy of the scattered primary electrons (PEs). The inelastic scattering process is described as follows:

$$\frac{d\sigma_{\text{in}}}{d\Omega} = \frac{\pi e^4}{E^2} \left(\frac{1}{\Omega^2} + \frac{1}{(1-\Omega)^2} + \left(\frac{\tau}{\tau+1} \right)^2 - \frac{2\tau+1}{(\tau+1)^2 \Omega (1-\Omega)} \right), \tag{2}$$

where σ_{in}, E, Ω, e, τ denote the inelastic scattering cross section, the incident electron energy, the energy transfer ΔE normalized with E, the basic charge, the electron kinetic energy normalized by the rest mass energy of an electron, respectively.

Furthermore, the inelastic mean free path can be written as:

$$\lambda_{\text{in}} = \frac{A}{N_a z \rho \sigma_{\text{in}}}, \tag{3}$$

where A, ρ, z, N_a, and σ_{in} are the atomic weight, the density of polymer, the mean atomic number, the Avogadro constant, and inelastic scattering cross section, respectively.

The electrons, including primary electrons (PEs), secondary electrons (SEs), and holes, eventually deposited on the polymer sample are either transported (drift and diffuse) because of the internal electric field and charge density gradient or trapped. The charge transport and trapping are neglected during electron scattering because the whole scattering process is extremely fast, that is, the scattering process is 10^{-5} s for the incident electron with an energy of 30 keV.

2.2. Charge transport and trapping

The electron density $n(z, t)$, trapped electron density $n_{\text{trap}}(z, t)$, hole density $h(z, t)$, trapped hole density $h_{\text{trap}}(z, t)$, electron current density $\boldsymbol{J}_n(z, t)$, hole current density $\boldsymbol{J}_h(z, t)$, and internal potential distribution $V(z, t)$ satisfy the continuity, transport and Poisson equations:

$$\frac{\partial \left(n(z,t) + n_{\text{trap}}(z,t) \right)}{\partial t} = \frac{\nabla \cdot \boldsymbol{J}_n(z,t)}{e} - Rn(z,t)h(z,t), \tag{4}$$

$$\frac{\partial \left(h(z,t) + h_{\text{trap}}(z,t) \right)}{\partial t} = \frac{-\nabla \cdot \boldsymbol{J}_h(z,t)}{e} - Rn(z,t)h(z,t), \tag{5}$$

$$\boldsymbol{J}_n(z,t) = -e\mu_e n(z,t)\nabla V(z,t) + eD_e \nabla n(z,t), \tag{6}$$

$$\boldsymbol{J}_h(z,t) = -e\mu_h h(z,t)\nabla V(z,t) - eD_h \nabla h(z,t), \tag{7}$$

where e denotes the absolute value of electron charge; R is the electron–hole recombination rate, which is set to 10^{-15} cm^3 s^{-1}(Le Roy et al., 2012); $V(z, t)$ is the internal potential; μ_e and μ_h are the electron and hole mobilities, respectively; D_e and D_h are the electron and hole diffusion coefficients, respectively. The mobility and the diffusion coefficient satisfy the Nernst–Einstein equation. Considering that the hole mobility is much less than the electron mobility in polymers, we use hole mobility μ_h 10^{-12} cm^2 V^{-1} s^{-1} (Sessler et al., 2004).

Electrons and holes that eventually deposit on the polymer will either drift or diffuse because of the internal electric field and charge density gradient or be trapped. Some charges may be trapped by trapping centers while being transported through the polymer. At the same time, electron–hole recombination will occur. In principle, the trapped charges may also be released again via detrapping based from several experiment data (Sessler et al., 2004). However, several experimental studies have shown that the charges in some polymers could persist for significant period of time (Sessler et al., 2004), which indicates that detrapping effect is often very weak and therefore negligible. The charge-trapping process in polymer is complex (Sessler et al., 2004; Touzin et al., 2006). Thus, space charges may either be free or trapped.

In this paper, we describe the trapping process and neglect the detrapping process to reduce the computation time as follows:

$$\frac{\partial \left(n_{\text{trap}}(z,t) \right)}{\partial t} = n(z,t)\,\mu_e E(z,t) S_e \left(N_e - n_{\text{trap}}(z,t) \right), \tag{8}$$

$$\frac{\partial \left(h_{\text{trap}}(z,t) \right)}{\partial t} = h(z,t)\,\mu_h E(z,t) S_h \left(N_h - h_{\text{trap}}(z,t) \right). \tag{9}$$

Here, $h_{\text{trap}}(z, t)$ and $n_{\text{trap}}(z, t)$ are densities of trapped holes and electrons, respectively. N_e and N_h are the electron trap and hole trap concentrations respectively, and S_e and S_h are the electron capture and hole capture cross sections, respectively. Trap rate ($N_e \times S_e$) is the product item of the trap concentration N_e and capture cross section S_e in a polymer position, which is subordinated to the Poole–Frenkel trapping/detrapping mechanisms (Sessler et al., 2004; Touzin et al., 2006). In addition, the internal electric field distribution $E(z, t)$ satisfies the charge continuity and transport equations.