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SINGLE POINT DIAMOND MACHINING OF FERROELECTRIC MATERIALS

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Abstract: *Ferrolectric ceramics and single crystals have attained an enormous importance in an ever-widening range of applications. Their exceptional combination of properties includes strong piezoelectric, pyroelectric and electro-optic effects. One of the most important and widely-used groups is the lead zirconate titanate solid solution series (PZT). The contemporary technology that has been used to machine these materials has been grinding and diamond sawing followed by lapping and polishing. The objective os this research program is to develop a highly efficient and precision machining process for this group of ceramic materials reducing sub-surface damage and thus eliminating the need for lapping and polishing, leading to reduced costs of production. The results show that "ductile regime"machining can be achieved with this group of brittle materials. The plasticity observed in PZT is apparently dependent on the poling direction, which has been shown to directly influence the ductile regime machining conditions. Other materials characteristics, such as porosity and hardness, also influence this behaviour.*
The research is helping in the understanding of the ferroelectric material mechanical and electrical characteristics when machined and also is being used to build up an optimised process model for the damage free diamond grinding of PZT.

Keywords: *lead zirconate titanate; PZT; x-ray diffraction; single point diamond turning; fracture mechanics.*

1. INTRODUCTION

Lead titanate $PbTiO_3$ and lead zirconate $PbZrO_3$ are perovskites which form a lead zirconate titanate (PZT) solid solution ($PbZr_x Ti_{1-x} O_3$), over the whole composition range (Shirane, Suzuki and Takeda, 1952). For $x \approx 0.52$, the piezoelectric, elastic and dielectric constants rise to their maximum values. This boundary has been termed the morphotropic phase boundary (MPB). Little information is available on the mechanical behaviour of the group of ceramics which have compositions near the MPB (Mabud,1980). A comparison of their machining properties is of particular interest. The contemporary technology that has been used to machine these materials has been diamond sawing and grinding followed by free-abrasive lapping and polishing. A wide range of products relies on the high-precision fabrication of piece-parts using ferroelectric ceramics, including: ultrasonic medical imaging transducers, ink jet printing heads, pyroelectric IR detection arrays, and optical modulation systems. Not only is precision important, but also the degree of sub-surface damage needs to be minimised because this is known to compromise performance by engendering depoling. It also leads to in-service problems due to ageing and noise effects caused by the movement of damage-induced domain walls and cracks. The objective of this study was to investigate a 'ductile mode' machining process for this group of ceramic materials reducing sub-surface damage and thus eliminating the need for lapping and polishing, leading to reduced costs of production. The possibility of machining ceramics using diamond turning and grinding in a "ductile mode" has been investigated by many researchers in recent years and is now recognised as an emerging technology with important applications. This is why ductile mode machining using different techniques is being investigated.

In the first stage indentation tests together with ruling machining trials using fracture mechanics techniques have been performed. Subsequently, single point diamond turning tests have also been tried.

2. MATERIAL PREPARATION

4mm thick disk shaped samples were diamond sawn from cylinders of PC4D (hard) and PC5K (soft) MPB PZT materials produced by Morgan Matroc Ltd (Unilator Divisison) (Commercial Literature, 1996). These were lapped and polished on a Logitech PM4 polishing unit fitted with a PP6 vacuum jig. The final flatness was to within better than half a wavelength of HeNe laser light (~300nm). Surface preparation was a two stage procedure. Initially, samples were lapped flat with 3 μm alumina in water slurry on a cast iron radially grooved lap. The second finishing stage consisted of polishing for one hour with colloidal silica on a polyurethane pad. The polishing pressure was $100 g/cm^2$ ($\sim 10{,}000\ N/m^2$) throughout. Samples of three different conditions of each composition were prepared. The conditions were a) poled in-plane, (or parallel to the surface), b) poled perpendicular to the surface and, c) unpoled. By observing the {002}/{200} X-ray diffraction (XRD) reflection doublet it could be seen that very little domain re-orientation had taken place in the near surface due to the final polishing.

3. QUASI-STATIC INDENTATION AND RULING

The crack system obtained in quasi-static indentation can serve as a basis for descriptions of material behaviour in processes such as machining. The response of materials to indentation provides information about wear, machining damage, fracture and yield strength. However, machining damage differs morphologically from isolated indentation damage with regard to the configuration of the plastic deformation zone and associated cracks, as well as the multiplicity of neighbouring damage sites (Marshall et al., 1983). The quasi-static indentation technique was used in this study to investigate the behaviour of PC4D and PC5K ceramics. Vickers indentation experiments were performed on a Matsuzawa Seiki MHT-1 micro-hardness tester with loads ranging from 10 to 500 grams. Six indentations at each load were made and analysed to obtain the hardness and fracture toughness values for both compositions. The values of PC4D hardness and fracture toughness were consistently higher than for PC5K. Poling direction had an important effect on fracture toughness results. Threshold loads and cracks were calculated and the results were found to agree with the Hagan (1979) model for brittle materials. Yield Stresses were calculated based in the model proposed by Studman, Moore and Jones (1977) and the results considering the stresses parallel (E_{33}) and perpendicular (E_{11}) to the polar axis.

Table 1. Yield Stress for PC4D and PC5K Ceramics

Poling direction relative to the sample surface	Stress direction relative to polar axis	Yield Stress PC4D (GPa)	Yield Stress PC5K (GPa)
Unpoled	N/A	1.46	1.12
Poled Parallel	E_{33}	1.46	1.16
Poled Perpendicular	E_{11}	1.57	1.32
Poled Parallel	E_{11}	1.62	1.39

Complementary to quasi-static indentation the process of single point diamond ruling as for diffraction-gratings was used for this study (Hirst and Howse, 1969). Tribological studies of ruling have demonstrated its relationship to quasi-static indentation (Hirst and Howse, 1969) and it has been shown that ruling is one of four fundamental material ablation processes categorised according to pre-set loading or depth and singularity or multiplicity of tool-points (Gee et al., 1983). Seven different loads from 21.5 to 113.4 grams (0.2109 to 1.112 N) were used in the ruling machine which used a hatchet-shaped tool. All samples were machined with groove direction parallel to the surface. For the samples poled in-plane, or parallel to the surface, two machining conditions were analysed: a) parallel to the poling direction and, b) orthogonal (90 degrees) to the poled direction. Three maximum ruling speeds of 22, 39.8 and 63.7 mm/sec were used for each load. The movement of the leadscrew was calibrated to maintain an index movement to avoid interference between adjacent grooves. XRD analysis using radiation CoKα was undertaken before and after ruling and the degrees of domain reorientation were compared. The ductile/brittle threshold depth of cut dependent upon material mechanical properties and the orientation of poling. PC4D exhibit a more ductile response when comparing with PC5K exhibiting this response over a range of loads and speeds. Using the model proposed by Bifano (1988) was possible to predict the critical depths of cut for ductile grinding as shown in Table 2.

Table 2. Critical Depth of Cut after Bifano (1988)

Poling direction relative to the sample surface	Stress direction relative to polar axis	Critical Depth of Cut of PC4D (μm)	Critical Depth of Cut of PC5K (μm)
Unpoled	N/A	0.3	0.4
Poled Parallel	E_{33}	0.6	0.7
Poled Perpendicular	E_{11}	0.4	0.3
Poled Parallel	E_{11}	0.2	0.1

These results show good agreement with the figures actually observed for PC4D and PC5K poled parallel to the surface and provide a basis for other machining processes to be interpreted.

4. DIAMOND TURNING

For some years single point diamond machining has been used routinely in many applications. Under normal engineering conditions diamond-turning of brittle materials is considered to be a crushing process producing surfaces characterised by conchoidal fractures and deep damaged layer (Bryan and Carter, 1985). Ductile machining phenomena have been observed in brittle materials when subjected to laterally moving indentors (scratching) in which a light cutting force has been applied. In such observations instead of brittle damage, material was seen to pile up either side of the machined groove (Taylor, 1949). This phenomenon has been described for single point diamond turning by Puttick et al. (1989), and it is apparent that, for cuts less than some critical depth of cut, together with appropriate machining conditions, glasses and other brittle materials can be machined in a ductile manner. As the need for machining glasses, crystals and infrared optics has grown, the technology of single point diamond machining has been adapted to machine brittle materials like BK7, silicon and germanium with very good results (Shore, 1995).

The ductile-brittle transition in single point diamond turning has been determined by machining a wedge grooved surface (Wills-Moren and Read, 1988), and by the shoulder analysis technique (Blake, 1988). The latter method requires removing the tool from the surface during a cut, leaving a shoulder in the shape of the tool radius. The work established general trends of the ductile-brittle transition as function of tool geometry and machining parameters (i.e. cutting speed). The critical cutting depth was obtained based in a straightforward analysis of the geometry shown in Fig 1 (Blake and Scattergood 1990).

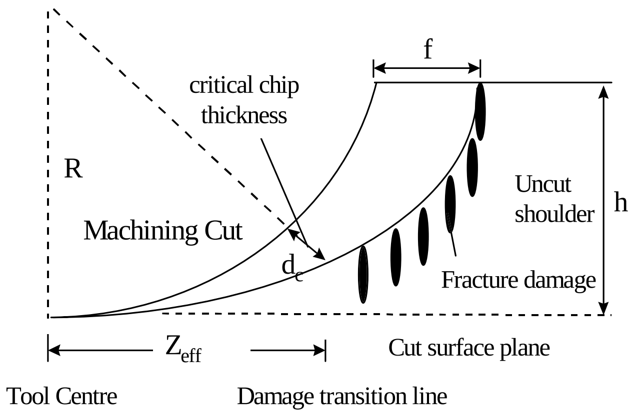


Figure 1- Geometry for relating the width Z_{eff} to the critical cutting depth d_c.

Using this geometry the critical cutting depth is obtained by measuring the ductile/brittle transition for several feed rates for each material, using the equation (Blackley and Scattergood, 1994):

$$d_c \cong \frac{f \cdot Z_{eff}}{R} \tag{1}$$

Where: f = feed rate

Z_{eff} = distance from centre of the tool to the ductile-brittle transition

R = Tool nose radius

Sintered PZT ceramics have been single point diamond machined by Nah (1995) and it was observed that the material composition was the most influential aspect in those tests. Feed rates and depths of cut were found to be the most important machining parameters when single point diamond machining these materials. This current investigation is aimed at identifying the conditions in which such ductile behaviour will be expected in hard and soft PZT ceramics.

5. EXPERIMENTAL PROCEDURE

5.1. Equipment and material preparation

Samples of PC4D and PC5K were single point diamond turned. The tests were carried out on surfaces which had a minimum amount of alteration from the bulk. The types of alteration to be avoided were, particularly, brittle grain pull-out and ferroelastic domain reorientation. Discs of PC4D and PC5K were lapped and polished with a Logitech[†] PM4 and the polishing route used was described in section 2. The polishing pressure was set to 100 gm/cm^2 and the platten rotational speed was set at 50 rpm throughout. The sample flatness obtained was better than one interferometer fringe of HeNe laser light (equivalent to $\lambda/2$ = 316.4 nm).

5.2. Single point diamond machining

Three unpoled samples of each composition were prepared and machined using a diamond tip on an air-bearing precision facing lathe. The diamond tip was obtained from Contour Fine Tooling Ltd (Commercial Literature, 1997) with 1.143 mm nose radius and a negative rake angle of 10°, and no cutting fluid was used. The cuts were done using a fast tool servo to remove the tool rapidly from the surface during the cut producing an uncut shoulder region to observe the ductile brittle transition. A Taguchi design experiment using two variables with three levels was prepared. The method was used in order to evaluate the sensitivity of the most important machining parameters based on previous tests (Nah, 1995). Two variables, feed rates and depths of cut, with three levels were chosen based on those used by Nah, although the PZT materials used for those tests had a higher level of porosity and therefore a lower mechanical strength. The Factors and levels used in these tests are shown in Table 3:

Table 3. Levels of factors chosen for the experiments

	Level		
Factor	(–)	(0)	(+)
Feed Rate (μm/ver)	0.1	0.7	4.9
Depth of Cut (μm)	0.1	0.7	4.9

In this case the factors are equally spaced in a logarithmic scale to cater for their wide range. The regions were machined with wedges varying in depth of cut from 0 to 400 nm, in order to obtain shallower depths of cut than the 316.4 nm (one fringe of HeNe laser light) which was the parallelism limit for the prepared samples. Nine runs were made for each composition three for each sample. Before and after machining the surface roughness was measured using a Wyko, Topo 3D phase shift (Linnik) interferometer, a non contacting white light interferometer fitted with a 40 times magnification objective, which provides a 250 μm^2 assessment area. Vertical resolution is claimed to be 0.6 Angstroms and the lateral resolution is 1 μm. After machining, three points in each region were measured and the average results of the surface roughness for each region was obtained. After the first assessment and the determination of the best feed rate and depth of cut, for both hard and soft PZT ceramics another set of tests was undertaken to investigate the effect of the negative rake angle, the influence of cutting speed and cutting fluid for the different poling conditions. The parameters

[†] Logitech Ltd, Erskine Ferry Road, Old Kilpatrick, Glasgow, Scotland, United Kingdom

used in these tests are listed in Table 4. All the combinations between these parameters were tested using a Taguchi design experiment.

Table 4. conditions used after the initial tests

Tool rake angle (degrees)	Cutting Fluid	Cutting Speed (rpm)	Poling condition	Material
-10	dry	500	unpoled	PC5K
		1000	poled perpend.	
-25	white spirit	2500	poled parallel	PC4D

5.3. X-ray diffraction analysis

X-ray diffraction permits the evaluation of crystallographic texture (Cullity, 1978, Cheng Lloyd and Kahn, 1992). In the tetragonal PZT, the diffraction {200}, {002} peaks form a doublet. The {200} {002} doublet was examined using CuKα radiation at a 2θ angle in the range of $43° < 2\theta < 45.8°$. A Siemens 5005 diffractometer operating under PC control was used for x-ray diffraction in small areas (3x2mm). The radiation was CuKα. The high lead content of PZT results in 90% of the CuKα radiation intensity being absorbed within the first 3.2 μm of the surface (Cullity, 1978). The {002}/{200} ratio was examined both before and after turning and the changes in domain reorientation were measured and quantified using *Traces* (1995) and *Peak Solve* (1996) software.

6. RESULTS AND DISCUSSION

The average values of the roughness R_a found in the polished regions of the three samples, were 15.3 nm for PC5K and 7.19 nm for PC4D. The best surface roughness average result in the hard PZT material was 5.02 nm, and the best surface roughness average result for the soft PZT material was 11.4 nm. None of the surface roughness average R_a results found in the hard material were better than that for the polished region. On the other hand the best surface roughness result found in the soft material was 9.69 nm in the second turned region, where the cutting conditions were 0.1 μm for depth of cut and 0.1 μm/rev for feed rate. The surface roughness R_a better than 20 nm was obtained in both compositions of PZT and it is possible to observe that the in the hard PZT material the surface roughness degrades less than the soft PZT material.

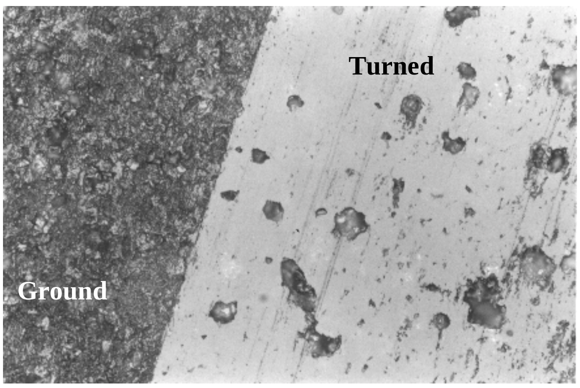


Figure 2- Optical microscope photograph of PC5K turned from the ground sample (The image is 360 microns wide)

It is possible therefore to use deeper cuts and faster feed rates to achieve the same surface quality. Nevertheless Fig. 2 shows ductile machining of soft PZT ceramics from the bulk material.Using the shoulders produced in the unpoled ceramics (Fig. 3) and the Eq. (1) the critical depths of cut calculated are shown in Table 5.

Table 5. Critical depth of cut using shoulder technique after (Blackley and Scattergood, 1994)

	PC5K	PC4D
Critical depth of cut (μm)	0.043	0.170

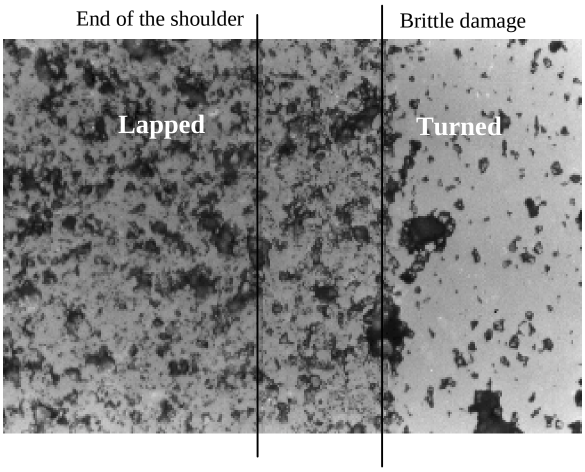


Figure 3- Shoulder in unpoled PC5K ceramic (The image is 360 microns wide)

The results from the x-ray diffraction tests show that, although good surface finishes have been achieved during the tests when using very fine feed rates and depths of cut, there were changes in texture on the sample surfaces. Based on the values used for these experiments the Table 6 shows the best conditions for each parameter, in order to minimise the surface textural effects in unpoled PZT materials.

Table 6. Conditions in which the textural effects on unpoled PZT ceramics were minimum in these turning tests.

	PC5K	PC4D
Feed Rate	4.9μm/rev	4.9μm/rev
Depth of Cut	4.9μm	4.9μm
Rake Angle	more negative	more negative
Coolant	dry cut	dry cut
Spindle Speed	no influence	no influence

These results show that in the range analysed, an increase in feed rate and depth increased the brittle damage producing more grain pull-out and reducing the internal strain on the bulk material. However although no improvement has been observed in the surface roughness with the use of more negative rake angles, the surface texture decreased with a tool of high negative rake angle of 25°. Dry cuts show superior surface roughness and less domain switching, and no influence was noted when using higher or lower cutting speeds. The advantages of poling PZT samples parallel to the surface after machining were not as noticeable during these tests as they were during the ruling and quasi-static indentation tests

(Beltrão et al., 1997). For these tests a facing lathe was used and therefore this produce constant changes in cutting direction on the sample surface during turning. During quasi-static indentation and ruling tests carried out in previous tests poling parallel to the surface showed strong anisotropy (Beltrão, 1998). A reduction in crack generation, grain pull-out and surface roughness was also observed during those tests in both compositions of PZT ceramic poled parallel to the surface. Unfortunately this phenomenon was not observed during turning because it was not possible to poled the samples in a radial or circumferential direction which was necessary to get an either orthogonal or parallel direction in the facing lathe used. The domain switching was also shown to be time-dependent. Turning is a process which has a much higher tool movement than quasi-static indentations or ruling which were processes for which the influence of poling direction was verified. They have a much smaller strain energy than single point turning and also the generation of heat due to the friction between tool tip and bulk material may have an annealing effect in these materials. However this fact could not be verified. The diamond wear rate was verified during the tests and is shown in Fig. 4 a) and b).

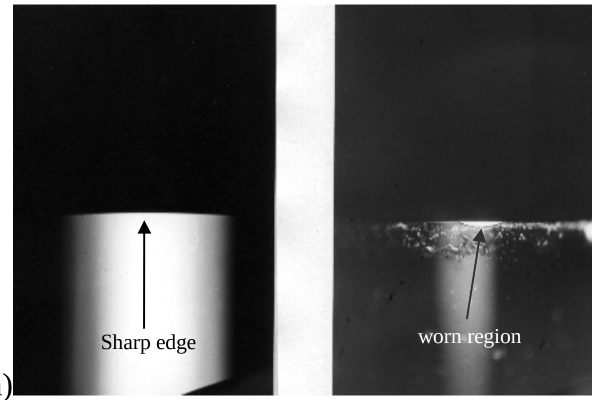
a)  b)

Figure 4- Diamond wear on the edges during PZT turning tests (each figure is ~1.0mm wide)

The diamond edge is seen to be highly worn (b) after ~ 6 km of machining. This may appear to be a long distance but in fact it does not represent a big machined area, as the feed rates used were in the order of 0.1 μm / rev.

7. CONCLUDING REMARKS

Quasi-static indentation techniques associated with ruling studies have been shown to provide some important insights into the mechanisms arising during the machining of PZT. Ductile behaviour was observed under some conditions, and poling procedures were found to change the machined behaviour of the same material composition. XRD analysis showed that the domain switching is associated with the ‘ductile’ machinability with this group of ceramics.

Ductile mode machining was achieved in both soft and hard PZT compositions when single point diamond turned. The hard material compositions showed a more stable behaviour than the soft material and they were easier to machine in a ductile mode.

X-ray tests indicate that negative rake angles (~ -25°) had a beneficial effect on the textural effects, reducing domain switching. Increases in feed rates and depths of cut reduced the domain switching because the brittle damaged releases the surface strain generated by the tool compression. Although the cutting forces were very small, the cutting areas were also small which increased the pressures on the tools over the surface. Diamond wear rate is also high when machining these materials, which together with the high levels of domain switching suggest that the single point diamond turning process should be used only for special applications when machining PZT ceramics. In order to solve the problem of diamond wear rate a multi-point diamond machining process (e.g grinding) was indicated.

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