THE APPROXIMATE REPRESENTATION OF THE TRANSFORMANT OF A SINGLE REFLECTION

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An analysis of the general formula for the transformant of a single reflection derived in [1] is presented. One of the approximations of the general formula most convenient from the point of view of computer programing is considered. The question of the error characterizing this approximation is examined, in particular, what conditions have to be satisfied so as to reduce this error below a certain preassigned value.

The transformant of a single reflection is one of the most important parameters characterizing the interaction of a rarefied gas with a solid surface [2]. The general formula of the transformant for reflection from a uniform, anisotropic, differentiable random surface was derived in [1]. However, the direct use of this formula is impeded by its fairly complicated expression for the probability of an intersection between the surface and the trajectory of a gas particle:

$$I(T)=\int\limits_{\dot{f}(t_0)}^{\infty} \rho\,[f(t_0),\ \dot{\xi}(t_0)\,|\,S(T)]\,[\,\dot{\xi}(t_0)-\dot{f}\ (t_0)]\,d\,\dot{\xi}\,(t_0) \tag{1}$$

Here ξ (t) is a random function characterizing the surface in the direction t, f(t) is a function describing the trajectory of the gas particle, t_0 is a fixed point (or moment) on the t axis; $\dot{\xi}$ (t_0) and $\dot{f}$ (t_0) are derivatives of the functions ξ (t) and f (t) taken at the instant t_0, T is a certain known interval preceding the instant t_0, S(T) is the condition that in the interval T, $\xi\,(t) < f\,(t)$, $\rho\,[f\,(t_0),\ \dot{\xi}\,(t_0)\,|\,S\,(T)]$ is the nominal density of the combined distribution of ξ (t_0) and $\dot{\xi}$ (t_0) for a value of $\xi\,(t_0)=f\,(t_0)$ and subject to the condition S(T).

In order to bring Eq. (1) to a form convenient for numerical calculations, it is easiest to use the approximation [1] according to which T is limited by the correlation interval T_k while S(T) is replaced by the condition that $\xi\,(t)<f\,(t)$ at a finite number of points $t_i \in T$, i = 1–n. If the points are taken at identical distances from one another and the first of them coincides with the beginning of the interval T while the final one coincides with the end of this interval, Eq. (1) may be written in the form

$$I(T)\approx I(t_i,\,i=1-n)=\int\limits_{\dot{f}(t_0)}^{\infty}\rho\,[f(t_0),\,\dot{\xi}(t_0)\,|\,S(t_i,\,i=1-n)]\,[\,\dot{\xi}(t_0)-\dot{f}\ (t_0)]\,d\,\dot{\xi}\,(t_0)=\int\limits_{\dot{f}(t_0)}^{\infty}\int\limits_{-\infty}^{f(t_1)}\cdots\int\limits_{-\infty}^{f(t_n)}\rho\,[f(t_0),\,\dot{\xi}(t_0),$$

$$\xi(t_1),\ldots,\xi(t_n)]\,[\,\dot{\xi}(t_0)-\dot{f}\ (t_0)]\,d\xi(t_n)\ldots d\xi(t_1)\,d\,\dot{\xi}\,(t_0)\left\{\int\limits_{-\infty}^{f(t_1)}\cdots\int\limits_{-\infty}^{f(t_n)}\rho\,[\xi(t_1),\ldots,\xi(t_n)]\,d\xi(t_n)\ldots d\xi(t_1)\right\}^{-1} \tag{2}$$

This form already allows reasonably simple computer programing, either by the expansion of the multidimensional integrals in convergent series of tetrachoric functions [3] or by means of the Monte Carlo method [4].

By taking the number n fairly large we might reduce the error arising from the substitution of (2) for (1) to practically zero, if it were not for the fact that the computing time rises sharply with increasing n. Hence one of the main problems arising in this connection with this approximation lies in estimating the minimum number of points required to prevent the error of the approximation

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$$\Delta \doteq \frac{I(t_i,\ i=1-n)-I(T)}{I(t_i,\ i=1-n)} \tag{3}$$

from exceeding an acceptable value. This paper is devoted to a solution of this problem. In deriving the formulas here employed, in individual cases we have made use of data obtained from an analysis of profile recordings of standard samples with surface finishes of classes 6-14 (All-Union State Standard 9378-60).

Let us therefore consider the problem of the minimum number of points, regarding the surface as a uniform, normal, differentiable random field and using the following terminology [5]. Any intersection of the particle trajectory $f(t)$ by the random function $\xi(t)$ we shall call an overshoot. If the intersection proceeds from bottom to top we shall call the overshoot positive, if from top to bottom we shall call it negative. The distance between neighboring overshoots of different signs we shall call the duration of the overshoot. If in a specified interval two, three, or more intersections occur, we shall speak of a twofold, threefold, and so on overshoot in this interval. Furthermore let A be the average number of realizations having a positive overshoot in the infinitely small interval $(t_0,\ t_0+dt_0)$ and B be the average number of realizations passing below the particle trajectory in the same interval. We separate these realizations into three types depending on the conditions $S(t_i,\ i=1\text{-}n)$ and $S(T)$ (Fig. 1):

1) realizations satisfying both conditions $(A_1,\ B_1)$;
2) realizations satisfying only the first condition $(A_2,\ B_2)$;
3) realizations satisfying neither of the conditions $(A_3,\ B_3)$.

Using these forms of nomenclature and also allowing for the fact that the instant t_1 directly precedes the instant t_0, while in an infinitely short interval $(t_0,\ t_0+dt_0)$ the quantities A, A_1, A_2, and A_3 are infinitely small compared with B, B_1, B_2, and B_3, we obtain

$$I(t_i,\ i=1-n)\,dt_0=(A_1+A_2)/(B_1+B_2),\quad I(T)\,dt_0=A_1/B_1$$

whence

$$|\Delta|=\left|\left(\frac{A_1+A_2}{B_1+B_2}-\frac{A_1}{B_1}\right)\Big/\left(\frac{A_1+A_2}{B_1+B_2}\right)\right|=\left|\frac{A_2}{A_1+A_2}-\frac{A_1}{A_1+A_2}\,\frac{B_2}{B_1}\right|<\max(\Delta_1,\Delta_2) \tag{4}$$

where

$$\Delta_1=A_2/(A_1+A_2),\qquad \Delta_2=B_2/B_1 \tag{5}$$

Let us first estimate the value of Δ_2. It is easy to see that this equals

$$\Delta_2=pr/(1-pr) \tag{6}$$

where pr is the probability of the appearance of even overshoots in the short intervals $\Delta t_i=(t_{i-1},\ t_i)$, $i=2\text{-}n$ subject to the condition $S(t_i,\ i=1\text{-}n)$. Remembering that in such intervals the probability of the appearance of repeated overshoots falls rapidly as their multiplicity increases, we may in the present case confine ourselves to considering simple twofold overshoots.

Let us first estimate the probability of the appearance of an overshoot of this kind in the interval Δt_i subject to the condition $[S(t_{i-1}),\ S(t_i)]$.

Let the overshoot start at the instant τ_1 and end at the instant τ_2. We denote the unknown probability by $p_{\Delta t_i}$ and the density by $W(\tau_1,\ \tau_2)$; then we have

$$p_{\Delta ti}=\int_0^{\Delta t_i}d\tau_1\int_{\tau_1}^{\Delta t_i}W(\tau_1,\tau_2)\,d\tau_2 \tag{7}$$

Further, let

$$\xi(\tau_1)=\xi_1,\qquad \xi(\tau_2)=\xi_2,\quad f(\tau_1)=f_1,\quad f(\tau_2)=f_2,\quad \dot f_1=\dot f_2=\dot f$$

Then [5]

$$W(\tau_1,\tau_2)=\int_{\dot f}^{\infty}\int_{-\infty}^{\dot f}(\dot\xi_1-\dot f)(\dot f-\dot\xi_2)\,\rho(f_1,f_2,\dot\xi_1,\dot\xi_2)\,d\dot\xi_2\,d\dot\xi_1 \tag{8}$$

where $\rho(f_1,\ f_2,\ \dot\xi_1,\ \dot\xi_2)$ is the density of the combined distribution of the quantities ξ_1, ξ_2, $\dot\xi_1$, and $\dot\xi_2$ for values of $\xi_1=f_1$, $\xi_2=f_2$.

We may show that the quantity $W(\tau_1,\ \tau_2)$ becomes a maximum if the trajectory of the particle is turned around a singular point lying at a height of $(f_1+f_2)/2$ before coincidence with the horizontal level (Fig. 2).

Enumerating the quantities ξ_1, ξ_2, $\dot{\xi}_1$ and $\dot{\xi}_2$ in the order of writing and allowing for the normality of $\xi(t)$, we obtain

$$W(\tau_1,\tau_2)=\frac{1}{4\pi^2M^{1/2}}\int_{\dot f}^{\infty}\int_{-\infty}^{\dot f}(\dot\xi_1-\dot f)(\dot f-\dot\xi_2)\exp\Big[-\frac{1}{2M}(M_{11}f_1^2+M_{22}f_2^2+ + M_{33}\dot\xi_1^2+M_{44}\dot\xi_2^2+2M_{12}f_1f_2+2M_{13}f_1\dot\xi_1+2M_{14}f_1\dot\xi_2+2M_{23}f_2\dot\xi_1+ + 2M_{24}f_2\dot\xi_2+2M_{34}\dot\xi_1\dot\xi_2)\Big]d\dot\xi_2d\dot\xi_1 \tag{9}$$

where

$$M=\begin{vmatrix}d_{11}&d_{12}&d_{13}&d_{14}\\d_{21}&d_{22}&d_{23}&d_{24}\\d_{31}&d_{32}&d_{33}&d_{34}\\d_{41}&d_{42}&d_{43}&d_{44}\end{vmatrix}$$

Here d_{ij} are the second central moments of the distribution of the random quantities with numbers i and j; M_{ij} are the algebraical complements of the elements d_{ij} in the determinant M. Let us denote the horizontal level $(f_1+f_2)/2$ by c, the interval $\tau_2-\tau_1$ by τ, and let us transform to new variables $u=\dot\xi_1-\dot f$, $v=\dot\xi_2-\dot f$. Then remembering that

$$M_{22}=M_{11},\quad M_{44}=M_{33},\quad M_{23}=-M_{14},\quad M_{24}=-M_{13}$$

we obtain

$$W(\tau_1,\tau_2)=\frac{1}{4\pi^2M^{1/2}}\exp\Big\{-\frac{\dot f^2}{M}\Big[M_{33}+M_{34}-\tau(M_{13}+M_{14})+ +\frac{\tau^2}{4}(M_{11}-M_{12})\Big]\Big\}\exp\Big[-\frac{c^2(M_{11}+M_{12})}{M}\Big]F(\tau,\dot f) \tag{10}$$

where

$$F(\tau,\dot f)=\int_0^{\infty}\int_0^{-\infty}\exp\Big\{-\frac{\dot f}{2M}[2(M_{33}+M_{34})-\tau(M_{13}+M_{14})](u+v)\Big\}\times \times\exp\Big\{-\frac{1}{2M}[M_{33}(u^2+v^2)+2M_{34}uv+2c(M_{13}-M_{14})(u-v)]\Big\}uvdudv \tag{11}$$

The expression

$$\Big\{-\frac{\dot f^2}{M}\Big[M_{33}+M_{34}-\tau(M_{13}+M_{14})+\frac{\tau^2}{4}(M_{11}-M_{12})\Big],$$

under the sign of the exponential in (10) cannot be positive [otherwise for vertical trajectories ($\dot f=\pm\infty$) the value of $W(\tau_1,\tau_2)$ would be equal to infinity]. Hence

$$W(\tau_1,\tau_2)\leqslant\frac{1}{4\pi^2M^{1/2}}\exp\Big[-\frac{c^2(M_{11}+M_{12})}{M}\Big]F(\tau,\dot f) \tag{12}$$

Let us find the maximum value of the integral $F(\tau,\dot f)$. Differentiating this with respect to $\dot f$ we obtain

$$\frac{\partial F(\tau,\dot f)}{\partial\dot f}=\int_0^{\infty}\int_0^{-\infty}\frac{1}{2M}[2(M_{33}+M_{34})-\tau(M_{13}+M_{14})](u+v)\times \times\exp\Big\{-\frac{\dot f}{2M}[2(M_{33}+M_{34})-\tau(M_{13}+M_{14})](u+v)\Big\}\exp\Big\{-\frac{1}{2M}\times \times[M_{33}(u^2+v^2)+2M_{34}uv+2c(M_{13}-M_{14})(u-v)]\Big\}uvdudv \tag{13}$$

In Cartesian coordinates the range of integration of the right-hand side of (13) occupies the fourth quadrant (Fig. 3). Let us divide this in two with the bisectrix OO_1 and compare the values of the integrand function at the points $A_1(a,-b)$ and $A_2(b,-a)$ lying symmetrically with respect to the bisectrix. It is not difficult to see that the sum of the values at these points vanishes if $\dot f=0$ and has a constant sign if $\dot f\neq0$. Further remembering that the range of integration in (13) may be represented as a set of points of the form A_1 and A_2, symmetrical with respect to the bisectrix OO_1, and replacing the actual integration by summation with respect to these points, we finally obtain

$$\frac{\partial F(\tau,\dot f)}{\partial\dot f}=\begin{cases}0, & \text{if}\quad \dot f=0\\ \neq0, & \text{if}\quad \dot f\neq0\end{cases}$$

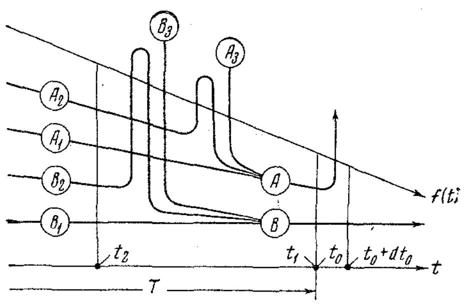

Fig. 1

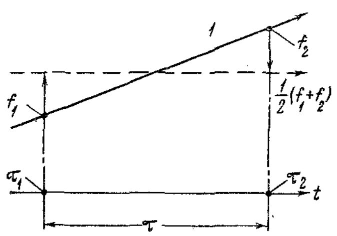

Fig. 2

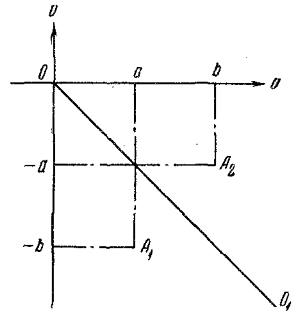

Fig. 3

TABLE 1

N_1/N_0	n, $\Delta = 0.01$	$\Delta = 0.02$	$\Delta = 0.05$	$\Delta = 0.10$
1	1	1	1	1
2	17	12	8	6
3	27	19	13	10
4	36	26	17	13
5	46	33	21	16
6	55	39	26	19
7	64	46	30	22
8	73	52	34	25
9	83	59	38	28
10	92	66	42	31

Thus the function $F(\tau, \mathring{f})$ has a single extremum with respect to the variable $\mathring{f}$ at zero. It is clear that this is a maximum, otherwise we should have one of the conditions

$$F(\tau, 0) < F(\tau, \infty), \quad F(\tau, 0) < F(\tau, -\infty),$$

Yet both of these are impossible, since $F(\tau, \infty) = F(\tau, -\infty) = 0$ and for any finite value of $\mathring{f}$ the quantity $F(\tau, \mathring{f}) > 0$.

The foregoing arguments enable us to write inequality (13) thus:

$$W(\tau_1\tau_2) \leqslant \frac{1}{4\pi^2 M^{1/2}} \exp\left[-\frac{c^2(M_{11}+M_{12})}{M}\right] F(\tau, 0) = \int_0^{\infty}\int_0^{-\infty} \dot{\xi}_1\dot{\xi}_2 \rho(c, c, \dot{\xi}_1, \dot{\xi}_2)\, d\dot{\xi}_2 d\dot{\xi}_1 \tag{14}$$

Q.E.D.

The integral at the end of Eq. (14) may be found by using [5]. After certain transformations we obtain

$$\int_0^{\infty}\int_0^{-\infty} \dot{\xi}_1\dot{\xi}_2 \rho(c, c, \dot{\xi}_1, \dot{\xi}_2)\, d\dot{\xi}_2 d\dot{\xi}_1 = \frac{M_{33}}{2\pi\sigma^6(1-R^2)^{3/2}} \exp\left[-\frac{1}{1+R}\left(\frac{c}{\sigma}\right)^2\right]\Psi(r, h) \tag{15}$$

$$\sigma = k(0), \qquad R = R(\tau) = k(\tau)/k(0)$$

where $k(\tau)$ is the correlation function of $\xi(t)$, and

$$r = \frac{M_{34}}{M_{33}}, \quad h = \frac{c\sigma^2(M_{13}-M_{14})}{M_{33}-M_{34}}\left(\frac{1-R^2}{M_{33}}\right)^{1/2},$$

$$\Psi(r, h) = (r+h^2)E(r, h) + \frac{(1-r^2)^{1/2}}{2\pi}\exp\left(-\frac{h^2}{1+r}\right) - \frac{h}{\sqrt{2\pi}}\exp\left(-\frac{h^2}{2}\right)[1-\Phi(a)],$$

$$E(r, h) = \frac{1}{2\pi(1-r^2)^{1/2}}\int_h^{\infty}\int_h^{\infty}\exp\left[-\frac{x^2+y^2-2rxy}{2(1-r^2)}\right]dxdy,$$

$$a = h\left(\frac{1-r}{1+r}\right)^{1/2}, \qquad \Phi(a) = \frac{2}{\sqrt{2\pi}}\int_0^a \exp\left(-\frac{x^2}{2}\right)dx$$

We note that the error Δ_2 will only be small (and it is this case which is of practical interest) if the intervals Δt_i are correspondingly small. In any such interval the quantity $R(\tau)$ may be expanded in a Maclaurin series:

$$R(\tau) = \sum_{n=0}^{\infty}\frac{R_0^{(2n)}}{(2n)!}\tau^{2n}, \qquad R_0^{(2n)} = \left.\frac{d^{2n}R(\tau)}{d\tau^{2n}}\right|_{\tau=0} \tag{16}$$

and limited to the first few terms. Remembering furthermore that $(\tau_1, \tau_2) \in \Delta_i$ and also allowing for (14), (15) and the general Rice formula for the average number of zeroes of the derivative $d^n\xi(t)/dt^n$ in unit length [6]

$$N_n = \frac{1}{\pi}\left|\frac{R_0^{(2n+2)}}{R_0^{(2n)}}\right|^{1/2} \tag{17}$$

we easily find

$$W(\tau_1, \tau_2) \lesssim \frac{\pi N_0^3}{8}\left[\left(\frac{N_1}{N_0}\right)^2 - 1\right]\tau\exp\left[-\frac{1}{2}\left(\frac{c}{\sigma}\right)^2\right]\Psi(1, h) \tag{18}$$

where

$$\Psi(1,h)=\frac{1}{2}(1+h^2)[1-\Phi(h)]-\frac{h}{\sqrt{2\pi}}\exp\left(-\frac{h^2}{2}\right),\quad h=\frac{c}{\sigma}\left[\left(\frac{N_1}{N_0}\right)^2-1\right]^{-1/2}$$

Subsequent substitution of (18) into (7) leads to the inequality

$$p_{\Delta t_i}\lesssim\frac{\pi^2N_0^3}{48}\left[\left(\frac{N_1}{N_0}\right)^2-1\right]\Delta t_i^3\exp\left[-\frac{1}{2}\left(\frac{c}{\sigma}\right)^2\right]\Psi(1,h) \tag{19}$$

It may be shown that this inequality remains valid not only for small values of Δt_i but also quite generally for any values. In addition to this, it follows from an analysis of the profile recordings that for real surfaces $N_1/N_0 \geq 1.5$. We may here easily convince ourselves that the right-hand side of inequality (19) reaches its maximum value at the middle level of the surface ($c=0$), whence finally we obtain

$$p_{\Delta t_i}\lesssim\frac{\pi^2N_0^3}{96}\left[\left(\frac{N_1}{N_0}\right)^2-1\right]\Delta t_i^3 \tag{20}$$

We remember that $p\,\Delta t_1$ is the probability of the appearance of a twofold overshoot in a single interval Δt_i subject to the condition $[S(t_{i-1}), S(t_i)]$. If we replace this condition by $S(t_i\ i=1\text{-}n>2)$, analysis of the profile recordings shows that the value of $p\Delta t_1$ becomes somewhat smaller. Allowing for this characteristic and also the earlier arguments regarding even overshoots (on page 683), and using $p\Delta t_i$ to denote the probability of the appearance of such overshoots in a single interval Δt_i subject to the condition $S(t_i,\ i=1\text{-}n)$, we shall have

$$p_{\Delta t_i}r\lesssim\frac{\pi^2N_0^3}{96}\left[\left(\frac{N_1}{N_0}\right)^2-1\right]\Delta t_i^3 \tag{21}$$

Let us consider the case in which the probability $p_{\Delta t_1}r$ is so low that the mean number of corresponding overshoots in the correlation interval Nr is much smaller than unity. Then these overshoots may be regarded as independent and their appearance described by the Poisson law [7]. For the probability pr we here obtain

$$pr=1-\exp(-Nr)\lesssim Nr\lesssim p_{\Delta t_i}rT_k\,/\,\Delta t_i \tag{22}$$

If the surface is normal, then according to [8] $T_K \approx 2/N_0$ and Eqs. (21), (22), and (6) lead to the following result:

$$\Delta_2\lesssim\frac{Nr}{48-Nr}\lesssim\frac{(\pi N_0\Delta t_i)^2\left[(N_1/N_0)^2-1\right]}{48-(\pi N_0\Delta t_i)^2\left[(N_1/N_0)^2-1\right]} \tag{23}$$

We note that the expression so found will only give a comparatively genuine estimate of Δ_2 under the condition $Nr<1$ (or $\Delta_2<0.02$). Otherwise it leads to a severe overestimate of the error in question, and then it may be considered simply as an upper limit beyond which the error cannot under any circumstances pass.

Let us now return to the error Δ_1. This is equal to the probability pr subject to the condition of a positive overshoot at the instant t_0. It is analytically difficult to estimate the effect of this condition. However, direct analysis of the profile recordings shows that this leads to a certain reduction in the probability under consideration and correspondingly to the inequalities

$$\Delta_1<p_4,\qquad \Delta<\Delta_2 \tag{24}$$

Thus on the basis of (4), (23), and (24) we obtain the following estimate of the number of points $t_i \in T$ sufficient for the error of approximation (2) to fall below Δ :

$$n\geqslant 1+2\pi\sqrt{\frac{1+\Delta}{48\Delta}\left[\left(\frac{N_1}{N_0}\right)^2-1\right]} \tag{25}$$

The values of n calculated from Eq. (25) are shown in Table 1. It should nevertheless be emphasized that these values were calculated for the most unfavorable (in the sense of the value of n) trajectories of the molecules and in any specific cases may be considerably reduced [1].

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