Characterization of nanoscale roughness in single point diamond turned optical surfaces using power spectral density analysis

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Power spectral density (PSD) distribution provides an accurate measure of roughness of an optical surface. This article presents an analysis of optical surface roughness generated by single point diamond turning (SPDT) using PSD. For this study, flat 60 mm diameter aluminium-6061 samples are machined for varying tool feed rates, while keeping the other machining parameters constant. The 1-D PSD distributions are computed from the surface roughness data obtained by mechanical profilometer. The PSD distribution of the surface roughness profile is composed of primarily three periodic components, which are correlated to the tool feed rate, material induced vibrations and machine-tool vibrations. An attempt has been made to identify their individual contributions in PSD estimates. This study helps in improving the surface quality by selecting optimum process parameters.

Surface roughness significantly affects the quality of optical systems, as it causes scattering and stray light, degrading the contrast and sharpness of the optical images. Smoother the surface, lesser will be the scattering, resulting in enhanced functioning of the optical component, whether in reflection or transmission mode. The measurement of roughness or surface finish of an optical surface is of great significance during as well as after the fabrication. Before quantifying roughness, one should look into the measuring technique as well as the parameters considered in the metrology.

There have been a multitude of measurement techniques including: total scattering, angle resolve scattering, mechanical and optical profiling, atomic force microscopy, white light interferometry, confocal laser scanning microscopy. Historically, the most common method of surface measurement has been to mechanically measure the variation of height of the surface along a line across the surface. Roughness is generally expressed by either the root mean square (rms) value \( R_q \), arithmetic average \( R_a \), or maximum departure \( R_t \) from the mean line. The limitation with either of these roughness parameters is that, they look at only the heights and depths of the peaks and valleys, and not at their spatial distribution, resulting in an incomplete representation of roughness features of the surface. To obtain an accurate representation of roughness of an optical surface with a random distribution of peaks and valleys, it would be worthwhile to see how the roughness ‘power’ is distributed among the different surface frequencies, i.e., by looking at the spectral distributions. To correct the anomaly of incomplete presentation of roughness by a single parameter, e.g., rms roughness, power spectral density (PSD), a comprehensive roughness distribution parameter is considered.

Machining effects on surface roughness generation

Single point diamond turning (SPDT) has been widely used to fabricate optical quality surfaces. Tool feed rates, cutting speeds, and depth of cuts are typically much lower in diamond turning process compared to turning with conventional machining tools. There are number of factors which affect simultaneously the surface roughness of the turned work-pieces. Prominent among them are tool geometry, tool feed rate, work-piece RPM, material induced vibrations and machine-tool vibrations. In this paper, the contributions of tool feed rate, material induced vibrations and machine-tool vibrations on surface generation are considered. These components would appear at different frequencies in the power spectrum density of surface roughness. There is a difference between the frequency of surface modulation caused by the material induced vibrations and that by the machine-tool vibrations. The former depends on the homogeneity and crystallographic
orientation of the work material being cut. The machine-tool vibrations induce surface modulation with a frequency, which depends on the ratio of frequency of vibrations between the tool and workpiece, and the spindle rotational speed.

The fundamental feed components appear at frequencies of \(\nu(\text{feed}) = 1/\text{feedrate} \) (\(\mu\text{m}/\text{rev}\)) in the PSD. Since an ideal surface produced by the tool nose is periodic but not sinusoidal, its FFT spectrum would have power spectral density at the harmonics of the feed frequency \(\nu(\text{feed})\). But fundamental frequency of the feed component is predominant and is used to characterize the effects of tool feed rate and tool geometry in the FFT spectrum analysis.

The small amplitude and low frequency exists relatively between the tool and the work-piece. These vibrations between the tool and work-piece cause waviness not only in the cutting direction but also in the tool feed direction. This effect has been termed as tool-work-piece vibrations. The frequency of the surface modulation will depend on the tool feed and work-piece revolutions and can be written as \(\nu(\text{tw}) = \frac{\phi}{2\pi}s\), where \(\phi\) is the phase shift of the vibration to one revolution of the work-piece, and \(s\) is the tool feed rate. The frequency of the tool-work-piece vibrations becomes higher with the increase of the phase shift or with the decrease of feed rate.

Material induced vibrations are caused due to the reaction of the material to the thrust force applied to cut the material. It causes the surface undulation of the frequency higher than machine-tool vibrations and denoted as \(\nu(\text{mat})\). These vibrations are caused because of variation in the material properties and the ductility of the material. Since the material chosen for this study is polycrystalline (aluminium alloy-6061), the variation of surface roughness will be independent of angle.

A better understanding of the effects of these factors on surface roughness will allow us optimising the parameters to get a good surface quality. In this paper, an experimental study on diamond turned surface is conducted by machining aluminium alloy at varying tool feed rates, while other machining parameters are kept constant. The contributions of material induced effects and machine-tool vibrations vis-à-vis tool feed rate towards surface roughness have been studied by using PSD analysis. The objective of this study is to find out the optimum range of tool feed rate, where the combined effect of the above three factors i.e. material induced vibrations, machine-tool vibrations and tool feed rate is minimum.

Surface evaluation

Machined surfaces suffer from three types of errors, i.e., form, figure and finish. It is impossible to say, at what point does finish error become figure error. It is better to separate these errors according to their cause, as this relates to the performance factors. Roughness (finish) of a surface is caused due to the irregularities inherent in the production process (e.g. cutting tool and tool feed rate). The roughness also depends on the material properties and tool wear\(^7\). Figure error may result from vibrations, chatter or work deflections and strains in the material. Form is the general shape of the surface, neglecting variations due to roughness and figure error.

The root mean square (rms) roughness \((R_q)\) is one of the important parameter calculated from the surface profile as given below:

\[
R_q = \left[ \frac{1}{N} \sum_{i=1}^{N} [z_i(x)]^2 \right]^{1/2}
\]  

where, \(N\) is the number of data points and \(z(x)\) is the height as a function of distance \(x\) above and below the mean line.

The value of rms roughness depends on the bandwidth of the surface spatial wavelengths that the instrument can sense. It means that two important parameters should be specified for rms roughness: the lowest spatial wavelength (lateral resolution) and the longest spatial wavelength (sampling length). It is important to know the values of these two limiting factors for any measuring condition and roughness analysis. Other derived statistical parameters include peak-to-valley heights, rms slope, curvature, skewness, mean spacing irregularities and autocorrelation length. Each of these parameters represents the roughness by a single number. A single characteristic analysis of a surface may be sufficient for some applications. However, for accurate analysis of a surface, a much more specific description that measures the spatial interaction is required. The profile descriptions discussed for rms roughness ignore any information about spatial wavelength. Fig. 1 shows a situation where two very different surfaces being represented by same value of rms roughness\(^8\).
The surface roughness profile of a machined surface provides information not only about the cutting process and material properties, but also about the tool-work-piece vibrations, material induced effects and other machining effects. Usual roughness parameters, e.g., $R_q$, $R_a$ or $R_t$ are inadequate to provide this information. Hence, for the comprehensive roughness analysis of an optical quality surface, PSD has been preferred. PSD represents the spatial frequency spectrum of the surface roughness measured in inverse-length units. The unit of 1-D PSD is nm$^3$. It can be calculated from the surface profiles made by an optical or mechanical profiler. The power spectrum of a surface roughness profile is composed of several periodical components, which can be correlated to different process parameters and mechanisms of surface generation. The lower spatial frequencies represent the waviness, whereas higher spatial frequencies represent the actual roughness. The PSD is closely related to the amount and distribution of light scattered by a rough surface. One of the most interesting properties of PSD between two designated spatial frequency limits is that, it is equal to square of rms roughness of the original profile, when the profile is measured or filtered to have same spatial frequency limits.

Calculation of power spectral density of surface roughness

The one-dimensional PSD can be computed from discrete data obtained from the mechanical profilometer. If $z(x)$ is the surface roughness height as a function of distance $x$, a finite-length Fourier transform may be written as:

$$Z(k)=\int_0^L z(x) \exp(-ikx) \, dx$$  \hspace{1cm} \cdots \hspace{1cm} (2)$$

where $i = \sqrt{-1}$ and $k$ is the wave number. In practice, we can measure only a finite number of values of $z(x)$. The surface roughness data set consist of $N$ values of $z(x)$, which are measured at equally spaced intervals $\Delta x$ over the total sample length $L$. The discrete equivalent of Eq. (2) is:

$$Z(f)=\sum_{n=1}^N z(x) \exp\left(\frac{-2\pi i(x-1)f}{N}\right)$$  \hspace{1cm} \cdots \hspace{1cm} (3)$$

Fast Fourier Transform (FFT) routine of MATLAB has been used to calculate the discrete Fourier transform (DFT) of the roughness data. The one-dimensional PSD is the complex conjugate square of the DFT of the linear surface profile divided by total number of discrete points, $N$.

$$\text{PSD} = \left(\text{Normalization factor} \right) \frac{Z(f) \cdot \text{conj}[(Z(f))]}{N}$$  \hspace{1cm} \cdots \hspace{1cm} (4)$$

The frequency range of a computed PSD starts at the lower end with $1/L$ and goes up to $1/2\Delta x$. A suitable multiplicative normalization factor has been used to compute PSD. To find out this normalization factor, the PSD over the Nyquist bandwidth limits of surface spatial frequency has been integrated to obtain the area. According to the Parseval’s theorem, the area under the PSD curve should equal to the mean-square roughness:

$$R_q^2 = \int_{f_{\text{min}}}^{f_{\text{max}}} \text{PSD}(f) \, df$$  \hspace{1cm} \cdots \hspace{1cm} (5)$$

This expression provides the correct normalization factor, $2\Delta x$, which is used to compute PSD in Eq. (4).

PSD calculated from a single profile is exceedingly noisy and non-reproducible. To obtain a true PSD of a surface that has random roughness, the average of PSD estimates is to be calculated from the profiles made at different places on a surface. The long profile can be subdivided into $j$ (1, 2, … $n$) small profiles.

$$\text{Average PSD} = \frac{1}{n} \left( \sum_{j=1}^n \text{PSD}_j \right)$$  \hspace{1cm} \cdots \hspace{1cm} (6)$$

Experimental Procedure

The machining is performed on Nanoform 250, a two-axis CNC lathe from Taylor-Hobson (Leicester, England). Aluminium-6061 is chosen for this study, as aluminium alloys are extensively used in precision
optical components for various applications. The material used is assumed to be isotropic. For SPDT, a single-crystal natural diamond tool with 0.5 mm nose radius, 100° included angle, 0° rake angle with designated waviness of 0.40 μm is used. A series of face cutting experiments are conducted on a 60 mm diameter work-piece with tool feed rate varying from 0.3 μm/rev to 30.0 μm/rev. The depth of cut is kept at 2 μm and spindle’s rate at 3000 rpm.

A standard Form Talysurf Series 2 (PGI) Profilometer from Taylor-Hobson, (Leicester, England) is used for the surface evaluation. A diamond conical stylus having the tip radius 2 μm and 10 mm vertical range is selected to measure the figure error and surface roughness. The stylus is held in a cantilever position from the measuring arm and the force of stylus is selected to be low, so that the machined surface is not damaged during measurement scan. Draughts and airborne vibrations are avoided during the measurements. Measurements are taken with the stylus movement speed of 0.5 mm/s in the radial direction. The roughness data is extracted from the scans of SPDT machined aluminium samples and used for the PSD calculation.

Results and Discussion

A spectrum analysis for varying tool feed rates has been conducted by computing the PSD distribution from the data extracted from Form Talysurf profilometer. Throughout this analysis, the lowest spatial wavelength (lateral resolution) is chosen to be 0.0025 mm and the longest spatial wavelength (sampling length) is selected to be 0.8 mm. The power spectrum of the roughness profile is determined by Fast Fourier Transformation (FFT) algorithm as explained earlier.

A single profile analysis often provides with a noisy and non-repeatable spatial distribution. In order to compute a realistic PSD of a typical surface, the average of PSD estimates has been calculated from the series of small profiles. For this purpose, a profile of 20 mm length has been selected and this is further divided into 20 small profiles with 1000 data points each. This data is then used to calculate the average PSD. The un-averaged and averaged PSD’s are shown in Fig. 2.

Figs 3a-3f represent the PSD distribution of roughness for tool feed rates 6, 10, 12, 15, 18 and 25 μm/rev respectively. The feed frequencies appear at 166, 100, 83.3, 66.6, 55.5 and 40 respectively. In these figures, ν(tw), ν(mat) and ν(feed) denote frequencies due to tool-work-piece vibrations, material induced vibrations and tool feed rate respectively. Feed component contribution is found to be predominant in terms of amplitude and is used to characterize the effects of feed rate in FFT spectrum analysis. As the tool feed rate increases (Figs 3a-3f), the feed components shift to a lower spatial frequency range. It is observed that, at low feed rate (Fig. 3a), amplitude components of tool-work-piece vibrations and material effects dominate over the feed component. At medium feed rates (Fig. 3b) the amplitude components of tool-work-piece vibrations and feed are comparable. But at higher feed rates (Figs 3c-3f), the amplitude component due to feed dominates over contributions due to tool-work-piece vibrations and material effects. It is also observed that the contributions of tool-work-piece vibrations and material induced vibrations gradually increase with the feed rate. The frequency corresponding to the relative tool-work-piece vibrations component shifts
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For the tool feed rate in the range of 1.5–8.0 μm/rev, the surface finish is mainly decided by low frequencies and the contribution of feed component (high frequency) is very less. The amplitude of low frequency component is almost constant within this range.

Additionally, using Parseval’s theorem the rms roughnesses have been obtained by integrating the PSD curves. The rms roughness from the PSD have been calculated (rms-PSD) and compared with the rms roughness values (rms-scan) obtained from the Form Talysurf. The average values (Av.rms-PSD and Av.rms-scan) of the 20 small profiles are also computed. Fig. 4 represents the comparison of rms-scan and rms-PSD values in un-averaged (Fig. 4a) and averaged (Fig. 4b) modes. The relative contributions of the tool feed rate, tool-work-piece vibrations and material induced vibrations to the rms roughness have also been computed by applying the Parseval’s theorem in their respective frequency bands. Fig. 5 represents relative average contributions of the tool feed rate (Av.rms_feed), material effects (Av.rms_mat) and of tool-work-piece vibrations (Av.rms_vib) to the rms roughness.

Conclusions

In this study, optical surface roughness has been presented in terms of PSD rather than by the conventional single parameter root mean square (rms) roughness. Following conclusions can be drawn from this study:

1. The surface roughness is composed of several periodical components, which are feed component, tool-work-piece vibrations and material induced vibrations.
2. Amplitude of feed component dominates at higher feed rate range, while at low feed rate the tool-work-piece vibrations dominate. At very low feed rate the feed component is almost negligible and tool-work-piece vibrations component determines the surface roughness.

3. Surface roughness is found to be small and constant in the range of 1.5 to 8.0 μm/rev. This is the optimum range of tool feed rate where the surface the surface quality is good for the work-piece under investigation.

4. The frequency corresponding to the relative tool-work-piece vibrations component shifts to the lower frequency range with the increased feed rate.

5. A single PSD profile gives noisy and non-reproducible estimates. Hence PSD estimates should be averaged before drawing any conclusion.

6. PSD analysis provides all the amplitude and frequency details of the surface and helps in establishing the relationship between manufacturing process and surface roughness generation.

References