JOURNAL OF SPACECRAFT AND ROCKETS
Vol. 43, No. 3, May–June 2006

Simulation of Electron Radiation on Outgassing of Spacecraft Materials

R. H. Khassanchine,* A. N. Timofeev,† A. N. Galygin,‡ and V. I. Kostiuk§
Joint-Stock Company "Kompozit," 141070, Korolev, Russia

In this work, mathematical models of influence of electron radiation on outgassing of spacecraft materials and condensation of generated volatile products are given. Data of experimental investigations of outgassing kinetics of materials irradiated with different electron flows and results of numerical analysis of the processes are presented.

Nomenclature

A_{i0}, A_{i1} = parameters depending on composition of material and electron radiation spectrum
a_i = parameter defining influence of electron radiation on desorption kinetics of i component
$C_i(x, t)$ = concentration of i component of outgassing process in material
D_i = effective coefficient of diffusion of i component
$F_i(t)$ = dependence of flux of i component emitted from material through the unit of surface on time t
h = thickness of material
k_{ci} = effective coefficient of remission of i component from the surface element
k_i = effective coefficients of desorption of i component
$M_{\mathrm{ci}}(t)$ = dependence of mass of i component deposited on a condensation surface element on time t
$M_{\mathrm{si}}(t)$ = dependence of mass of i component in sample on time t
R_i = concentration of i component in material at initial moment
$S_i^{\mathrm{rad}}(x, t)$ = i-type volatile-product source function determined by influence of electron radiation on material
S_0 = surface area of sample
α_{cs} = geometrical factor that depends on arrangement of volatile-product source with respect to the condensation surface
α_0, α_1 = effective coefficients of linear reduction of absorbed energy in spacecraft coatings from low-energy and high-energy spectrum parts of space electron radiation, respectively
β_i = effective first-order reaction rate with i component
$\delta M_s(t)$ = time dependence of a sample mass loss
λ_k = characteristic value of differential equation
$\sigma_{i\to j}^{\mathrm{rad}}$ = weighting coefficient of radiation-enhanced destruction of i component through j channel
υ = evaporation rate of material
Φ = electron flux
χ_{ci} = chemical reaction rates with involvement of i component on condensation surface
χ_i^{rad} = chemical reaction rates with involvement of i component

Introduction

OUTGASSING of the materials intended for application on outer spacecraft surfaces is the major source of volatile products (VP) that are able to condense on contamination-sensitive surfaces. Outgassing of polymeric materials subjected to electron radiation is the result of their radiochemical decomposition and thermal desorption of generated and existing VP. Deposition of outgassing products is caused by condensation of high-molecular VP and polymerization of low-molecular VP on spacecraft surfaces. The following factors exert influence on radiation-enhanced adsorption, desorption and diffusion, which are the basic mechanisms for VP outgassing and condensation processes that occur in the near-surface layer of a VP source and on condensation surface of individual outgassing components: 1) radiolysis of organic components in material and changes of VP diffusion, desorption and adsorption coefficients; 2) various radiation-induced defects generated on VP condensation surfaces under the action of ionizing radiation; 3) structural changes of the near-surface layers, both the VP sources (for example, loosening) and condensation surfaces; and 4) generation of electric fields as a result of accumulation of volume charge in materials.

Usually, absorbed dose in the near-surface layer of spacecraft materials is determined by the low-energy part of spectrum of space ionizing radiations. The profile of the radiation dose to which the spacecraft external surfaces are subjected can be simulated in laboratory by exerting influence of electron fluxes with different energies upon them.

Outgassing and Condensation Model

From mathematical models discussed in Refs. 1–3, it follows that change of the concentration of i type outgassing component in VP source under the exposure to electron radiation can be described with the help of the differential equation

$$\frac{\partial C_i(x,t)}{\partial t} = D_i \frac{\partial^2 C_i(x,t)}{\partial x^2} - \sum_{j=1}^{M} \sigma_{i\to j}^{\mathrm{rad}} C_i(x,t) - \chi_i^{\mathrm{rad}} C_i(x,t) + S_i^{\mathrm{rad}}(x,t)$$
$$\text{for}\quad x \in (0, h - \upsilon\cdot t), \quad t > 0, \qquad \upsilon \cdot t < h \tag{1}$$

that satisfy the initial condition

$$C_i(x,t)|_{t=0} = R_i, \qquad x \in [0, h] \tag{2}$$

and boundary conditions

$$\left.\left[D_i \frac{\partial C_i(x,t)}{\partial x} + (k_i + a_i) C_i(x,t)\right]\right|_{x = h - \upsilon\cdot t} = 0$$
$$\left. D_i \frac{\partial C_i(x,t)}{\partial x}\right|_{x=0} = 0, \qquad t > 0 \tag{3}$$

Received 30 December 2004; revision received 22 August 2005; accepted for publication 24 September 2005. Copyright © 2006 by the American Institute of Aeronautics and Astronautics, Inc. All rights reserved. Copies of this paper may be made for personal or internal use, on condition that the copier pay the $10.00 per-copy fee to the Copyright Clearance Center, Inc., 222 Rosewood Drive, Danvers, MA 01923; include the code 0022-4650/06 $10.00 in correspondence with the CCC.

*Head of Laboratory, 4, Pionerskay Street, Moscow Region.

†First Deputy Director General, 4, Pionerskay Street, Moscow Region.

‡Head of Department, 4, Pionerskay Street, Moscow Region.

§Senior Research Engineer, 4, Pionerskay Street, Moscow Region.

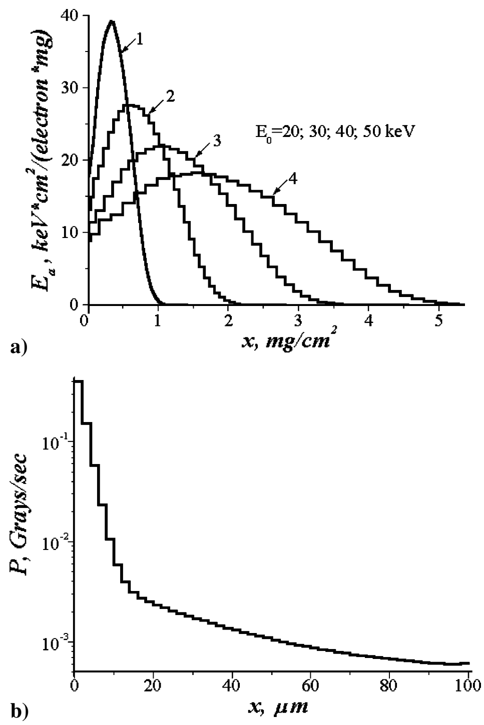

Fig. 1 Distribution of the absorbed energy in EKOM-1: a) for various values of electron energies in laboratory experiments: 1, 20 keV; 2, 30 keV; 3, 40 keV; and 4, 50 keV; and b) in material that is in service in GEO.

To determine the form of the source function, we have calculated, with the use of the Monte Carlo method, basic characteristics concerning interaction of electron radiation with materials under study. Figure 1 shows curves of distributions of absorbed energies in EKOM-1 polymer-based white conductive paint.[4] Curves in Fig. 1a give a distribution of the absorbed energy E_a for various values of electron energies in laboratory experiments; the curve in Fig. 1b gives a rough distribution of the absorbed dose P of electron radiation per time when material is in service in geostationary (GEO) orbit.

It was found from the computational results of absorbed energy of electron radiation in spacecraft coatings when in service that the VP source function can be represented as follows:

$$S_i^{\mathrm{rad}}(x,t)_i = A_{i0}\exp[\alpha_0(x+\upsilon\cdot t-h)] + A_{i1}\exp[\alpha_1(x+\upsilon\cdot t-h)] \tag{4}$$

Parameters A_{i0}, A_{i1} are equal in values to the ratio of absorbed dose rate in the near-surface layer of material to average energy required to generate an i-type VP molecule in material being under exposure to low-energy and high-energy spectrum parts of space electron radiation, respectively.

To calculate numerically VP distribution within the sample under test if exposed to electron radiation, we have found solution of Eqs. (1–3). As an example, next is given a solution for $\upsilon = 0$ where electron radiation has exerted influence on a sample of material before the time point t_0 and has stopped after it:

$$C_i(x, t \le t_0) = 2\sum_{k=1}^{\infty}\left\{F_k \exp\left(-b_i^0 t\right) + (G_{k,0} + G_{k,1}) \times \left[1 - \exp\left(-b_i^0 t\right)\right]\right\}\cos\lambda_k x$$

$$F_k = R_i \frac{\sin\lambda_k h}{\lambda_k}\frac{k_i^{0^2} + (\lambda_k D_i)^2}{k_i^0 D_i + h\left(k_i^{0^2} + (\lambda_k D)^2\right)}$$

$$G_{k,j} = A_j \frac{\lambda_k \sin\lambda_k h + \alpha_j\cdot\cos\lambda_k h - \alpha_j\exp(-\alpha_j\cdot h)}{h\cdot\left(\alpha_j^2 + \lambda_k^2\right)\cdot b_i^0}, \quad j = 0, 1$$

$$C_i(x, t > t_0) = \sum_{n=1}^{\infty} B_n \exp(-b_i\tau)\cdot\cos\lambda_n x$$

$$B_n = \frac{k_i^2 + \lambda_n^2 D_i^2}{k_i D_i + h\left(\lambda_n^2 D_i^2 + k_i^2\right)}\cdot\sum_{k=1}^{\infty} A_k^0 \cdot\left[\frac{\sin(\lambda_k - \lambda_n)h}{\lambda_k - \lambda_n} + \frac{\sin(\lambda_k + \lambda_n)h}{\lambda_k + \lambda_n}\right]$$

$$A_k^0 = 2\sum_{k=1}^{\infty}\left\{F_k\exp\left(-b_i^0 t_0\right) + (G_{k,0} + G_{k,1})\left[1 - \exp\left(-b_i^0 t_0\right)\right]\right\} \tag{5}$$

where the upper index 0 is attributed to values of parameters existing before the time point t_0:

$$\tau = t - t_0, \qquad b_i^0 = \beta_i^0 + \lambda_k^2 D_i$$

$$b_i = \beta_i + \lambda_n^2 D_i, \qquad k_i^0 = k_i + a_i$$

β_i^0, β_i are effective first-order reaction rates that occur in material

$$\beta_i^0 = \sum_{j=1}^{M}\sigma_{i\to j}^{\mathrm{rad}} + \chi_i^{\mathrm{rad}}, \qquad \beta_i = \sum_{j=1}^{M}\sigma_{i\to j} + \chi_i$$

and λ_k, λ_n are solutions of appropriate equations:

$$tg\lambda_k h = k_i^0 \big/ (\lambda_k D_i), \qquad tg\lambda_n h = k_i/(\lambda_n D_i)$$

Having found the distribution $C_i(x,t)$ of i component in a sample from Eqs. (1–3), dependences of VP mass in material and the flux through the unit surface of material-vacuum boundary on time t are, respectively, determined from the following expressions:

$$M_{\mathrm{si}}(t) = S_0\int_0^{h-\upsilon\cdot t} C_i(x,t)\,\mathrm{d}x$$

$$F_i(t) = (\upsilon + k_i + a_i)C_i(h - \upsilon\cdot t, t) \tag{6}$$

where $C_i(h - \upsilon t, t)$ is the concentration of i component in the near-surface layer of material at time t.

When studying outgassing kinetics of materials in onboard or laboratory experiments, the total VP flux

$$F_{\mathrm{total}}(t) = \sum_i^N F_i(t)$$

is usually observed. Part of this flux is deposited on a sensitive surface of the quartz microbalance that is intended to study outgassing kinetics of polymeric materials. Deposition rate depends on composition and energies of molecular flux components as well as on surface condition, temperature, and space environment (for example, electromagnetic or ionizing radiations).

Rate of change of i-component mass $M_{\mathrm{si}}(t)$ in sample and mass $M_{\mathrm{ci}}(t)$ deposited on unit area of condensation surface by time t are bound by the following system of equations:

$$\frac{\mathrm{d}M_{\mathrm{si}}(t)}{\mathrm{d}t} = -S_0(\upsilon + k_i + a_i)C_i(h - \upsilon t, t) \tag{7}$$

$$\frac{\mathrm{d}M_{\mathrm{ci}}(t)}{\mathrm{d}t} = -\alpha_{\mathrm{cs}}\frac{\mathrm{d}M_{\mathrm{st}}(t)}{\mathrm{d}t} - k_{\mathrm{ci}}M_{\mathrm{ci}}(t) - \chi_{\mathrm{ci}}M_{\mathrm{ci}}(t) \tag{8}$$

The outgassing rate of the VP source and deposition and reemission rates on/from the condensation surface respectively are defined mainly by the constants in Eqs. (7) and (8).

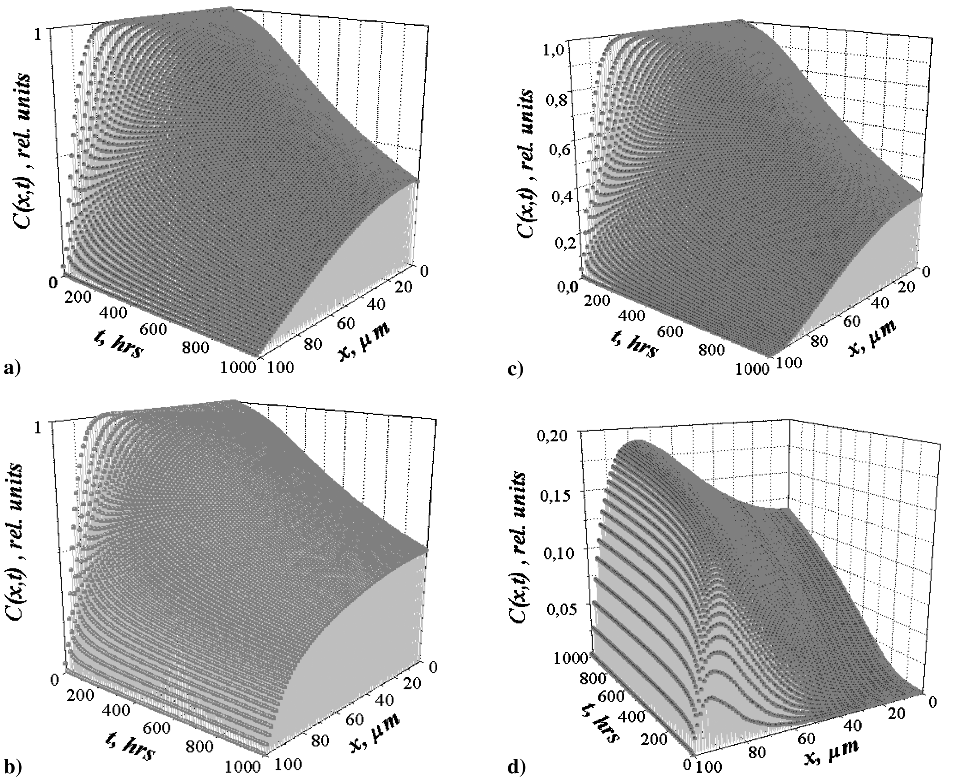

Fig. 2 **Distribution of VP in polymeric composite ($v = 0, \beta = 10^{-7}, \alpha_0 = 0.01, \alpha_1 = 0.01, k = 0.01, D = 0.001$): a) $A_0 = A_1 = 0, R = 1$; b) $A_0 = 0.01, A_1 = 0.002, R = 1$; c) $A_0 = 0.01, A_1 = -0.002, R = 1$; and d) $A_0 = 0.01, A_1 = 0.002, R = 0$.**

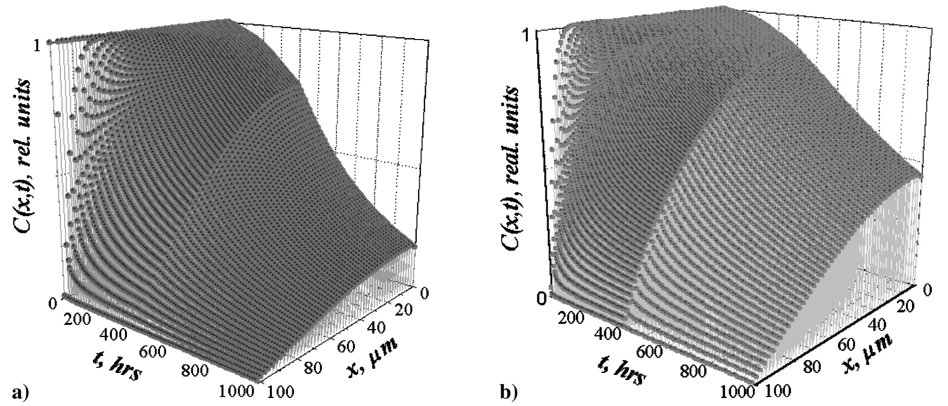

Fig. 3 **Space-time dependences of VP concentrations in material: a) stepwise increase of temperature of material and b) actuation of electron radiation source at $t = 400$ h.**

The total mass of VP deposited on the condensation surface, change of which makes the mass change sensor to response, can be determined by summarizing masses of individual components:

$$M_{\mathrm{c\,total}}(t) = \sum_{n=1}^{N} [M_{\mathrm{cn}}(t) + \Delta_n(t, \chi_{\mathrm{cn}})] \tag{9}$$

where $\Delta_n(t, \chi_{\mathrm{cn}})$ is part of n-component VP mass that has chemically reacted on the condensation surface by time t.

Results of Numerical Computation and Discussion

When calculating, the parameters were chosen in such a way that results would clearly show the outgassing processes described by the model.

Figure 2 shows influence of electron radiation on distribution of VP concentration in material at different model parameters. Figures 2a and 2b show changes of VP concentration in material at equal values of D, k, β and temperatures in material under thermal-vacuum action and when the thermal action is overlapped with the electron radiation influence, respectively. Figures 2a–2d show changes of concentrations of the same type VP in the sample.

Here it is seen that in the second case VP concentration in material becomes greater with time, because of radiation-enhanced generation of VP in material. Figure 2d is a distribution of VP concentration generating in material by electron radiation when there was no type of VP in initial material ($R = 0$); Fig. 2c gives the eventual case when radiation is responsible for the concentrations of some VP components to be reduced.

Figure 3 shows curves of VP concentrations in samples for the cases when temperature of material increases stepwise (Fig. 3a) and electron radiation ceases (Fig. 3b) at $t = 400$ h. In both cases VP concentration in material decreases more rapidly than before $t = 400$ h. It is caused by increasing the outgassing rate in the first case and by the fact that radiolysis products are no more generated in the second case.

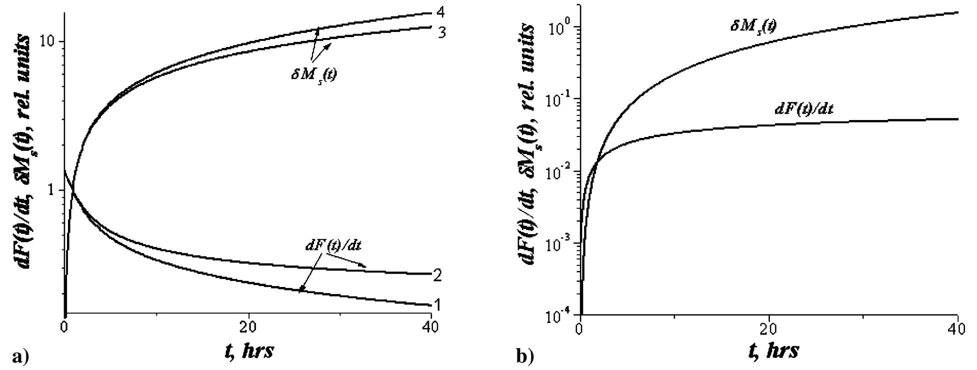

Fig. 4 Outgassing kinetics at different initial VP concentrations for electron action: a) $R = 1$: **1, 3—**$A_0 = 0, A_1 = 0$; **2, 4—**$\alpha_0 = 0.1, \alpha_1 = 0.01, A_0 = 0.01, A_1 = 0.002$; **and b)** $R = 0$: $\alpha_0 = 0.1, \alpha_1 = 0.01, A_0 = 0.01, A_1 = 0.002$.

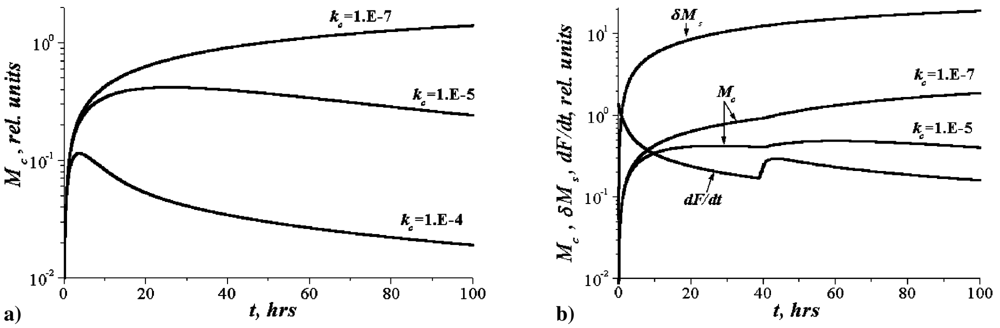

Fig. 5 Change of major parameters defining outgassing and VP condensation processes: a) VP deposition kinetics under thermal-vacuum action for different reemission coefficients k_{ci} **and b) responses of** $\delta M_{\mathrm{si}}(t)$, $\mathrm{d}F_i(t)/\mathrm{d}t$, **and** $M_{\mathrm{ci}}(t)$ **functions on electron radiation activated at** $t_0 = 40$ **h.**

The mass loss function can be determined from

$$\delta M_s(t) = S_0 \sum_{n=1}^{N} \left[hR_n - \exp(\beta_n t) \int_0^{h-v\cdot t} C_n(x,t)\,\mathrm{d}x \right] \qquad (10)$$

where hS_0R_n is the outgassing potential for n component.

Figure 4 shows functions of mass loss $\delta M_s(t)$ and outgassing rate $\mathrm{d}F(t)/\mathrm{d}t$ from the unit surface of VP source under thermal vacuum action and influence of electron radiation at various parameter values $R = 1$ (Fig. 4a) and $R = 0$ (Fig. 4b) with equality of other model parameters ($D = 0.001, k = 0.01, \beta = 10^{-6}$). Outgassing rate is maximum at initial times in the first case, and it grows up starting from zero value in the second case.

Effect of electron radiation that exerts influence on source material at different re-emission coefficients k_{ci} on VP deposition kinetics is given in Fig. 5, showing curves of VP mass deposited on the unit condensation surface $M_{\mathrm{ci}}(t)$ by time t. For great values of k_{ci}, VP deposited mass, initially grown as a result of the significant outgassing rate, reaches maximum and begins to reduce (Fig. 5a). VP mass chemically reacted on the condensation surface can be calculated with the help of Eqs. (7) and (8).

Curves in Fig. 5b represent the responses of the mass loss $\delta M_{\mathrm{si}}(t)$, mass deposited on the unit condensation surface $M_{\mathrm{ci}}(t)$, and outgassing rate $\mathrm{d}F_i(t)/\mathrm{d}t$ functions on a stepwise change of the model parameters resulted from the action of electron radiation at $t_0 = 40$ h. Electron radiation with time leads to the growth of VP concentration in the near-surface layer caused by radiolysis of material that sets off, to some extent, fall of the outgassing rate and leads to increase of the mass loss in VP source.

Experimental Results

Figure 6 shows the experimental curves of outgassing kinetics [functions of mass loss $\delta M_s(t)$] in EKOM-1 samples irradiated by electrons of different fluxes. To show the effect of electron radiation on the process under study, Fig. 6 also gives the experimental curve of outgassing kinetics for the thermal-vacuum influence ($\Phi = 0$). When comparing these curves, one can see that there is no linear dependence between amount of emerged VP and fluence of electron radiation, to which samples of VP sources were subjected.

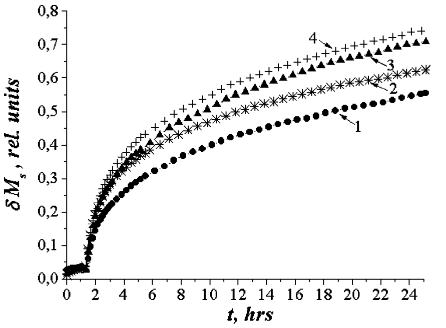

Fig. 6 Outgrassing kinetics of EKOM-1 irradiated by 10-keV electrons of different fluxes: 1, $\Phi = 0$ **(no electron flux); 2,** $\Phi = 5 \times 10^{15}$ **cm**$^{-2}$**, electron flux density** 5×10^{11} **cm**$^{-2}$ **s**$^{-1}$**; 3,** $\Phi = 5 \times 10^{16}$ **cm**$^{-2}$**, electron flux density** 5×10^{12} **cm**$^{-2}$ **s**$^{-1}$**; and 4,** $\Phi = 5 \times 10^{16}$ **cm**$^{-2}$**, electron flux density** 5×10^{11} **cm**$^{-2}$ **s**$^{-1}$**.**

When analyzing experimental data obtained for materials irradiated with electrons of the same flux, it was found that the electron flux density exceeds 10^{12} cm^2 s^{-1}, mass loss of irradiated VP source caused by the outgassing process reduces (see curves 3 and 4, Fig. 6).

Conclusions

Results of the numerical analysis of electron influence on outgassing kinetics show essential dependence of the process on absorbed dose distribution function and parameters of the mathematical model of outgassing.

Experimental results for samples irradiated by different electron flux densities confirmed the hypothesis that outgassing rate of materials depends on both the spectrum and the radiation flux densities.

Analysis of experimental data of outgassing kinetics of electron-irradiated polymeric materials shows that recommended electron flux density in such experiments should not exceed 5×10^{11} cm^2 s^{-1}.

References

[1] Khassanchine, R. H., Grigorevskiy, A. V., and Galygin, A. N., "Some Aspects of Simulation of Outgassing Processes Under Thermal Vacuum Exposure to Coatings Applied to Space Vehicles," *Protection of Materials and Structures from Space Environment*, ICPMSE-6, Toronto, 2002, pp. 327–334.

[2] Kostiuk, V. I., and Khassanchine, R. H., "On Simulation of Outgassing Processes Under Thermal Vacuum Exposure to Coatings Applied to Space Vehicles," *Cosmonautics and Rocket Engineering*, Vol. 28, No. 3, 2002, pp. 155–163.

[3] Khassanchine, R. H., Grigorevskiy, A. V., and Galygin, A. N., "Simulation of Outgassing Processes and Deposition of Volatile Products Under Thermal Vacuum Exposure to Space Vehicle Coatings," *Journal of Spacecraft and Rockets*, Vol. 41, No. 3, 2004, pp. 384–388.

[4] Grigorevski, A., Gordeev, Y., Gurov, A., Kiseleva, L., and Shuiski, M., "Study of Behaviour of the New Thermal Control Coating EKOM-1 in Flight and Laboratory Experiments Under Exposure to Simulated Separate and Complex Factors of Space Environment," *Proceedings of 8th International Symposium on "Materials in Space Environment" and 5th International Conference on "Protection of Materials and Structures from LEO Space Environment,"* Arcachon, France, 2000.

D. Edwards
Associate Editor