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SURFACE QUALITY EVALUATION OF DIAMOND TURNED SEMICONDUCTOR CRYSTAL BY MEANS OF ATOMIC FORCE MICROSCOPY

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Abstract. *The possibility of fabricating high quality components from brittle materials has been made possible by achieving material removal in the ductile mode. It is known that plastic behavior in brittle materials take place prior to the onset of fracture when the cut is restricted below critical cutting depth value. The surface integrity of any mechanical component, finished by means of mechanical material removal process, is considered to be critical for its performance. The importance of assessing surface integrity of mechanically finished brittle materials such as semiconductor crystals is strongly justified by the optical and electronic applications. In this paper, the use of AFM for the evaluation of diamond turned monocrystalline silicon surface finish is presented. (100) oriented monocrystalline silicon was single point diamond turned under conditions that lead to a ductile regime. 3-D image was used for the characterization of surface quality. The cut grooves can be clearly seen, regularly spaced and running parallel with cutting direction which confirm the absence of chatter vibration. A machined surface with the maximum peak-to-valley roughness of 25 nm can be generated at feedrate in the range of 1.5 and 2.0 μm/rev. The surface roughness measured is in the range of 2 nm Ra. This surface finish is slightly better than the polished samples used in the diamond turning tests. A closer examination at higher magnifications of the machined surface indicated that no microcracks are present. In this case single point diamond turning has achieved fully ductile material removal. The results demonstrate that the AFM is more suitable for the assessment of the of diamond machined surfaces because of the better accuracy of the surface roughness and evaluation of microtopography of the surface generated.*

Keywords: *AFM, Diamond Turning, Silicon Crystal*.

1. INTRODUCTION

The research on brittle materials machining has experienced great improvement with the possibility of cutting this materials with single-point diamond tools. Important applications of single point diamond turned optics are in the fabrication of unconventionally shaped optics, more generally, aspherics and particularly off-axis components such as paraboloids. It is worth mentioning that, in industry, ductile grinding is more widely used (as well as chemo-mechanical polishing) for plane surfaces of large silicon wafers, due to the rapid and deleterious diamond tool wear (**Abe et. al., 2000**).

The optical elements made from brittle materials demand high quality surface finish and integrity as well. High precision instruments are normally required in order to accurately evaluate optical surfaces fabricated by ultraprecision machining processes. Atomic Force Microscopy (AFM) has been successfully applied to the assessment of the microtopography of diamond turned non-ferrous metals and semiconductors crystals (**Yu et al. 1994, Brinksmeier and Riemer, 1998, Fang, 1998**). The use of AFM as sub-micrometer characterization technique of surface topography in other processes such as grinding of fine ceramics (**Ichida et al., 1993**) as well as polishing of hardened tool steel specimens and silicon wafers (**De Chiffre et al., 1996; Samitsu, 1993**) has been reported. Quantitative and qualitative features of surface finish characterization have been briefly discussed in a recent paper (**Jasinevicius et al. 1998**). The main advantages of AFM for structural and morphological analysis of materials, when compared with microscopy techniques such as SEM, in general, are: larger three-dimensional image resolution, there is no necessity of conductive surface layer, no preparation method is required and it allows the direct quantification of the surface roughness.

In this study, the inspection of the microstructure of single point diamond turned silicon surfaces is made by means of an AFM. As a result, the morphology and topography of the finished surface were imaged and measured as a function of the cutting conditions. The surface roughness of the cut surface, estimated by means of AFM, is in the range of 2 nm Ra. This surface finish is slightly better than the polished samples used in the diamond turning tests. The surface roughness Ra presented is expected to increase as the feed rate increases. However, this trend was better observed for Rmax and smaller depths of cut.

2. EXPERIMENTAL PROCEDURE

Single-point diamond turning tests were carried out on a commercially available ultraprecision diamond turning machine, the Aspheric Surface Generator Rank Pneumo ASG 2500. Facing cuts were performed on silicon substrates (10 mm x 10 mm). A single crystal p-type Si (100) surface orientation sample was used in this study.

The cutting fluid used was a synthetic water-soluble oil with the purpose of cooling and lubrication. This fluid was continuously mist sprayed onto the workpiece during machining. Round nose single crystal diamond tool geometry (Contour Fine Tooling®) was used. Only new diamond tools were used in the cutting tests. Table 1 describes the experimental conditions and tool geometries used in the cutting tests.

A specimen was machined for each combination of cutting parameters, i.e., feed rate and depth of cut, and the microtopography and morphology of the surface generated inspected by means of AFM. The atomic force microscope (AFM) was a Digital Nanoscope IIIa. It was operated with a standard 50-60^{o} conical silicon nitride stylus of 5 nm radius tip, with cantilever spring constant of ~ 0.06 N/m. Conventional contact mode was employed where the stylus is scanned raster style over, and in contact with the surface with contact forces of typically 10-100 nN. For the characterization of the examined diamond turned surfaces it was decided to used Ra and Rmax (Rt), representing the average and a maximum amplitude value of the surface roughness. The inspection process consisted of measuring the surface roughness and obtaining images of the surface in order to observe the reproduction fidelity of the tool edge profile into the surface cut grooves.

Table 1 - Tool geometry and dimensions used in the cutting tests.

Tool Specifications	Dimensions
Tool material	Single crystal diamond
Tool nose radius (mm)	0.657
Rake angle	-25^{o}
Clearance angle	12^{o}
Feed rate (μm/rev)	1.0, 1.5 , 2.0, 2.5, 5.0
Depth of cut (μm)	0.1, 1.0, 5.0, 10

3. RESULTS

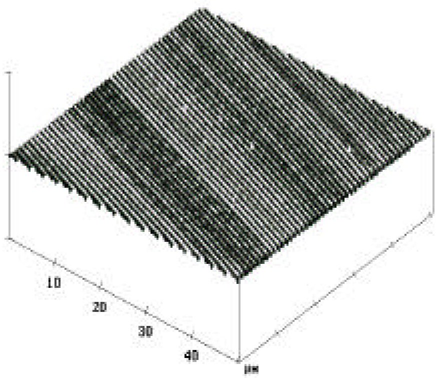
The final surface finish obtained during practical machining operation (such as in turning, milling, etc.) can be affected by several effects (chatter, built-up edge, etc.). The "ideal" surface roughness, which is a result of the geometry of the tool and feed rate is represented by the following formulation:

$$R_{max} = f^{2} \cdot (8r)^{-1} \qquad (1)$$

where f is the feed rate and r is the tool nose radius.

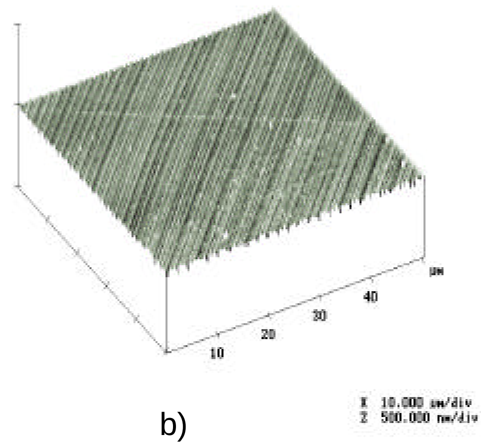
The results showed that the increase in feed rate presented the expected effect, i.e., the increase in surface roughness. However, this change was not much pronounced as can be seen in Fig. 1. Fig. 1 shows 3-D images of the micro-roughness of the silicon surfaces machined with different feed rate conditions. The morphology of the cutting grooves in all images shows equally spaced tooling marks according to the feed rate condition applied. No sign of cutting edge defect was found within the primary surface roughness structure. Although Fig. 1 e) shows a smooth surface finish it is worth mentioning that the surface does present microcracks. This is said in order to show a disadvantage of this technique to evaluate surface finish. Despite the possibility of proceeding a section analysis of the surface, which will show quantitative values of the micro-roughness, the image may not represent the real situation of the surface finish since it is only revealing a smooth and surface roughness profile. Fig.1 also shows the surface roughness values of the machined surfaces. The roughness R_a did not show a significant variation and is almost constant in the range of 2 nm. R_{max} shows some difference with the increase in the feed rate conditions. This can be considered as an expected result. However, the difference observed among the results cannot be explained. Figure 2 shows a closer examination of the surface machined presented in Fig 1 a). A three-dimensional image showing the microtopography of the diamond turned surface, is shown in Fig. 2 a). The cut grooves can be clearly seen, regularly spaced and running parallel with cutting direction which confirm the absence of chatter vibration. At this magnification, neither microcracks or sign of surface damage were detected. In Fig. 2 (b), the cross-feed of the cutting tool is advancing at 1.0 μm rev^{-1}. The surface roughness measured is 3.5 nm Ra. This average surface roughness is within the range required for optical parts used with infrared light (*Ra < 0.03 mm*). Another interesting aspect that can be observed is the spectrum of the *fast fourier transform* of the surface topography that shows a spectral period of 1.045 μm which can be attributed to the feed rate. The AFM can inform on the reproduction fidelity of the cutting edge during surface generation.

Ra = 2.46 nm
Rmax = 30.24 nm

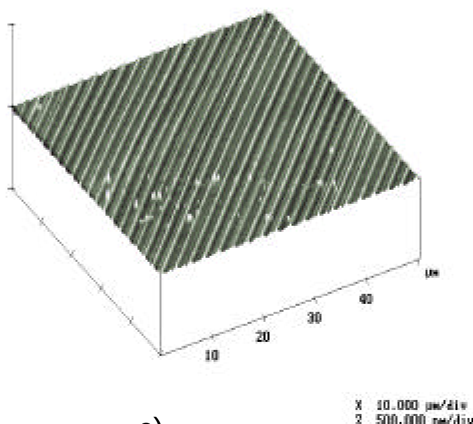


a)

Ra = 2.3 nm
Rmax = 25.6 nm



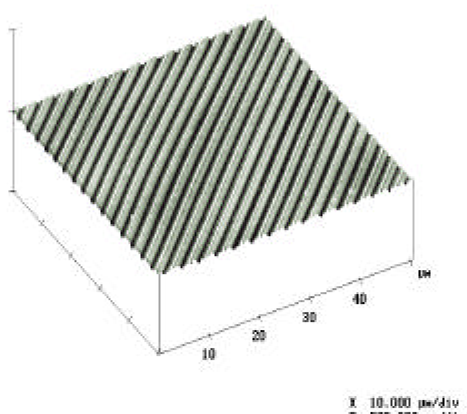
b)



Ra = 2.3 nm
Rmax = 26.5 nm

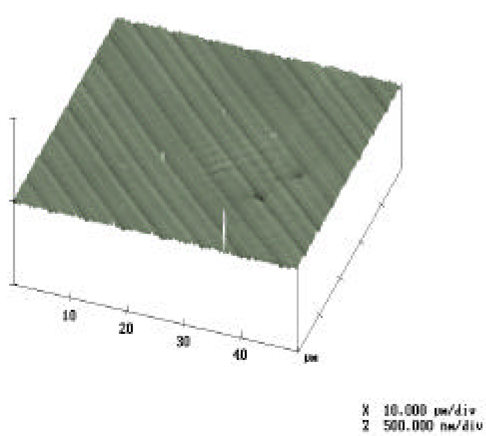
c)

Ra = 2.1 nm
Rmax = 34.7 nm



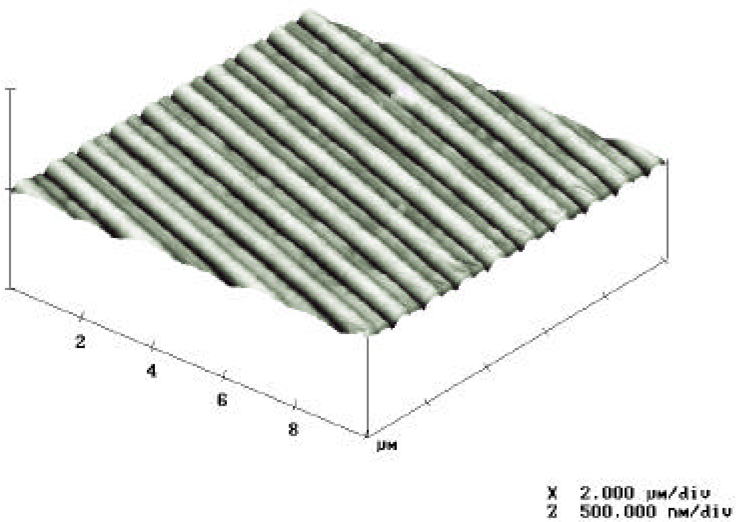
d)

Ra = 2.07 nm
Rmax = 33.4 nm

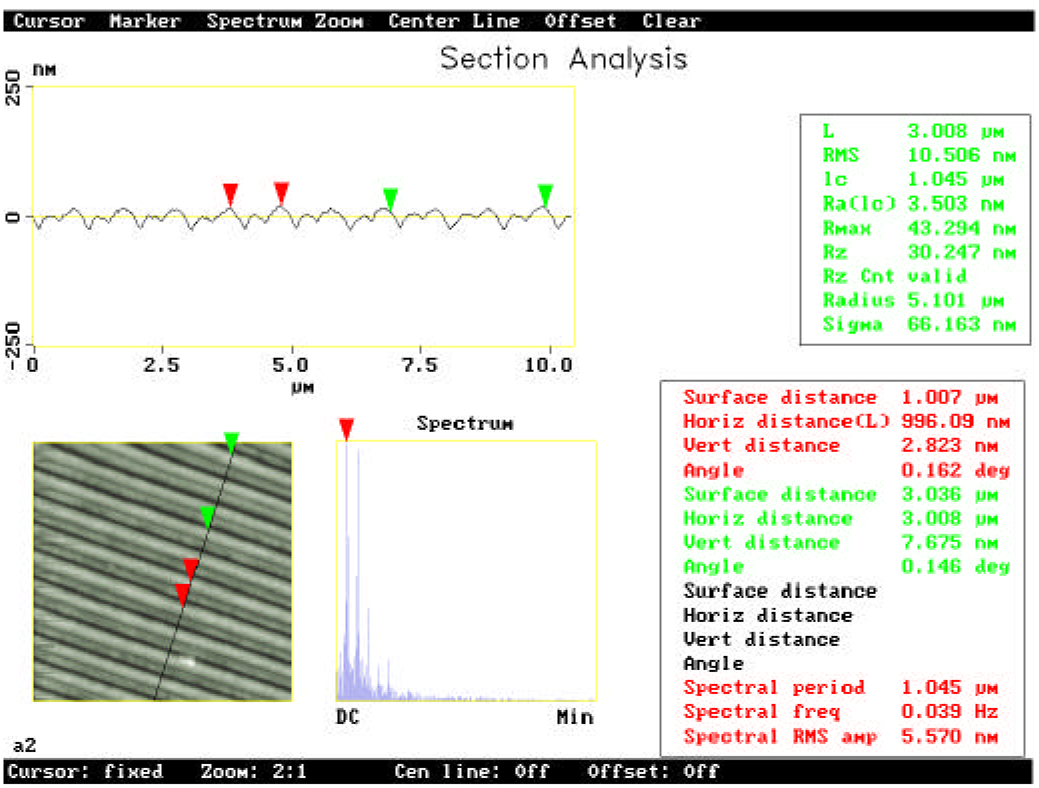


e)

Figure 1 – 3-D images of micro-roughness difference for the machined samples cut with different feed rates: a) 1.0 µm/rev, b) 1.5µm/rev, c) 2.0 µm/rev, d) 2.5 µm/rev, and e) 5.0 µm/rev.



(a)



(b)

Figure 2. Smaller portion of the surface can be analyzed by means of AFM technique. a) three dimensional image of the surface; b) cross-section analysis of the surface at this magnification

There is an interesting aspect which was found for the sample machined with different depths of cut. A decrease was observed in surface micro-roughness Rmax. This tendency can be observed in Fig.3. A possible explanation for this may be attributed to a more prominent spring back of the surface vicinity due to the back transformation to the amorphous phase, occurred during machining. It is generally accepted that at pressure of 11-12.5 GPa, silicon crystal with diamond cubic form transforms to the denser ***b****-tin* structure with 22% reduction in volume. When the pressure is withdraw, this metallic phase undergoes another phase change to a bcc structure with an intermediate density between the crystal and the metallic phase; the unit cell volume is some 8% denser than the silicon crystal phase(**Hu et al. 1988**). In this case, this may be promoting a size effect as a function of the increase in depth of cut.

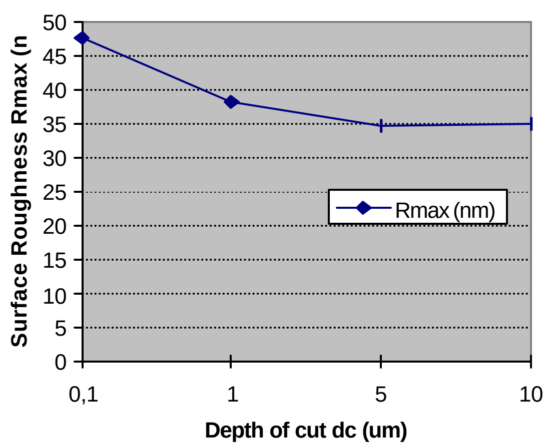


Figure 3. Rmax value as function of depth of cut.

As a result, the stress and strain distribution will tend to be higher in the tool-workpiece interface, so the workpiece under larger depth of cut will be likely to sustain most of the plastic deformation and make the machined surface profile be closer to the ideal surface profile. It is worth mentioning that the temperature during machining do not reach considerable values which could play a significant role in the surface generation mechanism (**Jasinevicius et al. 2001**). The phase transformation is not triggered by temperature, but certainly by mechanical interaction between cutting tool edge and material. The surface and subsurface damage has been investigated by means of Transmission Electron Microscopy technique (**Jasinevicius, 2000a,b**). The results show that the region beneath the amorphous layer is compound by dislocations loops and microcracks. This surface structural modification play an important role in the fabrication of optics, once a different diffractive index would be expected for this amorphous layer. Annealing tests were carried out and the surface probed by Raman spectroscopy. The results show that the crystalline state was recovered in the surface vicinity.

4. CONCLUSIONS

In this work, an investigation on the inspection of diamond turned surface of brittle material was carried out. Single crystal silicon specimens were machined in the ductile regime under different cutting conditions (i.e., feed rate and depth of cut) and the surface microtopography was examined by means of an Atomic Force Microscope (AFM). AFM 3-D images were obtained in order to inspect the surface morphology. The roughness parameters Ra and Rmax obtained were used as indicators of the effect of varying the cutting conditions. Although it was expected an increase in surface roughness with the increase in feedrate, the results did not show great variation. The phase transformation plays a fundamental role in the ductile regime during machining. This phenomenon has been investigated and extensive works has to be done in this field.

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