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DUCTILE MODE CHIP REMOVAL IN ULTRAPRECISION DIAMOND TURNING OF MONOCRYSTALLINE SILICON

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Abstract. *Ultraprecision diamond turning of single crystal semiconductor is an important field of brittle materials machining research. Considerable progress has been made in this sector since it was found that brittle materials could be machined in the ductile mode when appropriate cutting conditions and tool geometry were used. The observation of the material removed can provide interesting insights on the chip formation mechanism and surface generation process. Single crystal (100) oriented silicon was diamond turned at different cutting conditions (feed rate and depth of cut). A fresh diamond tool with 0.77 mm nose radius and 0° / 12° rake/clearance angles was used in the micromachining tests. The morphology and topography of the chips removed in the ductile mode are similar to chips observed with non-ferrous metals. Surface features of diamond turned surfaces are qualitatively analyzed through scanning electron microscope. The surface roughness of the surface machined in the ductile mode are smaller than 11 nm Ra. The ductile regime in the machining of semiconductor crystals is interpreted in terms of the pressure/stress-induced phase transformation generated by the cutting tool tip/edge from silicon crystal (Si-I) to a metallic phase (Si-II) during cutting and amorphous silicon (Si-III) after cutting.*

Key-words: *Diamond Turning, Ductile Regime, Silicon, Phase Transformation.*

1. INTRODUCTION

The demand for faster fabrication processes and surface with complex shape stimulate the search for alternative machining processes to cut brittle materials. The application of single point diamond turning to the manufacturing of large lenses from monocrystalline silicon and germaniun, is increasing because of the possibility of achieving surfaces with low tolerances of form accuracy, fine surface roughness and low surface and subsurface damage. The fabrication of optical components with complex forms such as aspherics is well attained by this process. Aspheric lenses have the main advantage of turning a multi-element lens assembly into a much simples system. This technique was initially applied for the manufacturing of optical reflecting components from non-ferrous metals, mainly, aluminum, copper, electroless nickel, etc. Machinability studies of semiconductor crystals involving continuous chip removal and higher removal rates has been widely reported. Ductile regime diamond turning of brittle materials has been investigated based on the transition from ductile to brittle damage observed along the uncut shoulder resulting from interrupted cutting tests (Blake and Scattergood, 1990; Blackley. and Scattergood, 1991). This transition was initially examined based on fracture mechanics concepts (Nakasuji et al. 1990, Hiatt and Strenkowski,1991). Using the fracture mechanics approach it was found that brittle materials could be machined in a ductile manner when the depth of cut was restricted below a critical value (Puttick and Franks, 1990). Plastic deformation during machining of brittle materials occurs by shear involving mechanisms of slip system activation and dislocation movement. However, silicon exhibit limited dislocation mobility and, consequently, brittle behavior below 650 °C (Suzuki and Ohmura, 1996). Based on this fact, how to explain the anomalous plastic behaviour of silicon during machining experiments at room temperature. Evidences reported on high pressure (Jameison, 1963) and indentation (Clarke et al. 1988) experiments have demonstrated that diamond-cubic silicon transforms to the denser metallic β-tin structure under hydrostatic pressure at room temperature and; upon release of the pressure, a reversion to another form, i.e., an amorphous semiconductor phase, with a cubic structure has been reported (Hu et al.1986). The critical pressure observed to cause a transformation to a metallic β-tin structure is in the range of 11.3-12.5 GPa, under pure hydrostatic conditions (Clarke et al. 1988). However, this is reduced to values as low as 8 GPa when shear stresses are present (Gilman, 1992). Hence, it is well known that during machining there is a strong shear stress component acting in the first deformation zone, i.e., at the tool tip/material interface. Based on these knowledge, new hypothesis were raised in the debate on the mechanism responsible for the material removal in ductile regime diamond turning of semiconductor crystals. According to some results reported, it has been asserted that the ductile mode has its origin in this phase transformation induced by pressure/stress (Minowa and Sumino, 1992; Morris and Callaham, 1994; Morris et al. 1995). Recently, it was demonstrated that ductile regime diamond turning of monocrystalline silicon induced structural disorder probed by Raman scattering (Pizani et al., 1999). This can be considered an indirect evidence that the material undergoes a phase transformation during the cutting tests. This results corroborates with the assert that the ductile regime material removal is resulting from a intermediate β-tin metallic phase induced by pressure/stress during machining. On the other hand, in the brittle regime the main mode of material removal is fracture and no sign of structural alteration was detected. Because of the amorphous state observed in both chips and surface after the diamond turning of silicon (Shibata et al. 1994) and germanium (Morris et al. 1995), it is suggested that the results favour the hypothesis of the intermediate metallic phase being responsible for the ductile material removal mechanism.

In this work, monocrystalline silicon (100) oriented was single point diamond turned at different cutting conditions (feed rate and depth of cut). The ductile regime material removal is discussed based upon the morphology and topography of silicon chips. It is demonstrated that chip formation during machining of monocrystalline silicon is similar to chip formation observed with ductile metals machining. Surface features of diamond turned surfaces are qualitatively analyzed through photomicrographs made by scanning electron microscopy (SEM). It is also discussed that the ductile regime in the machining of semiconductor crystals is a consequence of phase transformation induced by pressure/stress generated by the cutting tool tip/edge.

2. EXPERIMENTAL DETAILS

Ductile regime diamond turning tests were carried out on a commercially available diamond turning machine, the Aspheric Surface Generator Rank Pneumo ASG 2500. This is a T-base carriage configuration; and carriages (hydrostatic bearing, driven with pulse-width-modulated dc servomotors, rotary-to-linear motion through 5 mm pitch ballscrews and position feedback using laser interferometer. Facing cuts were performed on monocrystalline silicon polished samples (10 x 10 mm^2) with (100) surface orientation. Figure 1 gives the schematic diagram illustrating the machining geometry with round nose tool. When round nose tool are used the chip thickness varies from zero at the tool center up to a maximum at the top of the uncut shoulder. Consequently, when the feed rate increases, the brittle-to-ductile transition is shifted downward toward the tool center. When the feed rate is decreased the transition is shifted upward toward the uncut shoulder. If the microfracture damage does not replicate below the plane of the machined surface (dashed line in Figure 1), a "ductile regime" machining along with brittle fracture will take place, but a smooth-mirror like surface will be achieved. On the contrary, as the feed rate is increased and microfracture damage replicate below the plane of the machined surface, then a "opaque" damaged surface will be produced.

The crossfeed direction was outside to inside. Table I depicts some physical and mechanical properties of silicon. Form Talysurf 120 L (Taylor-Robson®) was used to measure the surface roughness of the machined samples. The stylus tip radius is 2.5µm. Four measurements were carried out using roughness filter ISO 2 CR, sample length of 560 µm and 0.08 mm cut off. Average and standard deviation were obtained from the measured values obtained. Surface roughness of the polished sample was measured to be less than 4 nm. Only fresh diamond tools were used to perform the cutting tests. The single point tools used in this work were round nose single crystal diamond tools fabricated by Contour Fine Tooling®. Figure 2 shows a photograph of the workpiece fixed in the vacuum chuck being cut. Table II describes the experimental conditions and tool geometry used in the cutting tests. Alkalisol 900 (synthetic water soluble oil made from a complex mixture of organic and chloride solvents developed by ALKALIS BRASIL - Rua Volta Redonda,21 Guarulhos - SP -Brazil) was used as the lubricant and coolant during turning. A Digital Scanning Microscope, Zeiss model DSM 960, operated at 20 kV was used to conduct the observation of chips, surface and cutting tool edge. The chips observed were those left on the machined surface after the cutting tests. Metallization coating provided enhanced visualization of detail in the chips as well as the diamond tool cutting edge at high magnifications.

Table I. Properties of Single crystal Silicon (Wortman and Evans,1965).

Material Property	Value
Density (g/cm^3)	2.328
Melting point (°C)	1420
Young Modulus (GPa):	131
Fracture toughness K_{Ic} (MPa.m$^{1/2}$):	0.9
Shear Modulus (GPa):	79.9
Poisson's Ratio (ν):	0.266
Hardness Hv (kgf/mm^2):	1000

Table 2. Tool geometry and cutting conditions used in the cutting tests.

Tool geometry	Dimensions
Tool nose radius (mm)	0.77
Rake angle (°)	0
Clearance angle (°)	12
Spindle speed (rpm)	1000
Feed rate (mm/min)	1.25, 2.5 and 5.0
Depth of cut (μm)	3

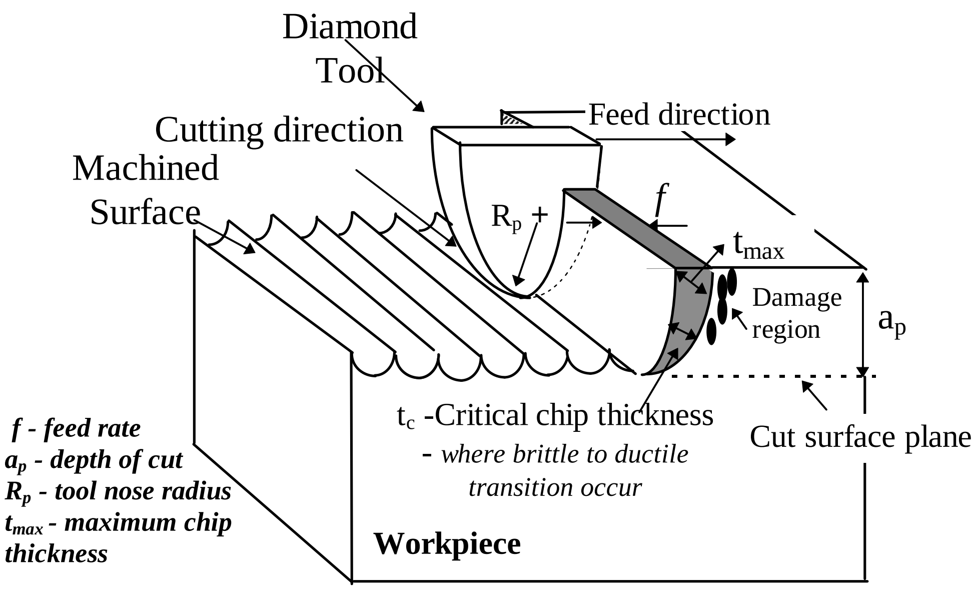

Figure 1 Schematic diagram illustrating machining geometry with round nose tool.

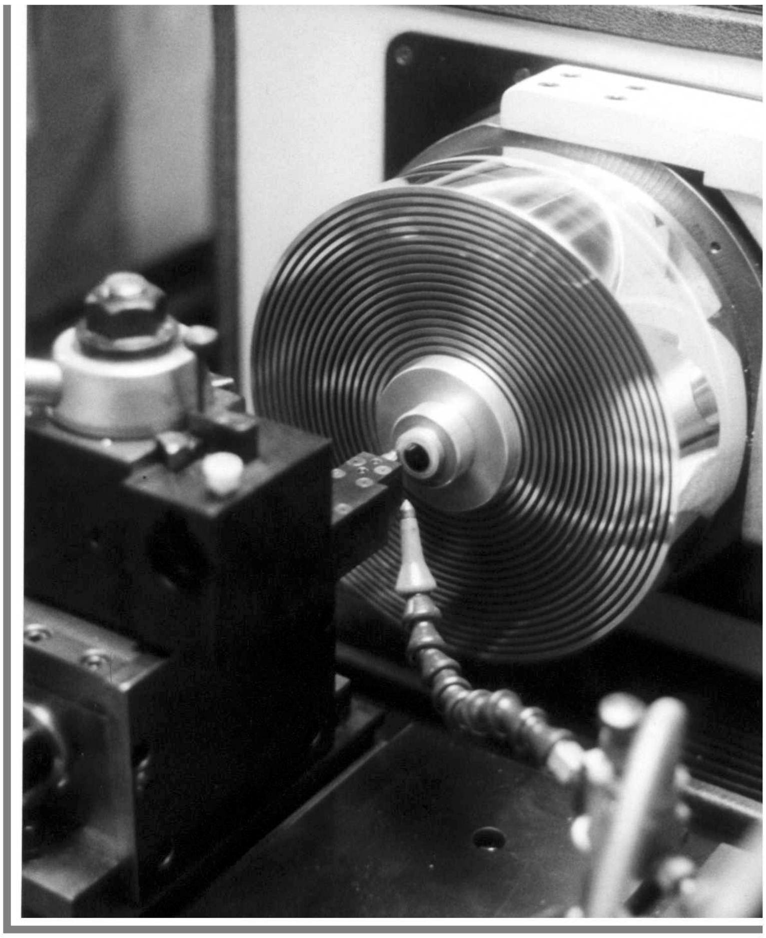

Figure 2 Photograph showing the workpiece fixed in the vacuum chuck.

3. RESULTS AND DISCUSSION

Experiments with three different feed rates were carried out. When silicon is machined in the ductile mode, ribbon-like chip are formed. Figure 3 is a photomicrograph illustrating a typical silicon chip removed in the ductile regime. Lamella structure is present and is similar to that observed in metal chips. Figure 4 shows a electroless copper (99.999% Cu) chip which depicts a different representation of the lamella structure. In this case the material is a polycrystalline aggregate and the orientation in each grain is different, consequently the lamellae size will be variable. The lamellae structure in the chip is formed as a result of shear deformation during chip formation process. There are three factors reported that can affect the lamella width. First, the increase in the thickness of cut will increase the lamella width (Black, 1979); second, the increase in the shear angle will decrease the thickness of the lamella (Blake & Scattergood, 1986); and third, there is the influence of the rake angle, positive rake angle produces thinner lamella structure and negative rake angle will generate thicker lamella structure (Jasinevicius et al. 1997).

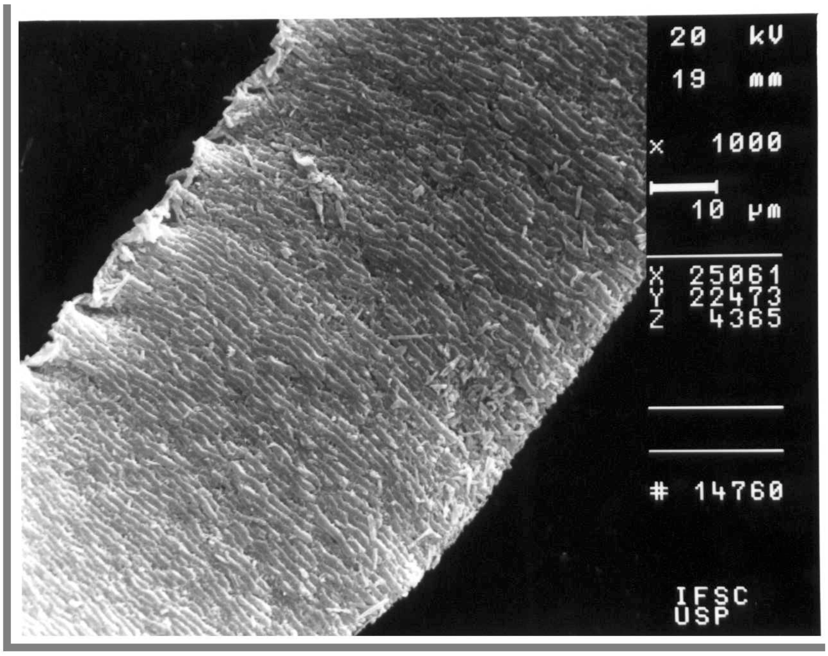

Figure 3. Photomicrograph made by SEM showing the typical morphology of chips removed in the ductile mode.

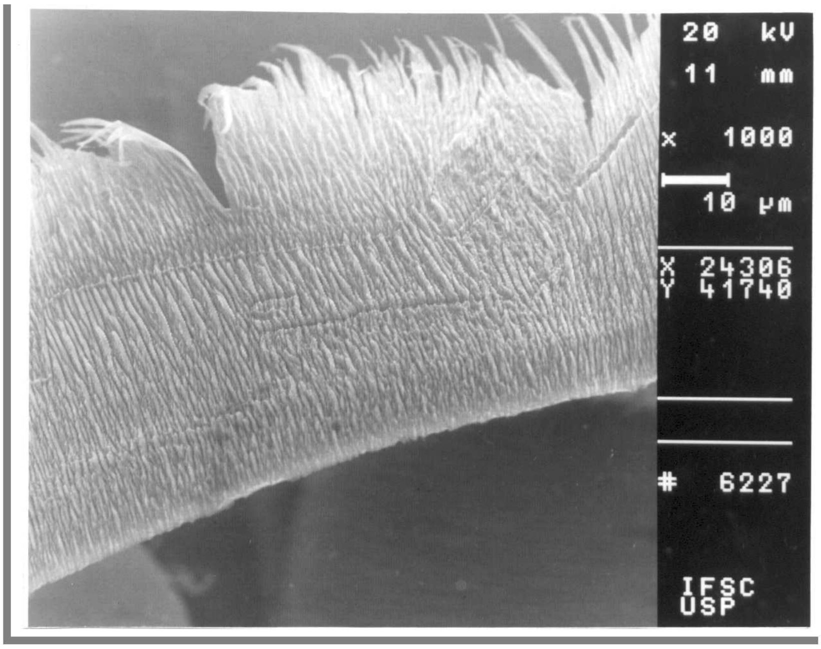

Figure 4. Photomicrograph made by SEM showing the morphology of electroless copper chip, the difference in the lamellae size is due to the different crystal grain orientation.

Figure 5 illustrates a surface machined in the ductile mode. In this case single point diamond turning has achieved fully ductile material removal and no sign of surface damage can be observed. This photomicrograph emphasizes the regularity of the machining grooves with a separation of 1.25 μm.

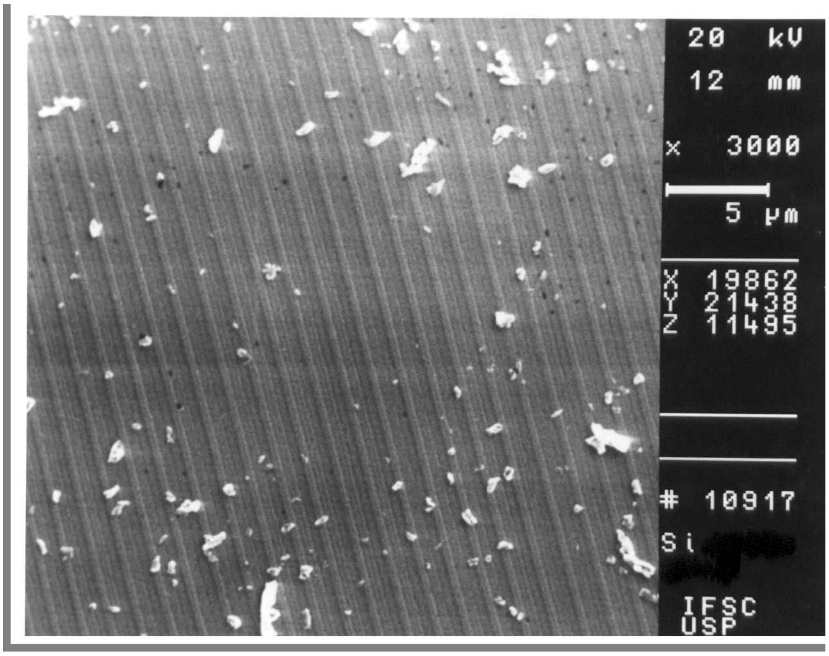

Figure 5 . Photomicrograph of the surface machined in the ductile mode. The cutting conditions f = 1.25 μm/rev and a_p = 3 μm, and the tool has 0.77 mm nose radius and 0° rake angle. Small debris are left on the surface after machining.

The mechanism responsible for chip formation process in the ductile mode still needs some discussion. It is possible that there are a second mechanism acting simultaneously in the chip formation process during diamond turning of semiconductor crystals. During cutting, the transformed metallic phase has a lower yield stress than the original cubic diamond structure, as a result, the ductile phase is pressed out at the tool/material interface. This make us believe that the lamellae formation might be also helped by plastic extrusion of this transformed metallic phase. This extrusion mechanism was previously observed by Phaar et al. (1991) during indentation with very low loads. Some clue on this discussion can be detected through the chips shown in Figure 6. This is a SEM photomicrograph illustrating a both side chip representation, where on the left side it is possible to observe the lamellae structure, and on the right side the face of the chip which contacts the tool rake face. The back of the chip is not smooth and mirror-like as it is observed in metal chips, on the contrary, it presents a kind of "scales" which could be termed as "lamellae tails", which seems to be a good clue to the extruding mechanism. It is worth mentioning that in this situation the plastic deformation can not be considered resulting from dislocation motion. Rather, this material might deform by ***viscous flow*** and the rate of deformation is proportional to the applied shear stress by the tool tip/cutting edge.

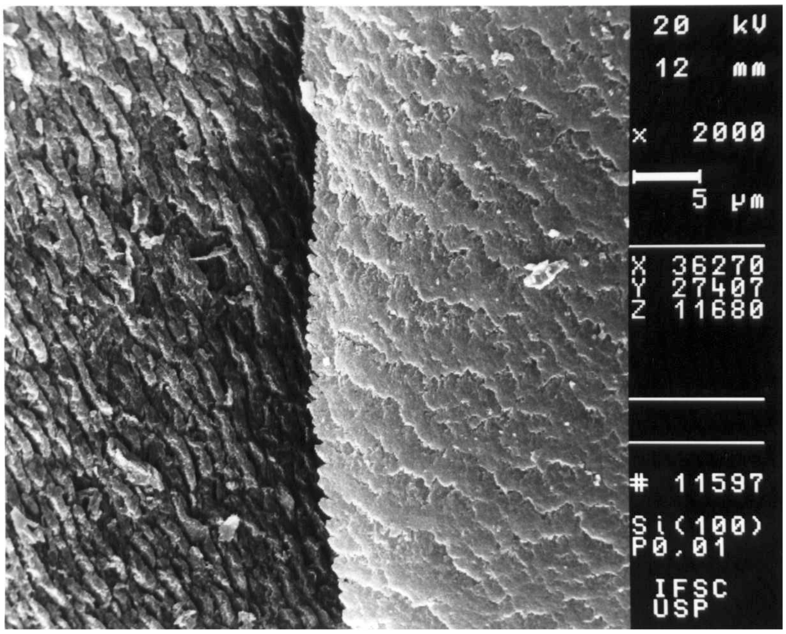

Figure 6 . Both side chip representation, where on the left side it is possible to observe the lamellae structure, and on the right side the face of the chip which contacts the tool rake face (after Jasinevicius et al. 1998).

The resultant silicon surfaces showed significant variations in surface roughness depending upon the machining condition, i.e., feed rate. This result is in agreement with expected tendency, i.e., the surface finish became very smooth as the feed rate was decreased below determined value. Figure 7 summarizes the surface roughness Ra data as obtained by Form Talysurf 120 L. The best finish was found at a feed rate of 1.25 μm/rev. When the brittle regime is present, the chips do not maintain its integrity. Silicon debris are found in the surface after machining and are resultant of brittle fracture. The 5 μm/rev feed condition surface roughness was the higher value encountered. The machined surface generated is illustrated in Figure 8. These surface defects leads to a diffraction effect from the otherwise mirror-like surface. The surface presents a “opaque” finish due to the large amount of microcracks. Despite the surface is machined in the brittle regime, it is still displaying the characteristic spacing of the marked grooves of 5 μm apart.

Finally, to produce a high quality mirror-like surface, it is necessary that no cracks or damage be generated in the surface and thus the machining process must be fully in the ductile regime. Appropriate cutting condition as well as tool geometry have to be found in order to achieving high performance during machining of brittle materials. Negative rake angle tools are more suitable to cut semiconductor crystals. The reasons may be related to the fact that negative rake tools generates higher shear stresses and the phase transformation is achieved with lower transition pressure. Lower feed rate also help obtaining the ductile regime as a consequence of the thickness of cut reduction. Recently, it was proposed that there exists a close relationship between the critical thickness of cut and the extension of the phase transformation induced by pressure and stress represented by the amorphous surface layer (Jasinevicius et al., 1998). More effort has been made in order to obtain more precise results in this direction.

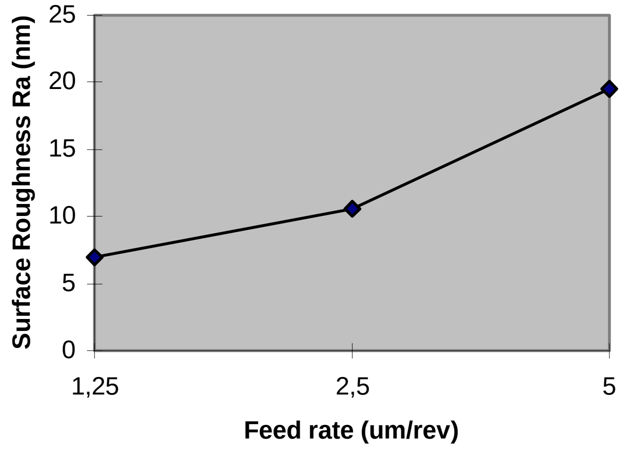

Figure 7. Ra surface roughness for Si (100) that has been single point diamond turned as function of feed rate. The tool radius was 0.77 mm and the lubricating/cooling fluid was Alkalisol 900.

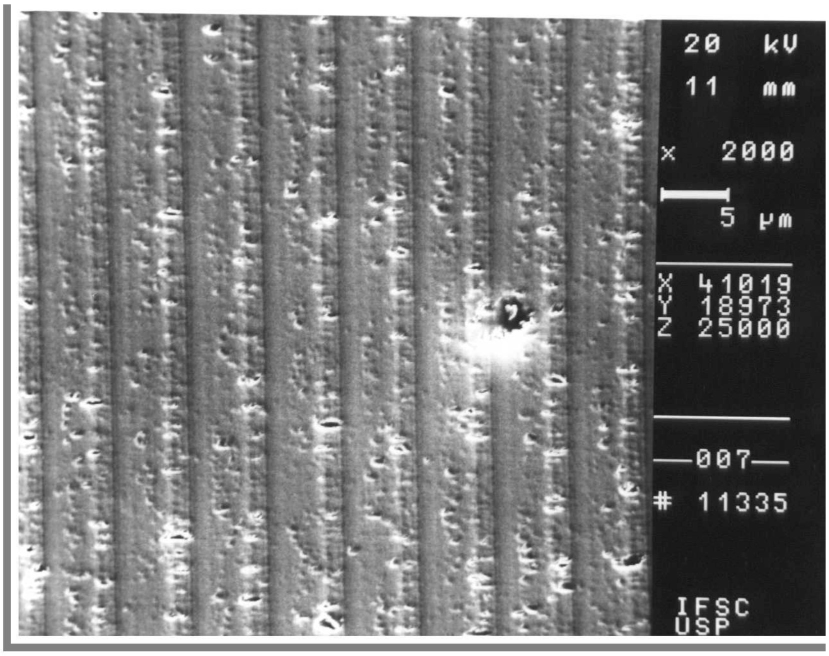

Figure 8 . Photomicrograph of the surface machined in the brittle mode. The cutting conditions are f = 5.0 μm/rev and a_p = 3 μm. and the tool has 0.77 mm nose radius and 0° rake angle. The surface presents a “opaque” finish due to the large amount of microcracks.

4. CONCLUDING REMARKS

The primary purpose of this work reported here was showing that ductile regime diamond turning of brittle materials is a viable technique. The process of ductile regime diamond turning brittle materials was investigated using monocrystalline silicon. Mirror-like surface, ductile material flow and continuous chip formation confirmed that ductile regime turning was achieved. It was briefly discussed that the mechanism involved in the process of ductile mode machining is a complex interplay of phase transformation induced by pressure/stress at the tool tip and plastic deformation occurring by shear involving mechanism of slip system activation and dislocation movement. The ductile response during SPDT exists when appropriate cutting conditions achieved. When fracture replicate bellow the cut surface plane, damaged surfaces are generated.

It was shown that when monocrystalline silicon is machined in the ductile regime, continuous chips are formed resembling those observed in the machining of nonferrous metals. The evaluation of chip topography and morphology can offer interesting information on material removal mechanisms involved during diamond turning of monocrystalline silicon.

Finally, the necessity of improved comprehension of the cutting process can help to extend this technology to be applied with other normally brittle materials.

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