9th INTERNATIONAL SYMPOSIUM ON MEASUREMENT AND QUALITY CONTROL (9th ISMQC)
November 21 – 24, 2007, IIT Madras

NUMERICAL GENERATION OF ANISOTROPIC 3D GAUSSIAN ENGINEERING SURFACES

Manesh K.K.[1,*], Ramamoorthy B. [2] and Singaperumal M.[3]
[1] Research scholar, [2] Professor, Manufacturing Engineering Section,
[3] Professor, Precision Engineering & Instrumentation Laboratory,
Department of Mechanical Engineering, Indian Institute of Technology, Madras
Chennai-600 036, India.
[*] Email address:maneshkk@iitm.ac.in

Abstract: *Prediction of the functional behaviour of precision engineering assemblies requires artificially generated three dimensional rough surfaces that have specific prescribed properties. In this paper, an algorithm is developed for the numerical generation of three dimensional anisotropic rough surfaces that have Gaussian height distribution and a given autocorrelation function with prescribed 3D spatial parameters. The procedure employs the non-linear Conjugate Gradient Method (NCGM) in order to cope with the memory and completing time limitations. The simulated surfaces are compared with those generated by 2-D Digital Filter method. The results show that both the methods can adequately produce rough surfaces at small correlation distances, where as at higher correlation distances, NCGM yields better results.*
Key words: *Autocorrelation function; Roughness; Spatial parameters; Anisotropy*

1. INTRODUCTION

The functional performance of engineering assemblies is closely linked to the geometric properties of the surfaces of its components. Prediction of the functional behaviour of these assemblies requires input of 3D surface data, which could be obtained from profilometer. But measured profiles cannot be used to determine an optimized surface roughness, in terms of 3D surface roughness parameters, for a specified application. Therefore, a simulation procedure for the generation of arbitrarily defined rough surfaces is needed.

A surface profile, being of random type, can be defined (in a statistical sense) by two characteristics: the height distribution and the autocorrelation function (ACF) (Whitehouse & Archard, (1970)). Hence, random process description of engineering surfaces makes it possible to generate a rough surface by numerical simulation. Patir (Patir, (1978)) proposed the linear transformation of a matrix in order to generate Gaussian rough surfaces that have a specified ACF. A major disadvantage of Patir's method was the storage space and time requirement of the numerical procedure used to solve non-linear system of equations.

Besides, time series modeling and Fourier analysis were also used to generate random rough profiles using autoregressive moving average method (ARMA) and AR time series models. But, as these models consider few order systems, the neighbourhood of the origin of the ACF only is simulated. Hu and Tonder (Hu & Tonder, (1992)) proposed a fast procedure based on 2D digital filter technique using Fourier analysis that also cope with storage space limitation of earlier methods. But this method can be applied for small autocorrelation lengths. As the autocorrelation length increases the deviation of the autocorrelation function become more and more significant. Hence, a procedure that will cope with the storage space and time limitations of the aforementioned surface generation methods and that can be applied to larger autocorrelation distances is required for generating anisotropic Gaussian 3D engineering surfaces.

In this paper, an algorithm has been developed, based on the linear transformation of matrices for generating 3D engineering surfaces numerically. For solving the non linear system of equations, Non linear Conjugate Gradient Method (NCGM) (Bakolas, (2003); Shewchuk) is used, in order to get convergence and minimize the storage requirements. Bakolas (Bakolas, (2003)) used NCGM for surface generation, but the 3D spatial surface roughness parameters are not considered. In the present work, random Gaussian surface data is generated representing the height values with a specified r.m.s value. Further, areal autocorrelation function is used for establishing dependency between the consecutive data points such that the generated surface is in conformance with the machining processes considered. Fast Fourier Transform technique is used to incorporate the areal autocorrelation function to the generated Gaussian surface data.

2. AREAL AUTOCORRELATION FUNCTION

The autocorrelation function describes the general dependence of the values of the data at one position on the values at another position. It provides basic information about the spatial relation and dependence of the data. Most of the statistical parameters of a rough surface can be derived from the two statistical functions namely, frequency density function of height distribution and auto correlation function. Since most engineering surfaces are approximately Gaussian in their roughness height distribution, a meaningful choice of autocorrelation function and its parameters are very important in the numerical generation of 3D Gaussian rough machined surfaces. For 3D surface generation, the ACF may be considered from an areal topographic point of view. Thus, the Areal Autocorrelation Function (AACF) is required. For a homogeneous surface $z(x,y)$, it is defined as

$$R(\tau_x,\tau_y) = E\{z(x,y)z(x+\tau_x, y+\tau_y)\} \qquad (1)$$

Where E is the expectancy (averaging) operator and τ_x and τ_y are the correlation distances. Also, $R(0,0)$ is equal to σ^2, where σ is the r.m.s roughness height. By digital approximation, AACF can be expressed as:

$$R(\tau_i,\tau_j) = \frac{1}{(N-i)(M-j)}\sum_{k=1}^{N-i}\sum_{l=1}^{M-j} z(x_k,y_l)z(x_{k+i},y_{l+j}) \qquad (2)$$

$$i = 0,1,\ \ldots,\ \mathrm{n} < N;\ j = 0,1,\ldots,m < M;\tau_i = i\Delta x;\tau_j = j\Delta y$$

Where n and m are the maximum numbers of the autocorrelation lengths in the x and y directions respectively.

The correlation length of a profile (τ^*) is defined as the length at which the AACF in the direction of the profile decays to a threshold r. Whitehouse et al. (Whitehouse & Archard, (1970)) have defined a threshold value of r=0.1, means the length where the AACF drops to 10% of its original value. Both deterministic and random surfaces may possess isotropic and anisotropic characters. Here, isotropic surface means the one that possess uniform statistical characteristics in all directions, and an anisotropic surface, the one with different statistical characteristics in different directions. Hence for an isotropic machined surface such as an EDM surface, correlation length (τ^*) will be same in all directions, whereas for anisotropic surface like Ground surface, it will be different. As the AACF of a rough surface has been found to be approximately exponential for a variety of engineering surfaces, the necessary variables to prescribe AACF for the generation of anisotropic engineering surfaces are the correlation lengths in two mutually perpendicular directions (τ^*_x, τ^*_y) .

In this study, Ground engineering surfaces are generated, for which an AACF of the form:

$$R(\tau_x,\tau_y) = \sigma^2 \exp\left\{-\left[\left(\frac{\tau_x}{\tau^*_x}\right)^2 + \left(\frac{\tau_y}{\tau^*_y}\right)^2\right]^{1/2}\right\} \qquad (3)$$

3. THREE-DIMENSIONAL SPATIALPARAMETERS

The feasibility and significance of parameters in characterising 3D surface topography are addressed by many researchers (Dong et.al.,(1994); Stout et.al.,(1993)) by conducting experiments on a wide range of engineered surfaces and proposed four parameters for 3D spatial characterization, under the set of so-called Birmingham 3D parameters, namely (i) The fastest decay autocorrelation length (S_{al}) (ii) Texture aspect ratio (S_{tr}) (iii) Density of summits of the surface (S_{ds}), and (iv) Texture direction of the surface (S_{td}). Among these, S_{al} and S_{tr} are particularly relevant to this study as they are more linked to anisotropy and wavelength property of the surface. The S_{al} can be defined as the shortest autocorrelation length in which the AACF decays to a threshold value, r =0.2 in any possible direction. Mathematically it is expressed as;

$$S_{al} = \min(\sqrt{\tau_x^2+\tau_y^2}), \qquad R(\tau_x,\tau_y) \le 0.2 \qquad (4)$$

A large value of S_{al} denotes that the surface is dominated by long wavelength components while a small value of the S_{al} denotes the opposite situation. In general, the ground and honed surfaces have smaller values of S_{al}, whilst the bored and the shaped surfaces have larger values of the S_{al}. For an anisotropic surface S_{al} is in a direction perpendicular to the surface lay.

The S_{tr} can be defined as the ratio of the distance that the normalized AACF has the fastest decay to 0.2 in any possible direction to the distance that the normalized AACF has the slowest decay to 0.2 in any possible direction.

The AACF of a surface which has similar texture aspects in all directions decays similarly along all directions (Dong et.al., (1994)). In principle, S_{tr} has a value between 0 and 1. Larger values of S_{tr}, S_{tr}>0.5, indicates stronger uniform texture aspect in all directions, whereas smaller values, S_{tr}<0.3, indicates stronger long crestness.

Since the exponential autocorrelation function is also found to fit a large number of surfaces (Whitehouse & Archard, (1970)), selection of the correlation distance (τ^*_x, τ^*_y) in Equation (3), for generating an engineered surface should be based on the 3D surface parameters namely S_{al} and S_{tr}. For isotropic surfaces, AACF can be expressed as

$$R(\tau) = \exp(-\frac{\tau}{\tau^*}) \quad \text{Where} \quad \tau = \sqrt{\tau_x^2+\tau_y^2} \qquad (5)$$

Using Equation (4), the value of S_{al} for exponential autocorrelation function is

$$S_{al} = 1.6\tau^* \qquad (6)$$

Hence, for generating anisotropic ground surface with AACF expressed by the Equation (3), τ^*_x, τ^*_y can be calculated.

4. NUMERICAL MODEL

According to Patir (Patir, (1978)), it is possible to generate an N x M matrix, representing the roughness amplitudes [z_{ij}], having Gaussian height distribution and given autocorrelation function using linear transformations.

Hence, an N x M matrix of roughness amplitudes [z_{ij}] can be generated from an (N+n) x (M+m) matrix [η_{ij}], with the components that are independent identically distributed Gaussian random numbers with zero mean and unit standard deviation, and an n x m autocorrelation matrix [R_{pq}] by the following transformation:

$$z_{ij} = \sum_{k=1}^{n} \sum_{l=1}^{m} h_{kl} \eta_{i+k,\, j+l} \; ; \quad \begin{matrix} i = 1, 2, ..., N \\ j = 1, 2, ..., M \end{matrix} \qquad (7)$$

where h_{kl} are the coefficients to be determined so as to produce the desired AACF.

Since η_{ij} are independent and have unit variance,

$$E(\eta_{ij}\eta_{kl}) = \begin{Bmatrix} 1 \text{ if } i = k,\, j = l \\ 0 \text{ if otherwise} \end{Bmatrix} \qquad (8)$$

According to the definition of the AACF:

$$R_{pq} = E(z_{ij} z_{i+p,\, j+q}) = \sum_{k=1}^{n-p} \sum_{l=1}^{m-q} h_{kl} h_{k+p,l+q} \qquad (9)$$

Where, $p = 0, 1, ..., (n\text{-}1)$
$q = 0, 1, ..., (m\text{-}1)$

Equation (9) represents a system of $n*m$ non-linear equations for the determination of the coefficients h_{kl} by an iterative solution procedure.

4.1 Non-linear Conjugate Gradient method

Equation (9) can be either solved by a direct root finding method or by treating it as a multidimensional unconstrained optimization problem. The application of direct root finding methods, like Newton's method, can lead to prohibitively large storage requirements and also to convergence problems. Conjugate Gradient Method (CGM) explicitly uses derivative information to generate efficient algorithm to locate optima, but at the same time it does not require the explicit form of the function $f(x)$.

Eq (7), the system of non-linear equations, can be rewritten as:

$$f\,'_{ij} = \sum_{k=1}^{n-p} \sum_{l=1}^{m-q} h_{kl} h_{k+p,l+q} - R_{pq} = 0 \qquad (10)$$

Hence, in this paper, an algorithm has been developed to solve Equation (4) for the coefficients h_{kl} by Non-linear Conjugate Gradient method, as it is described in (Shewchuk), which is briefed as follows:

In nonlinear conjugate gradient method, the residual is always set to the negation of the gradient $r_{(i)} = \text{-} f\,'(x_{(i)})$.The variable is updated in each iteration by the equation $x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)}$.The search directions $d_{(i)}$ are computed by Gram-Schmidt conjugation of the residuals. Once the search direction is decided the line search has to be performed for which, as in linear Conjugate Gradient method, a value of $\alpha_{(i)}$ that minimizes $f(x_{(i)} + \alpha_{(i)} d_{(i)})$ is found by ensuring that the gradient is orthogonal to the search direction. The Secant algorithm is used for the line search without computing $f\,''$, instead, approximating the second derivative of $f(x+\alpha d)$ by evaluating the first derivative at the distinct points α=0 and α=σ, where 'σ' is an arbitrary small nonzero number. By making use of Tailor expansion for $\frac{d}{d\alpha} f(x+\alpha d)$, line search problem yields;

$$\alpha = -\sigma \frac{[f\,'(x)]^T d}{[f\,'(x+\sigma d)]^T d - [f\,'(x)]^T d} \qquad (11)$$

The use of the Secant method for line search drastically reduces the space requirements as it does not calculate the Jacobian matrix. The Secant method iterations are terminated when each update αd falls below a given tolerance $(\|\alpha d\| \le \varepsilon_{\sec})$, or when the number of iterations (j) exceeds the given maximum number of iterations $(j_{\max})$. The given initial value (σ_0) determines the value of σ in Equation (11) for the first step of each Secant minimization. To calculate β in the Conjugate Gram-Schmidt process, Polak-Ribiere formula is used which is given by;

$$\beta_{(i+1)} = \frac{r_{(i+1)}^T (r_{(i+1)} - r_{(i)})}{r_{(i)}^T r_{(i)}} \qquad (12)$$

Non-linear CGM loop is restarted (by setting $d \Leftarrow r$) whenever Polak-Ribiere β parameter is negative. It is also restarted after every *n* prescribed number of iterations, to improve convergence, for small *n*. Hence, the outline of the nonlinear Conjugate Gradient method is:

Define: $-f\,'(x)$, x_0

$$d_{(0)} = r_{(0)} = -f\,'(x_{(0)})$$

$$x_{(i+1)} = x_{(i)} + \alpha_{(i)} d_{(i)}$$

(i) For $\alpha_{(i)}$:

Find $\alpha_{(i)}$ that minimizes $f(x_{(i)} + \alpha_{(i)} d_{(i)})$

(This is a line search problem to solve iteratively)

(ii) For $d_{(i)}$:

$$r_{(i+1)} = -f\,'(x_{(i+1)})$$

$$\beta_{(i+1)} = \frac{r_{(i+1)}^T (r_{(i+1)} - r_{(i)})}{r_{(i)}^T r_{(i)}}$$

$$d_{(i+1)} = r_{(i+1)} + \beta_{(i+1)} d_{(i)}$$

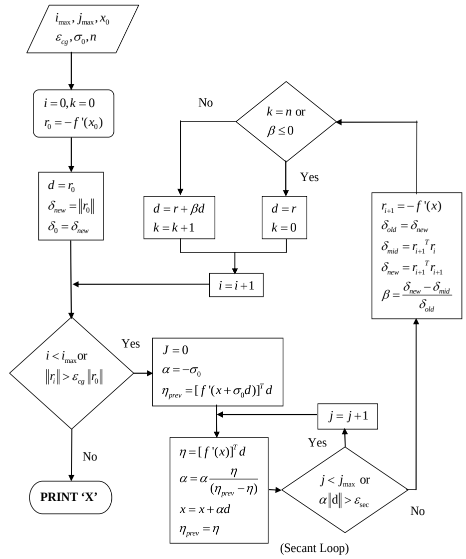

Fig.1 Flow chart of the implemented NCGM algorithm

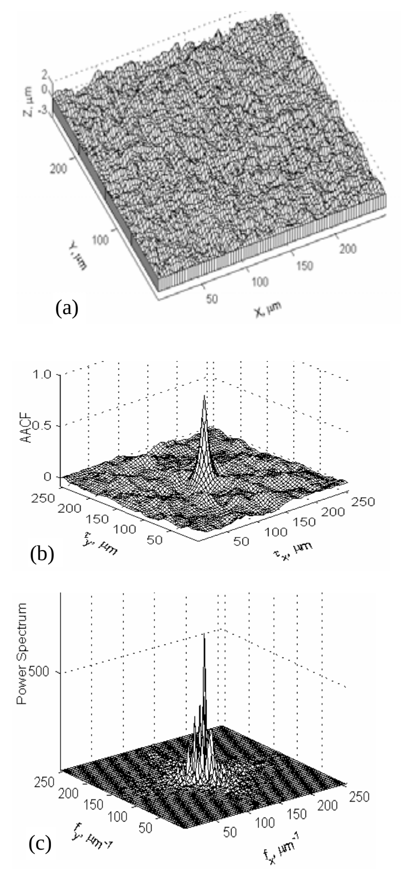

Fig. 2 (a) Typical isotropic surface generated by NCG method with $\tau_x^* = \tau_y^* = 10$;
(b) Its Areal Autocorrelation Function (AACF)
(c) and Power Spectrum

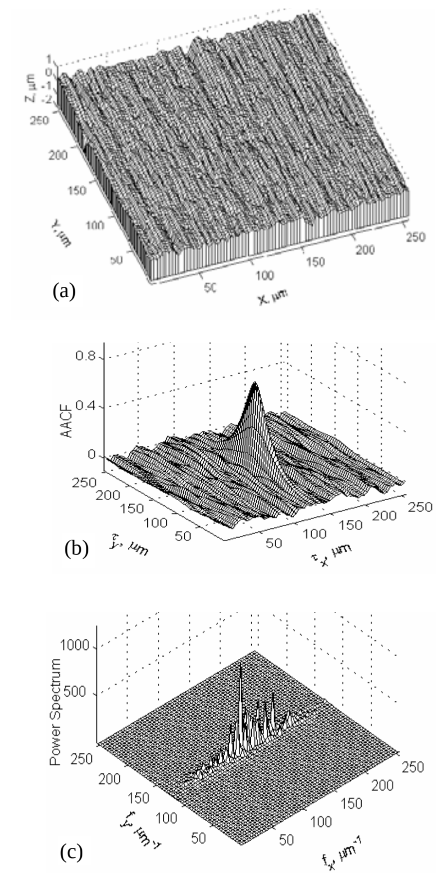

Fig. 3 (a) Typical anisotropic surface generated by NCG method with $\tau_x^* = 50$ & $\tau_y^* = 10$;
(b) Its Areal Autocorrelation Function (AACF)
(c) and Power Spectrum

An initial approximation to the coefficient vector h_{kl} may be obtained by the formulae [2]:

$$h_{ij}^0 = sc_{ij} \tag{13}$$

where, $$c_{ij} = \frac{R_{i-1,j-1}}{(n-i+1)(m-j+1)} \tag{14}$$

$$s^2 = \frac{R_{00}}{\sum_{i=1}^{n}\sum_{j=1}^{m} c_{ij}^2} \tag{15}$$

Given the overall error tolerance (ε_{cg}), the algorithm terminates when $\|r_i\| \le \varepsilon_{cg}\|r_0\|$, or when the number of Non-linear CGM iterations (i) exceed the given maximum number of iterations ($i_{\max}$). A flow chart of the implemented Non-linear CGM algorithm is shown in Fig.1.

4.2 2D Digital Filter Method

The term $h(k,l)$ in Equation (7) is the filter function that defines the system. By signal process theory, $z(i,j)$ will posses the same height distribution with the input sequence $\eta(i,j)$. The Fourier transform of Eq. (3) is given as (Hu & Tonder, (1992)) follows:

$$Z(\omega_x,\omega_y) = H(\omega_x,\omega_y) * A(\omega_x,\omega_y) \tag{16}$$

Where A and Z are Fourier transforms of η and z respectively, and H is the transfer function of the system, which can be calculated for a linear system as:

$$S_z(\omega_x,\omega_y) = |H(\omega_x,\omega_y)|^2 * S_\eta(\omega_x,\omega_y) \tag{17}$$

Where S_η is the spectral density of input sequence $\eta(i,j)$ which gives a constant value for a random sequence in white noise type, S_z is the spectral density of output sequence $z(i,j)$, i.e. the Fourier transform of the expected autocorrelation function, $R(\tau_x,\tau_y)$ given by the equation (3).Thus, the system transfer function $H(\omega_x,\omega_y)$ can be calculated by equation (17). Then, filter coefficient $h(i,j)$ can be obtained by applying inverse Fourier transform to $H(i,j)$.

5. RESULTS AND DISCUSSION

In order to evaluate the developed numerical model and to compare the results with that of the rough surfaces generated by 2D digital filter method, rough surfaces having specified spectral properties were generated with a spacing of 1 μm in x and y directions. The spectral properties were described by the areal autocorrelation function (AACF) given by the equation (3) with suitable decay rate and correlation distances in x and y directions (τ_x^*, τ_y^*) so as to get the required 3D spatial parameters, namely, the fastest decay autocorrelation length (S_{al}) and the texture aspect ratio (S_{tr}).

As the focus of this study is on the 3D spatial parameters S_{al} and S_{tr}, three cases were considered for the generation of rough surfaces:

i. Surfaces with $\tau_x^* = \tau_y^* = 10$

ii. Surfaces with $\tau_x^* = 50, \tau_y^* = 10$

iii. Surfaces with $\tau_x^* = 100, \tau_y^* = 10$

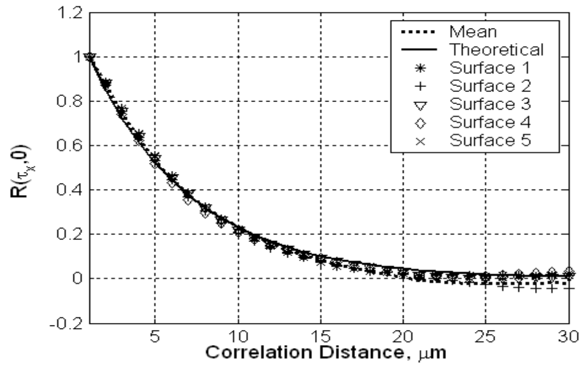

Fig.4 Autocorrelation of the generated isotropic surface with $\tau_x^* = \tau_y^* = 10$ by NCG method

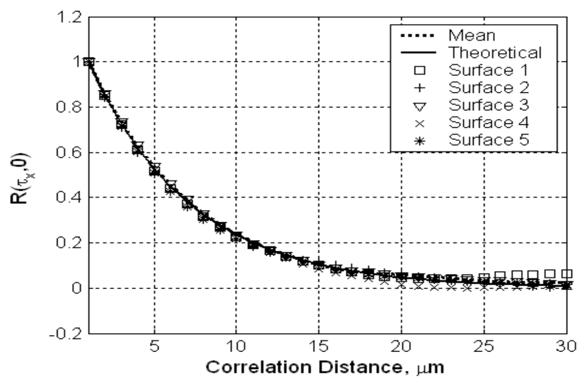

Fig.5 Autocorrelation of the generated isotropic surface with $\tau_x^* = \tau_y^* = 10$ by Digital Filter method

Table 1 S_{al} and S_{tr} values of the theoretical surface and the generated mean surfaces ($\tau_x^* = \tau_y^* = 10$)

	Theoretical Surface	Mean Surface by NCG	Mean Surface by Digital Filter
S_{al}	10.05	10.15	10.09
S_{tr}	0.985	0.979	0.973

Five surfaces were generated with dimension 256x256 μm² for the first two cases, by both the methods. For the third case, mean surface is generated with dimension 512x512 μm², by both the methods.

As the approximation of the AACF depends on the quality of the random number generator, a mean surface of fifty generated rough surfaces also used for the evaluation.

A typical isotropic rough surface generated by NCG method with $\tau_x^* = \tau_y^* = 10$, its Areal autocorrelation function (AACF) and the power spectrum plots are presented in Fig.2. Fig.3 shows the same for a typical anisotropic rough surface generated by NCG method, with $\tau_x^* = 50, \tau_y^* = 10$.

Fig.4 shows the plot of autocorrelation function (ACF) of the five generated surfaces and the mean surface, with $\tau_x^* = \tau_y^* = 10$ by NCG method, along with the theoretical ACF, in x direction.

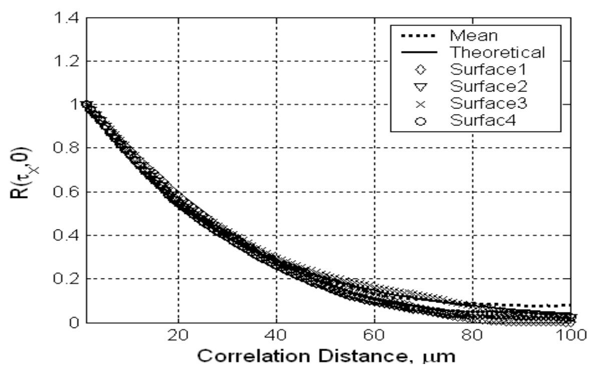

Fig.6 Autocorrelation of the generated anisotropic surface with $\tau_x^* = 50, \tau_y^* = 10$ by NCG method

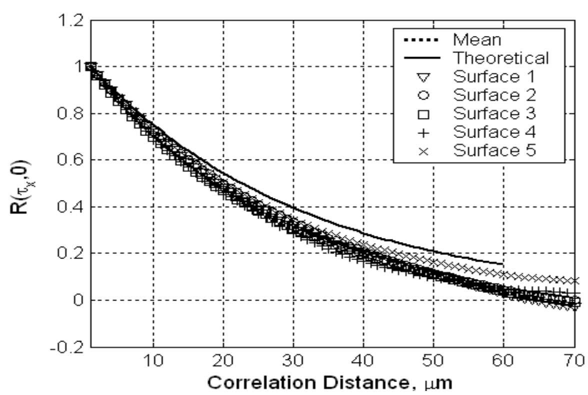

Fig.7 Autocorrelation of the generated anisotropic surface with $\tau_x^* = 50, \tau_y^* = 10$ by Digital Filter method

Table 2 S_{al} and S_{tr} values of the theoretical surface and the generated mean surfaces ($\tau_x^* = 50, \tau_y^* = 10$)

	Theoretical Surface	Mean Surface by NCG	Mean Surface by Digital Filter
S_{al}	10.15	9.79	9.85
S_{tr}	0.205	0.225	0.266

Fig.5 shows the same by 2D Digital Filter method. The produced surfaces have ACFs that match excellently with prescribed ones for both the cases. Table 1 show the S_{al} and S_{tr} values of these mean surfaces by both the methods.

Fig.6 shows ACF plots of the five generated surfaces and the mean surface, with $\tau_x^* = 50, \tau_y^* = 10$, by NCG method, along with theoretical ACF in x direction and Fig.7 shows the same by 2D Digital filter method. The S_{al} and S_{tr} values of these mean surfaces by both the methods are presented in table 2. From Fig.6 and Fig.7, it can be seen that the ACF of the generated surfaces by 2D digital filter method deviate more from the theoretical one compared to that by NCG method. This point is more evident in Fig.8, which compares the ACFs of the generated mean surface of dimension 512x512 μm^2, with $\tau_x^* = 100, \tau_y^* = 10$ by both the methods.

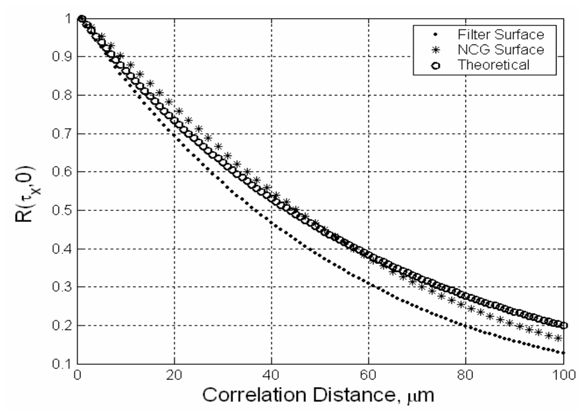

Fig.8 Autocorrelation of the generated anisotropic mean surface with $\tau_x^* = 100,\ \tau_y^* = 10$ by NCG & Digital Filter methods

6. CONCLUSION

An algorithm has been developed for the numerical generation of Gaussian 3D anisotropic rough surfaces with prescribed 3D spatial roughness parameters. The procedure is based on the linear transformation of matrices. To reduce the memory requirements and for easy convergence in solving non linear equations, non linear conjugate gradient (NCG) method is used in the procedure. The method is then compared with the 2D digital filter method .It is found that even though both methods provide good results at smaller correlation distances, at higher correlation distances NCG method yields better results. As the surfaces produced by grinding processes that have higher correlation distances, it is observed that the NCG method will be useful for the generation of ground 3D engineering surfaces.

7. REFERENCES

Bakolas, V. (2003). Numerical generation of arbitrarily oriented non-Gaussian three-dimensional rough surfaces. Wear, 254, 546-554

Dong, W.P.; Sullivan, P.J. & Stout, K.J. (1994).Comprehensive study of parameters for characterizing three-dimensional surface topography IV: parameters for characterising spatial and hybrid properties. Wear, 178, 45-60

Hu, Y.Z. & Tonder, K. (1992). Simulation of 3-D random rough surface by 2-D digital filter and Fourier analysis.Int.J.Mach.Tools Manufacture, 32, 1/2, 83-90

Patir, N. (1978). A numerical procedure for random generation of rough surfaces. Wear, 47,263-277

Shewchuk, J.R. An introduction to the Conjugate Gradient Method without the agonizing pain, http://www.cs.cmu.edu/~quake-papers/painless-conjugate-gradient.ps

Stout, K.J.; Sullivan, P.J.; Dong, W.P.; Mainsah, E.; Luo, N.; Mathia, T. & Zahouani, H. (1993). The development of methods for the characterization of roughness in three dimensions, Commission of the European Communities, Luxembourg

Whitehouse, D.J. & Archard, J.F. (1970). The properties of random surfaces of significance in their contact. Proc. Royal Society (London), A316, 97-121