Charging of substrates irradiated by particle beams

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A simple dynamical model for studying the charging of substrates irradiated by particle beams is developed. The charging potential for positive ion beams can be as large as the beam voltage. For negative ion beams, the charging potential is significantly lower and is governed by the secondary electrons. A closed form expression derived for the charging voltage in the case of negative ion beams agrees well with our numerical work. The results are consistent with observations on charging of isolated substrates during ion implantation with positive and negative ion beams. © 1997 American Institute of Physics. [S0003-6951(97)00548-2]

Positive ion beams, commonly used in materials processing applications such as ion implantation, etching, and lithography, causes substantial substrate charging. In ion implantation processes the charging and the associated damage have been recognized¹ and these are of serious concern.^{2–4} In substrate etching by ion beams, charging also poses a potential for serious damage to the devices. 5^{-11} Special techniques, such as electron or plasma flooding and plasma immersion.^{2,3,12-16} have been used to reduce the charge buildup. Negative ion beams have merits for achieving low charge-up voltage of substrates, without the aid of external neutralizing sources. Experimental results in the context of ion implantation together with Monte Carlo simulations show dramatic reduction in the charging voltage of substrates in comparison with the positive ion beam case. $^{17-20}$ In this letter, we present a novel, simple model for studying, both numerically and analytically, the charging of isolated substrates irradiated by particle beams. For the negative ion beam case, we have derived an analytic expression for the charging voltage.

The charging of a substrate irradiated by a particle beam is described by the system of equations:

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x} (nv) = 0, \tag{1}$$

$$\frac{\partial v}{\partial t} + v \,\frac{\partial}{\partial x} \,v = \frac{qE}{m} - \nu H(x - L)v, \qquad (2)$$

$$\frac{\partial E}{\partial x} = 4 \pi n (q + e \gamma n_s), \qquad (3)$$

$$n_{s} = \int_{e(\phi_{c}(L) + |\phi_{c}(L)|)/2}^{\infty} f(E) dE, \qquad (4)$$

with

$$f(E) = \frac{2E_p E}{(E+E_p)^3}.$$

The dynamics of the ions, with charge q, density n, and velocity v, are represented by the plasma fluid Eqs. (1) and (2). The electrons are secondary electrons produced by the beam impinging on the substrate. Their number density is

 γnn_s , where γ is the number of secondary electrons emitted per ion impact, and n_s is the fraction of secondary electrons relative to the ion density, as defined by Eq. (4). The electric potential is obtained from Eq. (3) for the given charge densities. The beam is assumed to propagate from x = 0, where an incoming flux is specified, to the substrate at x = L. The beam slows down at the rate ν when it encounters the substrate at x=L, characterized by the Heaviside function H(x). The first term on the right-hand side of Eq. (3) is the source for the self-field due to the beam and the second term is the net positive charge on the substrate due to the loss of secondary electrons. The net positive charge is an integral of the secondary electron distribution function f(E) over the energy space. The energy E_p , corresponding to the peak of the distribution function f(E), is dependent on the substrate and is typically in the range 0.5-2.0 eV for different materials.¹⁷ If the substrate is charged positive, the electrons with the energy less than charging voltage $\phi_c(L)$ will not escape and the net positive charge will be reduced. However, if the charging voltage is zero or negative, all secondary electrons will be lost. The lower limit of the integral in Eq. (4) reflects this. The factor γ is a function of the beam energy and we will use empirical data to choose the value of γ for different beam energies.

The equations are rendered dimensionless by normalizing distance to the size of the system *L* (typically 10–15 cm) and time to L/v_0 . The velocity is normalized to the initial beam velocity v_0 , the density to the beam density n_0 , the potential ϕ , and energy E_p to the initial beam energy $(mv_0^2/2=e\phi_0)$ and the charge *q* to the magnitude of electronic charge *e*. There are four dimensionless parameters, $\beta = (L/L_D)^2$, *q*, γ , and E_p , with $L_D = \sqrt{mv_0^2/8\pi n_0}$, the effective Debye length computed using the beam energy. The charging potential ϕ_c is the normalized potential at the substrate.

The first set of numerical runs is for a positive ion beam with $\gamma = 3.0$, $\beta = 1.0$, q = 1, and $E_p = 10^{-4}$. This would be typical for a beam with an energy of 10 keV, density n_0 $= 2.45 \times 10^7$ cm⁻³ and L = 15 cm. The damping coefficient is arbitrarily chosen to be $\nu = 10^4$, and typically any large number suffices. The boundary conditions that we use are the following. At x=0, $\phi=0$ and at x=L, $d\phi/dx=0$. For the ion density, dn/dx=0 at x=0, and n=0 and at x=L and similarly for the ion flux, p=nv, we demand that dp/dx

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FIG. 1. (a) potential ϕ , (b) ion density *n*, (c) ion momentum *p*, and (d) ion velocity *v* vs *x* for t=1 (solid line), t=2.0 (dotted line), and t=5.0 (dot-dash line) with q=1 (positive ions), $\gamma=3.0$, and $\beta=1.0$.

=0 at x=0, L. Our initial conditions are $\phi=0$, n=1.0 and p=nv=1.0 for all x.

The time evolution of the potential (ϕ) , ion density (n), ion momentum (p), and ion velocity (v) as functions of x are shown in the four panels at three different instants of time in Figs. 1(a)–1(d). The four quantities (solid line) are at t=1. The potential maximum is at the substrate and is 0.80 of the beam voltage. The ion momentum (or flux) as well as the density are close to unity for most of the region, but are very large at the substrate due to the rapid slowing down and accumulation of the incoming ions. The small dip in the flux before the rapid rise is due to the reduction of the number density and the ion velocity due to the repulsion from the accumulated ions. At t=2 (dotted lines), the charging voltage at the substrate is now 1.6, and the repulsion force has led to a further decrease in the ion density. Furthermore there is a significant reduction in the ion velocity and even the incoming velocity at x=0 has been reduced to 0.44 of the original velocity. There is now a reversal of the ion flux near the substrate. At this point the self-consistent fields strongly dominate the dynamics. Finally, at t=5 (dot-dash lines), the potential at the substrate has decreased. The ion momentum and velocity are now dominantly negative, implying that the self-consistent field due to the build up of positive charge has led to a strong repulsion of the incoming ions. The slowed down ions at the substrate now move in the negative x direction and this reduction in the ion density leads to the drop in the voltage at the substrate.

In Fig. 2, we plot the time history of the charging potential for $\beta = 0.1$, 1.0, and 10.0. The charging voltage maximum is seen to increase with β . The self-consistent field, which affects the ion dynamics and prevents buildup of charge at the substrate, plays a significant role in determining the maximum potential. In the very early phase of the charging secondary electrons are emitted. However, with the buildup of the positive voltage on the substrate, the electrons do not have enough energy to escape and are held back. Thus, for positive ion beams the maximum charging voltage is comparable to the beam voltage.

The next set of runs are for negative ion beams with $\beta = 1.0$, q = -1, and $E_p = 10^{-4}$. For this case, the charging



FIG. 2. The charging voltage ϕ_c vs time for $\beta = 0.1$, 1.0, and 10.0 for q = 1 (positive ions), $\gamma = 3.0$.

voltage reaches a constant value in a fraction of a microsecond as shown in Fig. 3 for $\gamma = 3$, 4, 5, and 6. The charging voltage increases with γ . These results are in good agreement with the experimental work of Sakai *et al.*¹⁷ Another interesting result is that the charging voltage is independent of the parameter β unlike the positive ion case as shown in Fig. 2.

The negative ion case is amenable to an analytical solution. If we examine, Eq. (3), a steady-state solution can be reached if the total charge at the substrate is zero or constant. Since the number density of the incoming negative ions increases, at the substrate, the steady state is achieved by making the total charge go to zero. The charging voltage adjusts to a value such that the number of secondary electrons emitted are exactly equal to the number of negative ions at the substrate:

$$\int_{E_c}^{\infty} f(E) dE = 1$$
(5)

and this yields

$$E_{c} = [(\gamma - 1) + \gamma^{1/2} (\gamma - 1)^{1/2}] E_{p}, \qquad (6)$$

where $E_c = \phi_c/e$. The charging voltage is found to scale linearly with energy at the peak of the secondary electron distribution function, which depends on the material. This



FIG. 3. The charging voltage ϕ_c vs time for $\gamma = 3.0$, 4.0, 5.0, and 6.0 for q = -1 (negative ions) and $\beta = 1.0$.

dependence on γ is found to be consistent with the values obtained in Fig. 3. Also there is no dependence on β , in accordance with the numerical results.

In conclusion, the present study provides a simple, novel model for investigating the dependence of the charging voltage of a substrate on the nature of the irradiating beam and the energy at the peak of the secondary electron distribution function. For positive ion beams, we find that the maximum charging voltage is comparable to the beam voltage. The negative ion beam case yields a steady state for the charging voltage. This is because the charging voltage adjusts to a value for which the negative ion density exactly balances the number density of the lost secondary electrons, thereby maintaining complete charge neutrality at the surface of the substrate at the equilibrium state. This criterion gives us a simple expression for the charging voltage given by Eq. (6). Thus in addition to providing an insight into the charging problem due to the simplicity of the model, the present study reinforces earlier work.^{17–20} The negative ion beams are thus potentially attractive for etching, ion implantation, and surface treatment due to the fact that the charging voltage is low enough to avoid structural damage to the substrate material.

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