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TWO–DIMENSIONAL NUMERICAL ANALYSIS OF PLASMA IMMERSION ION IMPLANTATION OF CYLINDRICAL BORES

A.G. Liu[1,2], *X.F. Wang*[1)], *L.P. Wang*[1)], *S.Y. Wang*[1)], *B.Y. Tang*[1)] *and P.K. Chu*[2)]

1) Advanced Welding Production Technology National Key Laboratory, HIT, Harbin 150001, China

2) Department of Physics and Material Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kang, China

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Plasma immersion ion implantation (PIII), unrestricted by sight–light process, is considered a proper method for inner surface strengthening. Two–dimensional simulation of inner surface PIII process of cylindrical bores were carried out in this paper using cold plasma fluid model, and influence of the bore's dimension on impact energy, retained dose and uniformity of inner surface were investigated.

KEY WORDS *plasma immersion ion implantation, plasma sheath, inner surface modification, computer simulation*

1. Introduction

Plasma immersion ion implantation (PIII)[1] unrestricted by sight–light process, is considered a proper method for inner surface strengthening. In recent years, researchers have paid a lot of attention on applying PIII in inner surface modification. T.E.Sheridan[2,3] has simulated the inner surface PIII process of a bore using one–dimensional fluid model, and presented the low impact energy problem for the first time. Zeng et al[4,5] presented an idea to improve the impact energy using an auxiliary electrode, based on similar analysis. We presented a method to improve both impact energy and retained dose of inner surface using deflecting electric field[6], and uniformity was investigated experimentally[7]. An assumption of infinite long bore was used in these works, and analyzing a real bore with finite length using these results will lead to no–conservation of energy. So, we set up a two–dimensional fluid model to analyze sheath evolution and development of ion density and ion velocity in PIII process of a finite long bore. Uniformity of inner surface PIII for different pulse duration had been reported[8] and in this paper, influnce of the bores' dimension on impact energy, retained dose, and uniformity were investigated.

2. Model

The applied voltage φ_t is usually several tens of kV in PIII, and the kinetic energy of ions and electrons can be neglected compared with $e|\varphi_t|$. And under the common pressure used in PIII, the average mean free path of a paticle is much larger than the sheath. So, the inner surface PIII process can be described using collisonless cold plasma fluid model. And, density of electron is assumed to satisfy Boltzman's distribution. So, ion density and velocity can be described using mass continuity equation and momentum continuity equation of compressable fluid in conservative form,

$$\frac{\partial n_i}{\partial t}+\nabla\cdot(n_i\vec{v})=0 \tag{1}$$

$$\frac{\partial}{\partial t}(n_i v)+\nabla\cdot(n_i v\vec{v})=-\frac{en_i}{m_i}\nabla\varphi \tag{2}$$

where n_i is the ion density, t is the implant time, $\vec{v}$ is the ion velocity, e is the charge of an electron, m_i is the mass of the ion, and φ is the potential. Distribution of the potential can be derived using Poisson's equation,

$$\nabla^2\varphi=-\frac{e}{\varepsilon_0}(n_i-n_e) \tag{3}$$

where ε_0 is the vaccum permitivity, and n_e, the electron density, satisfies Boltzman's distribution,

$$n_e=n_0\exp(\frac{e\varphi}{kT_e}) \tag{4}$$

where n_0 is plasma density, k is the Boltzman constant, and T_e is the electron temprature.

Due to the axial symmtry of the bore, implantation is symmetry axially, so the process can be simulated using cylindrical coordinate system. Under cylindrical coordinate system, applying equation (4) to (3), equation (1)–(3) will change to,

$$\frac{\partial n_i}{\partial t}+\frac{1}{r}\frac{\partial}{\partial r}(rn_i,v_r)+\frac{\partial}{\partial z}(n_i,v_z)=0 \tag{5}$$

$$\frac{\partial}{\partial t}(n_iv_r)+\frac{1}{r}\frac{\partial}{\partial r}(rn_iv_rv_r)+\frac{\partial}{\partial z}(n_iv_rv_z)=-\frac{en_i}{m_i}\nabla\varphi_r \tag{6}$$

$$\frac{\partial}{\partial t}(n_iv_z)+\frac{1}{r}\frac{\partial}{\partial r}(rn_iv_zv_r)+\frac{\partial}{\partial z}(n_iv_zv_z)=-\frac{en_i}{m_i}\nabla\varphi_z \tag{7}$$

$$\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial\varphi}{\partial r})+\frac{\partial^2\varphi}{\partial z^2}=-\frac{e}{\varepsilon_0}(n_i-\exp(\frac{e\varphi}{kT_e})) \tag{8}$$

where r and z are radial and axial coordinates respectively, v_r and v_z are radial and axial components f ion velocity. Apply equation (5) to (6) and (7) and simplify them, and let $\rho=\frac{r}{S}$, $Z=\frac{z}{S}$, $\phi=\frac{\varphi}{\varphi_t}$, $N=\frac{n_i}{n_0}$, $V_\rho=\frac{v_r}{v_{\max}}$, $V_z=\frac{v_z}{v_{\max}}$, and $T=t\omega_{pi}$ to normalize the equations. where $S=\sqrt{\frac{-4\varepsilon_0\varphi_t}{en_0}}$, is the overlapped sheath radius, $v_{\max}=\sqrt{\frac{-2e\varphi_t}{n_i}}$, is the maximum ion velocity, and $\omega_{pi}=\sqrt{\frac{n_0e^2}{\varepsilon_0 m_i}}$, is the ion frequency of plasma. When $n_i\neq0$, equation (5)–(8) change to,

$$\frac{\partial N}{\partial T}+\frac{}{\sqrt{2}}(V_\rho\frac{\partial N}{\partial\rho}+N\frac{\partial V_\rho}{\partial\rho}+\frac{NV_\rho}{\rho}+V_z\frac{\partial N}{\partial Z}=N\frac{\partial V_z}{\partial Z})=0 \tag{9}$$

$$\frac{\partial V_\rho}{\partial T}+\frac{1}{\sqrt{2}}V_\rho\frac{\partial V_\rho}{\partial\rho}+\frac{1}{\sqrt{2}}V_z\frac{\partial V_\rho}{\partial Z}=\frac{1}{2\sqrt{2}}\frac{\partial\phi}{\partial\rho} \tag{10}$$

$$\frac{\partial V_z}{\partial T}+\frac{1}{\sqrt{2}}V_\rho\frac{\partial V_z}{\partial\rho}+\frac{1}{\sqrt{2}}V_z\frac{\partial V_z}{\partial Z}=\frac{1}{2\sqrt{2}}\frac{\partial\phi}{\partial Z} \tag{11}$$

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\phi}{\partial\rho}) + \frac{\partial^2\phi}{\partial Z^2} = 4(N - \exp(\frac{e\varphi_t}{kT_e}\phi)) \tag{12}$$

To linear Poisson's equation, assume ϕ_{last} is the potential distribution at last time step, then if

$$\left|\frac{e}{\varphi_t}kT_e\phi - \frac{e\phi_t}{kT_e}\phi_{last}\right| \ll 1,$$

$$\begin{aligned}\exp(\frac{e\varphi_t}{kT_e}\phi) &= \exp(\frac{e\varphi_t}{kT_e}\phi)\cdot\exp(\frac{e\varphi_t}{kT_e}\phi_{last} - \frac{e\varphi_t}{kT_e}\phi_{last}) \\ &\approx \exp(\frac{e\varphi_t}{kT_e}\phi_{last})(1 + \frac{e\varphi_t}{kT_e}\phi - \frac{e\varphi_t}{kT_e}\phi_{last})\end{aligned} \tag{13}$$

and Poisson's equation changes to,

$$\frac{1}{\rho}\frac{\partial}{\partial\rho}(\rho\frac{\partial\phi}{\partial\rho}) + \frac{\partial^2\phi}{\partial Z^2} = 4(N - \exp(\frac{e\varphi_t}{kT_2}\phi_{last})(1 + \frac{e\varphi_t}{kT_e}\phi - \frac{e\varphi_t}{kT_e}\phi_{last}) \tag{14}$$

Digitizing equation (14) and equations (9)–(11) in the simulation area, and solving the digitized equations, principle of ion density and velocity evolution can be got.

Simulation was done on bores of different size. Left boundary of the simulated region is the bore's axis, down boundary is the symmetry plane of the bore, and the right and upper boundary is plasma region far enough. Far enough means that the boundaries are chosen so that the sheath will not reach them in the simulation process, and their states will not affect the implant process. The boundary conditions are as follows. On the upper and right boundary, $\phi|_\infty=0$, $N|_\infty=1$, $V_\rho|_\infty=0$, $V_z|_\infty$. On the left boundary, $\frac{\partial\phi}{\partial\rho}|_{\rho=0}=0$, $\frac{\partial N}{\partial\rho}|_{\rho=0}=0$, $V_\rho|_{\rho=0}=0$, and this is determined by the symmetry of the bore. On the down boundary, $\frac{\partial\phi}{\partial Z}|_{Z=0}=0$, $\frac{\partial N}{\partial Z}|_{Z=0}=0$.

3. Result and Discussion

Fig.1 shows retained dose and impact energy on inner surface versus radius of the bore. Pulse duration is 100. It is very evident that if radius of the bore is almost the "sheath overlapping radius"[2], the retained dose and impact energy are both lowest. With increasing of radius of the bore, both retained dose and impact energy increase. This is

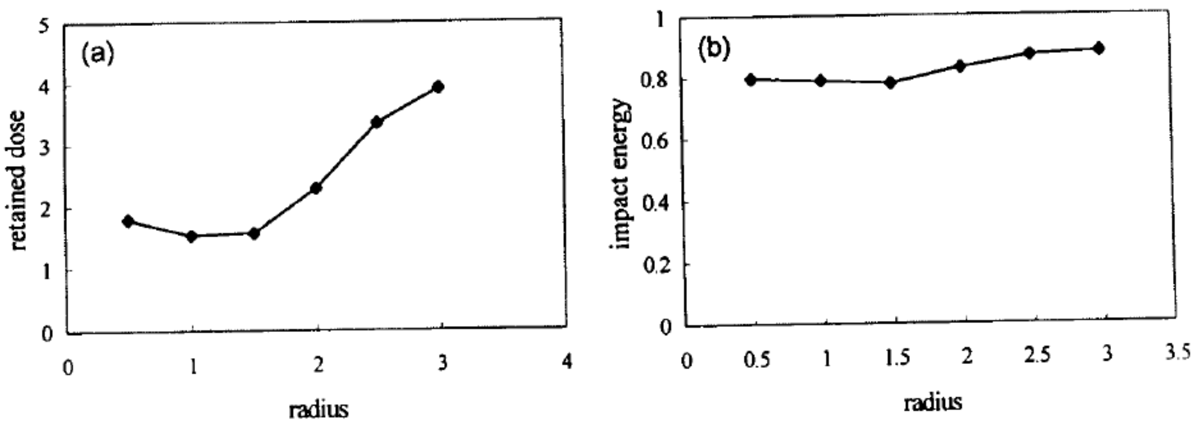

Fig.1 Retained dose and impact energy on inner surface versus radius of the bore:
(a) Retained dose on inner surface versus radius of the bore;
(b) Impact energy on inner surface versus radius of the bore.

the direct result of postponed sheath overlapping. Fig.2 shows evolution of retained dose on inner surface versus time of different radius. It can be found that, for bore of little radius (R=0.5), sheath overlaps after the pulse is set up, so ions on inner surface are mainly from outside the bore. For there is enough time for ions come into the bore, the retained dose is not the lowest. While for R=1.5, most of the pulse duration is consumed by the process of sheath overlapping, so the retianed dose and impact energy are lowest. For bore of large radius, sheath does not overlap during implantation, so retained dose and impact energy increase all the time.

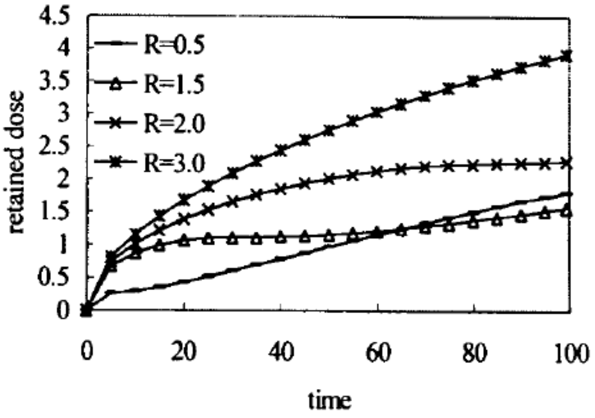

Fig.2 Retained dose on inner surface versus time of different radius.

Fig.3 shows evolution of retained dose and impact energy on inner surface versus the bore's length. With increase of the bore's length, retained dose and impact energy decrease. For the bore of little length, it is easy for ions accelerated by sheath at edge of the bore to get into the bore. This not only keeps ion density in the bore from decreasing too fast but also postpones sheath overlap. These two aspects form the higher retained dose and impact energy together.

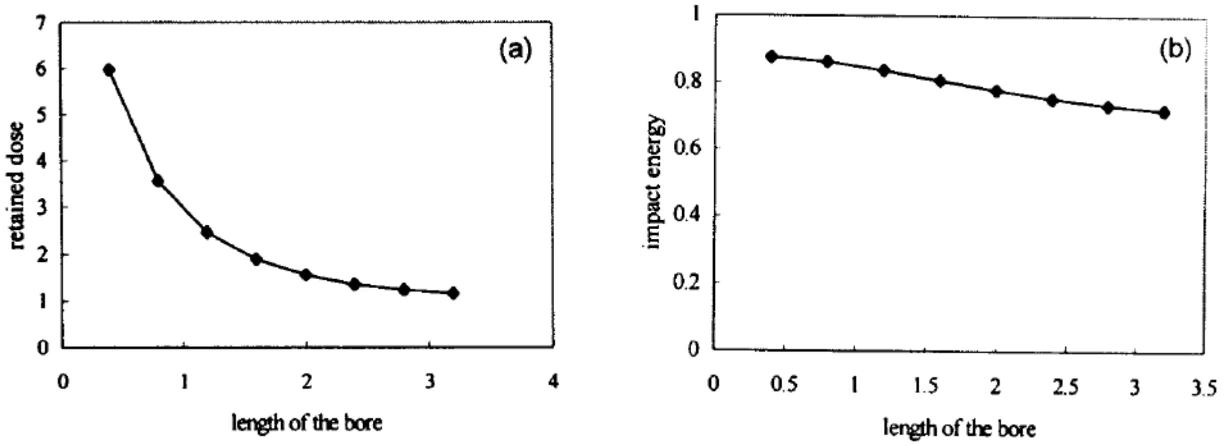

Fig.3 Retained dose and impact energy on inner surface versus the bore's length:
(a) Retained dose on inner surface versus the bore's length;
(b) Impact energy on inner surface versus the bore's length.

Dimension influences not only retained dose and impact energy on inner surface, but also uniformity of retained dose. Fig.4 shows distribution of retained dose on inner surface of bores of different radius at T=100. Though the distribution trend of retained dose is similar, uniformity is different. Maximum relative difference of retained dose is shown in Fig.5. Uniformity of little bore (R=0.5) and large bore (R=3.0) are better than the medium one. It is worst when R=1.5. This is because sheath in different bore overlaps at different time. For the little bore (R=0.5), sheath in the bore overlaps at the beginning,

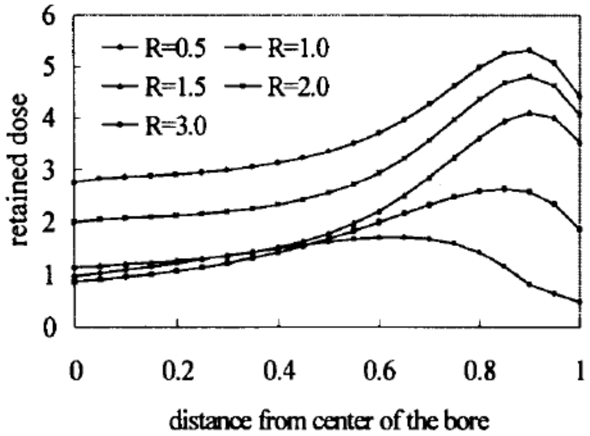

Fig.4 Distribution of retained dose on inner surface of bores of different radius at T=100.

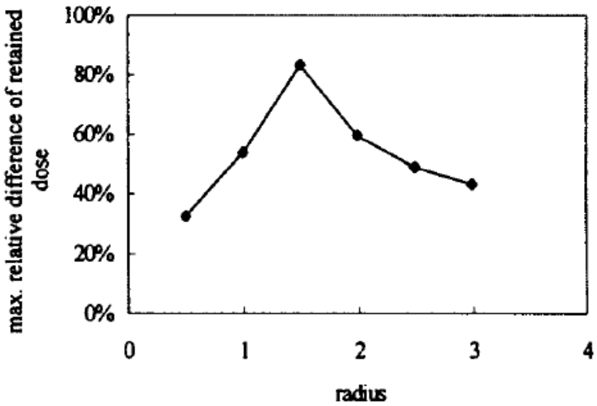

Fig.5 Maximum absolute difference of retained dose versus radius of the bores.

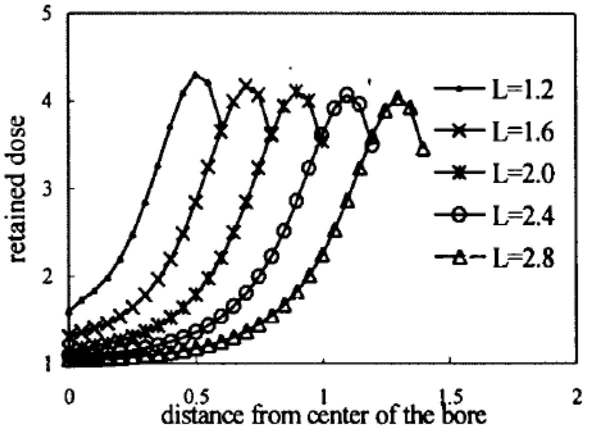

Fig.6 Distribution of dose on inner surface of bores of different length at T=100.

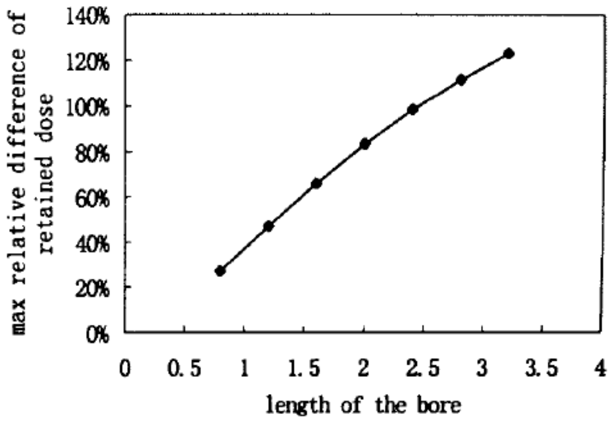

Fig.7 Maximum relative difference of retained dose versus length of the bore.

and there is no sheath expansion. The implanted ions are mainly from out of the bore, so the retained dose is comparatively uniform. While for the large bore, sheath does not overlap till end of implantation, and implanted ions are mainly primary ions in the bore, so it is uniform too. For the medium size bore (R=1.5), sheath overlaps before end of the pulse, and the implanted ions include not only the ones primarily in the bore but also the ones out of the bore. So more ions are implanted near edge of the bore, and the retained dose is not uniform. Fig.6 shows distribution of dose on inner surface of bores of same radius but different length at T=100. Fig.7 is maximum relative difference of retained dose versus length of the bore. With increase of length of the bore, uniformity gets worse. If ions from out of the bore were not considered, sheath expansion and overlapping should be the same. But ions come from out of the bore do influence ion density and velocity in the bore, and further sheath expansion and overlapping. For the short bore, ions are easy to reach center of the bore, and axial ion flux exists even before sheath overlapping. This lessen difference of retained dose of edge and center, so uniformity is good. While for the long bore, ions are difficult to reach center of the bore through electric field. So only after sheath overlapping and electric field getting weaker, the axial ion flux appears. This enlarge difference of retained dose of edge and center, so uniformity is not good.

4. Conclusion

Two–dimensional simulations were done on different size bores, and retained dose, impact energy and uniformity were analyzed in this paper. The result showed that, retained dose, impact energy and uniformity were all worse when radius of the bore was almost the same size of "sheath overlapping radius", and all getting worse with increasing of length of the bore.

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