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Numerical Simulations on Machining of Silicon Carbide

Jerry Jacob

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NUMERICAL SIMULATIONS ON MACHINING OF SILICON CARBIDE

by

Jerry Jacob

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Jerry Jacob
Experiments were conducted to determine the critical depth of cut for machining of single crystal silicon carbide through Single Point Diamond Turning (SPDT) and fly-cutting, and of CVD coated Silicon Carbide through scratching. The ductile nature of these nominally hard and brittle materials is believed to be the result of a high pressure phase transformation, which generates a plastic zone of material that behaves in a metallic manner. The SPDT experiments have shown chip formation similar to that in metal machining. This metallic behavior is the basis for using AdvantEdge, metal machining simulation software, for comparison to experimental results. The cutting and thrust forces generated from the experiments and the simulations compared favorably when the simulation depth is below the critical depth of cut. The differences in the results that do arise are due to a difference in the actual simulated machining depth versus the expected machining depth as a result of workpiece deflection.
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1.1 Silicon Carbide: An Advanced Engineering Ceramic

The term ceramic is often assumed to imply "classical" ceramics, which are the clay-based ceramics and whitewares such as porcelain (china). This is easily understood considering the major role these ceramics have played in the progress of human kind. According to the American Ceramics Society, the first use of functional pottery vessels is thought to be in 9,000 BC, while the first production of glass began around 1,500 BC. Since these ancient times, the manufacturing technology and applications of ceramics has steadily increased and today industries that benefit from their use include the refractory industry, the construction industry, the electrical and electronics industry, the communications industry, the medical industry and the aircraft and space industry. This has resulted in newer categories of ceramics that can be broadly classified as follows:

- structural clay products
- whitewares
- refractories
- glasses
- abrasives
- advanced (engineered) ceramics
Of these, the advanced engineered ceramics are considered for the purposes of the present work.

The definition of advanced ceramics has been vague for many years but several classifications have been made based on their chemical nature and functionality. In terms of their chemical nature, they can be classified broadly into oxides and non-oxides. The oxides include alumina and zirconia while the non-oxides include carbides, nitrides and borides (Srinivasan and Rafaniello, 1997). In terms of functionality, advanced ceramics are broadly classified as structural (cutting tools and engine components), electrical (capacitors, insulators, IC packages), optical (mirrors, windows, and lenses), and chemical (catalysts and catalyst supports). The functional benefits made possible by their unique properties include wear resistance, high temperature oxidation resistance, high hardness, high toughness, resistance to attack by chemical gases and hot molten metals and glasses. The unique combination of properties, such as: high thermal conductivity with electrical insulation, high strength to weight ratio, and optical and electronic properties, permit a wide array of potential applications in mechanical, electrical and optical components and systems.

According to Srinivasan and Rafaniello (1997), silicon carbide (SiC) is the leader among the various non-oxide ceramics that have found commercial applications. The properties of SiC such as – good strength and Young’s modulus as a function of temperature, relatively low weight (or high strength to weight ratio), corrosion resistance, and erosion resistance, make it an attractive engineering material. The raw materials used to make SiC are also relatively inexpensive, thus providing further
incentive for its commercialization. Thus the final products can be cost-competitive, besides offering a technical performance advantage, if economical manufacturing operations can be achieved.

1.2 The Structure of SiC

SiC has a close-packed structure with more than a 100 polytypes. (Powell et al., 1993). All SiC polytypes consist of 50% carbon atoms covalently bonded with 50% silicon atoms so that each Silicon (Si) atom has exactly four neighboring Carbon (C) atoms, and vice-versa, making a tetrahedral bond. The resulting structure is called zinc-blende or sphalerite and shown in Figure 1.1.

Figure 1.1: Zinc-blende crystal structure. White (open) atoms are Si and black (closed) atoms are C (Zetterling and Östling, 2002).

The different polytypes of SiC are actually composed of different stacking sequences of Si-C bilayers (also called Si-C double layers), where each single Si-C bilayer can simplistically be viewed as a planar sheet of silicon atoms coupled with a planar sheet of carbon atoms. The plane formed by a bilayer sheet of Si and C atoms is known as the basal plane, while the direction defined normal to the basal plane is
called the stacking direction. Using Ramsdell notation, the most common stacking arrangements are the 3C (cubic or β phase), 4H, 6H, 15R, and 27R (Rafaniello, 1997). The hexagonal (H) and rhombohedral (R) forms constitute α-SiC and vary by stacking sequence in the [0001] direction (see Figure 1.4) (Rafaniello, 1997). Figure 1.2 shows the stacking sequence of the most common polytypes being developed for electronics applications (Neudeck, 1998), which is one of the most promising applications of SiC.

![Diagram](image)

Figure 1.2: Stacking sequence of three polytypes of SiC (Zetterling and Ostling, 2002). Each layer (A, B or C) represents Si-C bilayer.

To help with future explanations in the present work, it is useful to further explain the 6H-SiC structure. While the three Miller indices h, k, l are used to describe directions and planes in the cubic crystal, for hexagonal crystal structures, four principal axes are commonly used: a₁, a₂, a₃ and c. Only three are needed to unambiguously identify a plane or direction. The three a-vectors (with 120° between them) are all in the close-packed plane also called the a-plane, whereas the c-axis is perpendicular to this plane (Zetterling and Ostling, 2002) as shown in Figure 1.3.
Figure 1.3: Principal axes for hexagonal crystals (Zetterling and Ostling, 2002).

Figure 1.4 schematically depicts the stacking sequence of 6H-SiC polytype, which requires six Si-C bilayers to define the unit cell repeat distance along the c-axis [0001] direction. The [1100] direction is often referred to as the a-axis direction.

Figure 1.4: Cross-sectional plane (1120) of 6H-SiC polytype (Neudeck, 1998).

SiC is polar across the c-axis, in that one surface normal to the c-axis is
terminated with silicon atoms while the opposite normal c-axis surface is terminated with carbon atoms. These surfaces are typically referred to as “silicon face” and “carbon face” surfaces, respectively (Neudeck, 1998).

1.3 History of Silicon Carbide Manufacturing

Naturally occurring SiC is called moissanite, first discovered in fragments of the meteorite at Diablo Canyon (Meteor Crater) in Arizona (Kelly, 2002). The creation of artificial SiC is credited to Edward Goodrich Acheson (in 1880) who in an attempt to create diamond from carbon and corundum ended up creating SiC (Guichelaar, 1997). He devised the trademark ‘carborundum’ because he at first mistakenly thought the crystals were a compound of carbon and alumina. The Acheson process provides the raw material for a number of industries. The highest tonnage produced is a material termed metallurgical SiC for the iron casting industry, while purer SiC is used in the abrasive and refractory industries, and powders are used for structural ceramics applications (Guichelaar, 1997). In addition, the process can provide irregularly shaped crystal platelets that can be further processed and used in electronic devices. Figure 1.5 shows platelets of SiC created as a result of the Acheson process.

According to Neudeck (1998), an improvement to the Acheson process is the Lely process invented in 1955, followed by the modified Lely process developed in the late 1970’s by Tairov and Tsvetkov. This process established the principles of a modified sublimation growth process of 6H-SiC.
At the genesis of the semiconductor electronics era, SiC was considered an early transistor material candidate along with germanium (Ge) and silicon (Si). Seed crystal growth techniques such as the Czochralski method helped produce large single-crystals of Si. But SiC cannot be grown by conventional melt-growth techniques, because SiC sublimes instead of melting at reasonably attainable pressures. Thus while production of small crystals in the laboratory permitted some basic SiC electronics research, they were clearly not suitable for semiconductor mass production. As such, Si became the dominant semiconductor fueling the solid-state technology revolution, while interest in SiC-based microelectronics was limited. The realization of SiC crystals suitable for mass production did not happen until the late 1980’s when improvements to the modified Lely process led to the creation of Cree Research in North Carolina, which began selling 2.5 cm diameter semiconductor wafers of 6H-SiC as shown in Figure 1.6, in 1989 (Neudeck, 1998).
Figure 1.6: Mass-produced 2.5 cm diameter 6H-SiC wafer manufactured circa 1990 via seeded sublimation by Cree Research (left), and 6H-SiC Lely and Acheson platelet crystals (right) representative of single-crystal SiC substrates available prior to 1989 (Neudeck, 1998).

Today a number of companies including SiCrystal AG, Nippon Steel, HOYA, SiCED and SiXON provide 3C, 4H and 6H polytypes of SiC wafers for electronics applications. While the production standards are improving, SiC is still behind Si, in terms of market penetration and technology maturation, due to limitations in manufacturing including the number and type of defects (particularly micropipes), size of wafers (currently limited to a maximum size of 4-6") and cost of equipment, all resulting in a wafer that is much more expensive (per unit area of volume) than Si wafer based products. These challenges posed by manufacturing are currently being addressed (primarily the difficulty of forming and fabricating and the resultant cost)
in the hope that the large number of attractive applications, taking full advantage of the materials enhanced properties, will be realized in the near future.

1.4 Applications of SiC

Srinivasan and Raniello (1997) provide examples of a variety of applications for SiC. According to them, the largest use of sintered SiC in the wear resistant material market is for fluid sealing applications such as mechanical shaft seals. Further, the resistance to acids and alkalis allows SiC to perform in demanding applications involving pumping of chemicals. The high thermal conductivity, and high emissivity in the infrared, in addition to the excellent creep resistance and oxidation resistance, have made reaction-bonded SiC (RBSC) the material of choice as burner materials to transfer heat efficiently to the surroundings. The high electrical resistance of SiC has been used to advantage in resistive heating applications such as igniters for natural gas furnaces. Laser mirrors are another application that is ideally suited for SiC because of its high section stiffness, ultra low weight, and thermal stability, besides being a cost-effective alternative to beryllium. SiC is also well suited for soft x-ray mirrors for synchrotron systems owing to its high hardness, good thermal properties and radiation resistance. The use of CVD coated SiC can help overcome the porosity problem, as a fully dense structure can be obtained for its use in mirror applications while being economical.

According to Schwier et al. (1997), SiC components with the highest density and strength may be produced by direct sintering, hot-pressing or hot-isostatic-pressing
HIPped SiC) from fine SiC-powders with sintering additives. High performance structural components require a sophisticated and controlled processing technology which necessitates the use of fine SiC-powders, which are generally characterized by high homogeneity and purity.

SiC has also found applications in the electronics industry in the form of LED, metal-semiconductor field effect transistors (MESFETs), power switching devices, laser diodes for next generation DVDs and semiconductor wafers (Cree, 2000).

1.5 Background of Research and Literature Review

The widespread use of SiC is limited, despite the demand, by the relatively high costs associated with finishing operations, especially in the semi-conductor and optics industries. The traditional fabrication processes include grinding with diamond wheels followed by lapping or polishing with diamond abrasives (Yin et al., 2003). These operations are used to achieve nanometer range surface finishes, which are not uncommon in these industries. Controlling or minimizing the sub-surface damage is one of the crucial factors during the machining operation, since this can severely limit the performance of these brittle materials (Morris et al., 1994). Compared to grinding, lapping, and polishing, single point diamond turning (SPDT) has the capability to precisely control the machining contour through high precision numerical control (Patten et al., 2004). Advances in the precision machining of brittle materials have led to the discovery of a “ductile regime” of operation, wherein material removal is accompanied by plastic deformation (Blake and Scattergood, 1990), which is capable
of producing fracture free surfaces. A review of the development and science of ductile regime machining of ceramic and semi-conductor materials is useful to understand the current status of the research. The rest of this chapter presents this overview of the state of the art and science of ductile regime machining of normally brittle materials.

1.6 Studies on the Ductility of Ceramics

Preliminary Diamond Anvil Cell (DAC) work on Silicon Nitride (Si$_3$N$_4$) conducted in the late 1990s demonstrated a high pressure phase (HPP) and was reported by Patten (2004). The HPP, formed at pressures in the GPa range, is believed to be responsible for the ductile nature of the ceramics at room temperature. A summary of experimental developments in nanoindentation of silicon (Si) by Domnich et al. (2000) revealed the elastic-plastic response and hysteresis of these normally brittle materials. Si transforms from the cubic diamond phase to a metallic phase at elevated pressures. Conductivity measurements confirmed the metallization of Si during nanoindentation, while scanning and transmission electron microscopy revealed amorphous Si and plastically extruded material around the indentations.

Scratching and nanocutting are other methods of studying ductile behavior, plastic deformation and material removal in ceramic materials at small size scales (generally limited to the nanometer to micrometer range). These methods are perhaps the closest analog to actual precision machining, although the stress fields associated with scratching are different due to the use of a stylus. The geometry of the stylus is
different than a cutting tool; in particular the rounded tip radius (typically rotationally symmetric and measured in micrometers) is not similar to a tool’s cutting edge, which typically has a large nose radius (millimeters) and a sharp cutting edge radius (nanometers) (Patten 2004). The unique advantage of scratching and nanocutting experiments is that they have helped to clearly identify a ductile-to-brittle transition depth by incrementally loading the workpiece material in a controlled and instrumented experimental condition. Nanocutting work done by Gao et al. (2000), and Patten and Gao (2001) have demonstrated the ductile response of Si. The critical aspects of this earlier work were the recording of the forces, the effect of the rake angle, and the determination of the DBT depth of cut. Further evidence of the metallic nature of Si was demonstrated during scratching of Si with a diamond stylus, where the electrical resistance was reported to have dropped approximately three orders of magnitude by Hirata et al. (2002).

1.7 Factors Contributing to the Ductile Regime Machining of Ceramics

Precision machining of germanium and silicon was studied using SPDT by Blake and Scattergood (1990), where special attention was directed to the ductile regime. In this work, an equation was developed to determine a parameter called the critical chip thickness. This parameter governs the transition from plastic flow to fracture along the tool nose and is given by

\[ t_c = \Psi \frac{E}{H} \left( \frac{K_c}{H} \right)^2 \]  
(1.1)
where $H$ is the hardness, $K_c$ is the fracture toughness, and $\Psi$ is a dimensionless constant that depends in a complex fashion upon machining parameters and tool geometry.

The SPDT operation is shown schematically in Figure 1.7 for the case of a round nosed tool. Here the geometry of the turning operation has an important effect on the process in that the effective chip thickness varies as a function of angular position along the tool nose (Blake and Scattergood, 1990).

![Figure 1.7: Schematic of SPDT operation with chip formation (Blake and Scattergood, 1990). $d$ is the depth of cut.](image)

Figure 1.8 shows the classic plane-strain condition for orthogonal machining. The nominal depth of cut ($d$) is defined as the height difference between the final cut and the initial uncut surfaces (also referred to as the uncut chip thickness, $t$). The critical depth of cut is a useful parameter as it helps obtain a basic estimate for depths below which machining will be dominated by ductile material removal as opposed to brittle
fracture i.e. $d < t_c$ to avoid fracture (Blake and Scattergood, 1990).

![Diagram of classical plane-strain orthogonal cutting geometry](image)

Figure 1.8: Classical plane-strain orthogonal cutting geometry (Blake and Scattergood, 1990).

It is worth noting from Figure 1.8 that a negative rake angle is specified for the tool geometry. The beneficial result of a highly negative rake angle tool has been demonstrated for a number of ceramic and semiconductor materials including,

Si - Nakasuji et al. (1990), Blake and Scattergood, and Patten and Gao (2001), Yan et al. (2001)


$\text{Si}_3\text{N}_4$ – Patten et al., (2004) and

$\text{SiC}$ – Patten et al., (2005).

A $-45^\circ$ rake angle appears to be the most advantageous (a range of -30 to -60 appears to be most useful), similar to results obtained in SPDT by Patten (1998). The advantage of a large included angle in machining brittle materials originates from the tool induced compressive stress state (hydrostatic pressure). The hydrostatic stress determines the strain at fracture which in turn determines the ductility or the
brittleness of the material under the state of stress. Diamond turning with a negative rake angle tool thus creates the conditions of high hydrostatic pressure that can be generated immediately underneath the cutting tool with a highly negative rake. Such a high hydrostatic pressure becomes a prerequisite for machining brittle materials by plastic flow at room temperatures. Due to the HPPT to a metallic state, the initially brittle material becomes sufficiently ductile (metallic) to sustain plastic flow (Patten 2004).

The other effect of the negative rake angle tool, due to the imparted compressive stress field is that it tends to suppress fracture, as compressive rather than tensile stresses dominate the stress field in front of the tool (the latter being more conducive to brittle fracture). Similarly, in the wake of the tool, in the trailing stress field, a negative rake angle tends to reduce the magnitude of this trailing tensile stress and also tends to move the location of the maximum tensile stress upwards-towards the surface, which tends to minimize the potential damage resulting from brittle fracture, i.e. the fracture is more likely to be contained to the near surface rather than subsurface region and is thus less catastrophic (Patten 2004).

Another factor to be noted in promoting a HPPT is the edge radius. Generally, a sharper cutting edge, such as an up-sharp edge for the tool, produces a higher pressure at its point of contact with the workpiece, and this promotes the formation of the HPP. A ratio of at least 5:1 is preferred when trying to cut a ceramic material, i.e. the depth of cut should preferably be 5 times the cutting edge radius, assuming the use of a highly negative rake angle tool. This promotes cutting as opposed to plowing or
rubbing at the tool-workpiece interface. However, work by Arefin et al. (2005) has indicated that ductile mode cutting of Si is possible if the undeformed chip thickness is smaller than the cutting edge radius of the tool.

During machining test, cutting forces \( (F_c) \) and thrust forces \( (F_t) \) are recorded (using force dynamometers) and the apparent coefficient of friction \( (\mu_a) \), which is \( F_c/F_t \), is studied for signs of ductile and brittle behavior. This is because \( \mu_a \) decreases as the depth of cut is reduced and eventually approaches the friction coefficient \( (\mu) \) for ductile machining. The relative value of the cutting and thrust forces as a function of the depth of cut, is also an indicator of whether machining took place in the ductile or brittle regime. Ductile machining is characterized by higher cutting forces (force per volume of material removed or energy per unit volume) as it takes more energy to remove material in the ductile mode rather than in a brittle fashion (Patten et al., 2005), i.e. it takes less energy to generate and propagate a crack (in a brittle material) than it takes to plastically deform the material, at the microscopic to macroscopic (but not necessarily at the nanometric) size scale.

In general, the cutting force is larger than the thrust force \( (F_c > F_t) \) for positive rake angle tools and the opposite behavior \( (F_t > F_c) \) is noticed for machining test with negative rake angle tools. Patten and Gao (2001) reported that the thrust force was greater than the cutting force while performing nanometric cuts on Si with \(-45^\circ\) and \(-85^\circ\) rake angle tools. They found that the thrust force increased with increasing negative rake angle, but the cutting force stayed about the same. Recent work (not published) conducted by Gao and Yasuto at Tohoku University also showed that the
thrust forces were larger than the cutting forces when using a -45° rake angle tool with 5° clearance, at depths of 50 nm and 250 nm.

The high pressures generated as a result of the negative rake angle and the sharp cutting edge of the tool can lead to ductile machining if the pressures are greater than or equal to the hardness of the material (Patten et al., 2005). Further, the HPPT region must extend sufficiently throughout the chip formation zone to avoid a brittle response resulting in fracture. This latter condition is generally provided by the highly negative rake angle tool, or when cutting at very small depths, where d < r. Patten’s model (1998) defines two zones of potential brittle behavior. One is a zone normally associated with a trailing tensile stress field in the wake of the tool and the other is the leading stress field in front of the tool, which acts to generate the chip. If the magnitude of this latter stress (within the chip formation zone) is at least equal to the hardness of the material and the spatial extent of it encompasses the chip formation zone, then the ceramic will undergo a phase transformation and chip formation will take place similar to machining of metals. This proposed model specifies

$$1 < \frac{r}{d} < 25$$  \hspace{1cm} (1.2)

as the criterion to achieve the HPPT, where r is the effective tool edge radius and d is the uncut chip thickness (or penetration depth). The practical upper limit, suggested above, of a value of 5 is taken as the limit for chip formation and material removal, whereas values between 5 and 25 represent plastic deformation in the form of plowing. Values above 25 would generally result in elastic contact for small depths (d) and brittle fracture for large depths.
Using these guidelines, experiments and machining conditions can be setup to increase the probability of ductile mode material removal in ceramics. However, multiple iterations on the process may be necessary before a proper understanding of the process parameters that influence the mode of material removal can be achieved, i.e. the DBT or the critical depth of cut is typically not known a-priori. Further, to induce phase transformation (to a metallic and more ductile state) through high pressures at room temperature as opposed to thermally induced phase transformations as suggested by Puttick et al. (1998), the machining is conducted at very slow speeds thereby separating out the thermal effects. In cases where tool wear is significant, the cost of tooling substantially contributes to the overall cost of the process. The significance of simulations in reducing the number of costly iterations becomes obvious and the need for such software (machining simulations) is realized.

1.8 Developments in Simulations of Ceramic Machining

While a significant portion of the machining literature relating to finite element (FE) modeling is related to metal machining, only a limited amount of work has been published in developing models to predict machining of ceramics. A notable publication includes recent work by Zhang and Feng (2004) that demonstrated the ability to simulate intragranular microplasticity and intergranular microdamage in polycrystalline α-6H SiC loaded under high confinement. The polycrystalline microstructure was simulated using 2-D Voronoi tessellation followed by a volume contraction. The resulting intergranular space was filled with grain boundary material.
Particularly impressive is their ability to simulate tensile cracks under load. Also, most FEA machining simulations are from micro-macro scale, and not nanoscale as needed to accurately represent ductile machining of these nominally brittle materials.

Noreyan (2005) developed molecular dynamics simulations to study nanoindentations in 3C and 6H-SiC and nanoscratching in 3C-SiC. With respect to nanoindentations, the work studied the dependence of elastic-plastic transition on the indentation velocity, size and workpiece temperature. Additionally, the dependence of pressure and critical indentation depth for the elastic-to-plastic transition on the indenter size was studied. The nanoindentation simulations were followed by nanoscratching on Si terminated (001) surface of 3C-SiC to investigate the dependence of the friction coefficient, scratch hardness, normal force, tangential force, wear of Si and SiC on indentation-scratching depth, scratching velocity, scratching direction, indenter size and indenter shape.

At present, the only commercially available simulation software for simulation of ceramic machining is AdvantEdge, developed by Third Wave Systems. This software is the outgrowth of a Ph.D. dissertation by Dr Troy D. Marusich from Brown University who went on to develop this software for commercial applications. AdvantEdge was primarily written as a finite element (FE) metal machining simulation software developed to optimize machining time and reduce tool wear. The software makes use of Lagrangian techniques to perform numerical modeling of metal cutting. Unlike simulation software that makes use of a predetermined line of separation at the tool tip (to cause separation of the chip from the workpiece),
AdvantEdge implements adaptive remeshing schemes along with explicit dynamics and tightly coupled transient thermal analysis to model the complex interactions of a cutting tool and workpiece (Marusich and Askari, 2001).

In addition to metal machining, AdvantEdge was used in the recent past to simulate, for the first time, 2-D orthogonal machining of the ceramic Silicon Nitride (Kumbera (2002), Ajjarapu (2004)). Over the years, the software has been improved to accommodate machining depths down to the nanometer range. Recently, simulations with depths of cut as small as 25nm have been successfully conducted. Further, to incorporate the pressure sensitive material model for machining of ceramics in the ductile regime, a Drucker-Prager yield criterion has been implemented in the software package as part of the material model in an effort to simulate or account for the effects of the HPPT.

In the present work, AdvantEdge is used to simulate 2-D orthogonal machining of SiC as well as a newly introduced 3-D scratching (grooving) module for simulations of Si and SiC. While both single crystal and polycrystalline machining data are available, the strain rate sensitivity of SiC during machining has not yet been properly characterized and as a result, the effect of this parameter on the simulation is purposely limited by adjusting parameters in the material model. Additionally, bulk material properties of SiC are considered in the simulation, i.e. directional dependencies of single crystal SiC have not been considered. The software presently cannot predict brittle fracture of ceramics. However insight into the likelihood of brittle, versus ductile, behavior can be obtained through analyzing and evaluating the
stress and pressure fields for indications of or the possibility of fracture and/or a ductile response, via the HPPT. Thus, the forces generated from the simulation are comparable to experimental results in cases where material removal was achieved through a ductile mode and not brittle fracture. In the case of brittle fracture, the experimental machining forces will be much smaller than that predicted by the simulation (which assumes completely ductile/plastic behavior) and care must be taken when making comparisons.

In the following chapters, simulations of machining of SiC and scratching of Si and SiC are presented and discussed to determine how well the simulated work compares with experimental results. This in turn will help determine the feasibility of using simulations to understand the mechanics of ceramic machining and possibly help reduce costly experimental testing iterations.
CHAPTER 2

MATERIAL MODEL FOR SIMULATIONS

2.1 Introduction

Currently, no known commercially available simulation software can successfully predict the behavior of ceramic materials such as silicon carbide (SiC) during machining operations. However, by confining the scope of the simulation to a ductile mode of material removal, it is possible to use the metal machining simulation software AdvantEdge to predict the behavior of SiC under machining operations such as 2-D orthogonal cutting and 3-D scratching.

The HPPT induced in semiconductors and ceramic, leading to ductile behavior has been documented to be metallic (β-tin) for some semiconductors (silicon and germanium) and is possibly, metallic for other semiconductors and ceramics, such as silicon nitride and SiC (Patten et al., 2004). Additionally, relatively long ductile (metal like) chip formation has been demonstrated in SPDT of SiC under nanometer scale machining conditions (Patten et al., 2005). Thus, under ductile material removal conditions (at the nanoscale), the simulation software could be used to accurately predict the forces and pressures generated by the tool-workpiece interaction for a given set of process conditions, assuming an appropriate material model is used. Properties that need to be specified to simulate machining include elastic and plastic behavior, heat transfer and thermal softening, and strain rate sensitivity.
2.1.1 Elastic and Plastic Behavior

The elastic behavior is specified by providing the Elastic (Young's) modulus and Poisson's ratio. The strain hardening behavior is specified by a power law model given by

\[ g(\varepsilon^p) = \sigma_0 \cdot \theta(T) \left( 1 + \frac{\varepsilon^p}{\varepsilon_0^p} \right)^{\frac{1}{n}} \]  

(2.1)

where, \( g(\varepsilon^p) \) is the flow stress, \( \sigma_0 \) is the initial yield stress determined using the Drucker-Prager yield condition (see section 2.2 on determination of initial yield stress), \( \theta(T) \) is the thermal softening factor, \( n \) is the strain (work) hardening exponent and \( \varepsilon^p \) and \( \varepsilon_0^p \) are the accumulated plastic strain and reference plastic strain respectively (AdvantEdge Theoretical Manual, 2004).

2.1.2 Heat Transfer and Thermal Softening

The value of thermal softening varies between 0 and 1 and is determined by

\[ \theta(T) = C_0 + C_1 T + C_2 T^2 + C_3 T^3 + C_4 T^4 + C_5 T^5 \text{, if } T \leq T_{\text{cut}} \]  

(2.2)

and

\[ \theta(T) = \theta(T_{\text{cut}}) - \left( \frac{T - T_{\text{cut}}}{T_{\text{melt}} - T_{\text{cut}}} \right) \text{, if } T > T_{\text{cut}} \]  

(2.3)

as given by Kumbera et al. (2001). In the present work, thermal softening is not considered as the speeds at which machining is performed are relatively slow and as such do not create any significant temperature effects. The thermal softening effects are not included in the simulations by disabling the thermal computations in the code.
For the polynomial shown in equation 2.2, $C_0$ is set to 1 while $C_1$ through $C_5$ are set to 0. Thus the value of thermal softening is 1 for temperatures below or equal to the cutoff temperature of the material and then drops linearly for temperatures greater than the cutoff temperature, reaching a value of zero at the decomposition or sublimation temperature (taken to be 2200 °C for this work). This behavior is shown in Figure 2.1.

![Figure 2.1: Variation in thermal softening with change in material temperature.](image)

### 2.1.3 Strain Rate Sensitivity

The strain rate sensitivity is given by

$$
\left( 1 + \frac{\dot{E}^p}{\dot{E}_0^p} \right) = \left[ \frac{\bar{\sigma}}{g(E^p)} \right]^{m_1}, \text{ if } \dot{E} \leq \dot{E}_i^p
$$

(2.4)

$$
\left( 1 + \frac{\dot{E}^p}{\dot{E}_0^p} \right) \left( 1 + \frac{\dot{E}_I^p}{\dot{E}_0^p} \right)^{m_2} = \left[ \frac{\bar{\sigma}}{g(E^p)} \right]^{m_1}, \text{ if } \dot{E} > \dot{E}_i^p
$$

(2.5)

where $\bar{\sigma}$ is the effective von Mises stress, $g$ the flow stress, $\dot{\varepsilon}$ the accumulated
plastic strain rate, $\dot{\varepsilon}$ is the reference plastic strain rate, and $m_1$ and $m_2$ are low and high strain rate sensitivity exponents, respectively. $\dot{\varepsilon}_0$ is the threshold strain rate which separates the two regimes.

Using the above constitutive models it is possible to generate a material model for SiC. One such material model was developed to simulate the machining of single crystal SiC. Using a value of 1 for thermal softening factor, 50 for the strain hardening exponent and published material data (Kamitani et al. 1997, www.coorstek.com, www.ceramics.org, and Gilman 1975), the stress-strain curve using equation 2.1 can be generated as shown in Figure 2.2. The values for input are shown in Table 2.1.

![Figure 2.2: Stress-strain curve of SiC developed for simulation.](image)
Table 2.1: Input values for stress-strain curve.

<table>
<thead>
<tr>
<th>Material property</th>
<th>Value</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Modulus, $E$</td>
<td>427.5</td>
<td>GPa</td>
</tr>
<tr>
<td>Thermal softening factor, $\theta(T)$</td>
<td>1</td>
<td></td>
</tr>
<tr>
<td>Hardness, $H$</td>
<td>26.0</td>
<td>GPa</td>
</tr>
<tr>
<td>Initial yield, $\sigma_0$</td>
<td>$H/2.2 = 11.8$</td>
<td>GPa</td>
</tr>
<tr>
<td>Reference plastic strain, $\varepsilon_0^p$</td>
<td>$\sigma_0/E$</td>
<td></td>
</tr>
<tr>
<td>Accumulated plastic strain, $\varepsilon^p$</td>
<td>$\varepsilon^p$ to 1</td>
<td></td>
</tr>
<tr>
<td>Strain hardening exponent, $n$</td>
<td>50</td>
<td></td>
</tr>
</tbody>
</table>

It should be noted that initial references on hardness of SiC were limited to polycrystalline material data and simulations were conducted using this value. Looking at Figure 2.2, the plastic part of the curve does not have a significant slope to it (minimal strain or work hardening). This is because the material model was developed to simulate a single crystal material where grain boundaries are nonexistent. Thus by setting the value of the strain hardening exponent to a high value (say 50), the strain hardening effects in the simulated material can be minimized.

The strain rate sensitivity in SiC for the ductile phase is presently not well understood and as a result $m_1$ and $m_2$ are set to high values to minimize the strain rate effects (Kumbera et al., 2001). Figure 2.3 shows a plot of the effect of $m_1$ on the strain rate sensitivity according to equation 2.4.
Figure 2.3: Effect of varying $m_1$ on strain rate sensitivity according to equation 2.4.

Thus for larger values of $m_1$, the slope drops and thus the effect is minimized. The value selected for simulations is $m_1 = m_2 = 100$. While there is limited data available from high speed ballistic testing of SiC (Grady and Kipp, 1993), further data was to be made available (through experiments by other facilities) during the course of the present research, but these data never materialized.

### 2.2 Determination of Initial Yield Stress

To reflect the ductile behavior in ceramics promoted by the HPPT, a pressure sensitive Drucker-Prager constitutive model as proposed by Ajjarapu et al. (2004) was specified as detailed below.

The Drucker-Prager Yield criterion is given by

$$\sqrt{3} J_2 + I_1 \alpha - \kappa = 0$$  \hspace{1cm} (2.6)
where, $I_1$ ($I_1 = \sigma_1 + \sigma_2 + \sigma_3$) is the first invariant of the stress tensor, $J_2$ is the second invariant of the deviatoric stress tensor is given by

$$J_2 = \frac{1}{6} [ (\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2 ] \quad (2.7)$$

$\alpha$ is the pressure sensitivity coefficient, $\kappa$ is the initial yield stress. The quantity $\kappa$ is given by,

$$\kappa = \frac{2.0}{\alpha - \sigma_1} \quad (2.8)$$

where, $\sigma_1$ and $\sigma_c$ are the yield stress in tension and compression respectively. The quantity $\kappa$ is equal to the Mises stress in the case when $\sigma_c = \sigma_1$, i.e. no pressure dependency.

The hardness of the SiC material is given to be 26 GPa (CoorsTek material data sheet) and the initial tensile yield stress ($\sigma_1$) is taken to be 11.82 GPa based on a proposed value of $H/2.2$ (Gilman, 1975) for brittle materials. The compressive yield ($\sigma_c$) is set to equal the hardness of the material (Ajjarappu et al, 2004).

For a uniaxial stress state ($\sigma_2$ and $\sigma_3$ are zero),

$$I_1 = \sigma_1 \quad (2.9)$$

and from equation 2.7,

$$J_2 = \frac{\sigma_1^2}{3} \quad (2.10)$$

Now using equation 2.8, $\kappa$ equals 16.25 GPa, and from equation 2.6, $\alpha$ equals -
0.375. These two parameters are set in the software material model, to provide a pressure-sensitive yield criterion; brittle fracture material behavior is not included in the model.

2.3 Material Model Validation

A material model validation study for SiC was recently conducted at the University of Tennessee (UT) using the Finite Element Analysis software Abacus (Shim et al., 2005). The result from this study was compared to the 6-H SiC material model used in AdvantEdge for simulations, as shown in Appendix A. 2-D simulations of SiC have shown plastic strain values as high as 8. However the UT model had values of plastic strain below 1. The curve was extrapolated up to a value of 8 for comparison purposes. It was determined that the curves showed different trends. The UT model showed noticeable strain hardening with flow stress reaching values close to 28 GPa for a plastic strain of 8 while the calculated curve stayed flat. This shows that there is a difference in the simulated material model and the model determined through the validation study.
CHAPTER 3

COMPARISON BETWEEN NUMERICAL SIMULATIONS AND EXPERIMENTS FOR SINGLE POINT DIAMOND TURNING OF SINGLE CRYSTAL SILICON CARBIDE

3.1 Introduction

The mechanical and thermal properties of silicon carbide (SiC) have traditionally allowed for its use in refractory linings and heating elements for industrial furnaces, as an abrasive in manufacturing processes, and in wear resistant rotating machinery such as pumps and engines. In the electronics industry SiC is used for high-powered/high temperature devices, where the high thermal conductivity, high electric field breakdown strength, and high maximum current density make it more promising than silicon (Si) (Zolper and Skowronski, 2005). The successful use of SiC in these industries impose stringent requirements on form accuracy and sub-surface damage (O’Connor et al., 2004) where surface finishes better than 10 nm are considered standard specifications (Blake et al., 1988). Brittle mode grinding and chemical-mechanical polishing (CMP) have been used to address these issues. Traditional grinding induces micro-cracks in the machined surface of brittle materials (Arefin et al., 2005), while polishing is widely accepted as an inherently slow and costly process (O’Connor et al., 2004), which is used to remove the surface and subsurface damage caused by grinding. Ductile mode machining or cutting technology has been studied as a replacement for grinding of optical devices and semi-conductors, such as Si
3.2 Background

Experiments conducted in recent years on Si (O'Connor et al., 2004, Arefin et al., 2005) and Silicon Nitride (Ajjarapu, 2004) have demonstrated a ductile mode of material removal similar to that seen in metals. Ductile mode implies a process dominated by ductile or plastic material deformation and removal rather than brittle fracture, resulting in a smooth surface (similar to a polished surface) free of fracture damage (Patten et al, 2005). The ductile nature of these hard and brittle materials has been attributed to the high pressure phase transformations (HPPT), which occur at or near room temperature. The HPPT is created as a result of the contact between the sharp tool and the workpiece at or below the critical depth of cut (Patten et al, 2004). This critical depth has been demonstrated to be in the nanometer range for SiC (O'Connor et al, (2004), Ajjarapu (2004), Patten et al, (2004 and 2005)).

Recent work (Patten et al, 2005) involving Single Point Diamond Turning (SPDT) of single crystal SiC was conducted to study, among other things, the effect of varying the rake angle and the depth of cut on the cutting and thrust forces, the resultant surface finish and the ductile to brittle transition (DBT). The forces from the experiment directly indicate whether the material removal is ductile or brittle during processing, while the final surface finish demonstrates achievement of ductile or brittle material removal. Ductile machining is characterized by higher cutting forces, as it takes more energy to remove material in a ductile mode as opposed to brittle
material removal for the same depth or volume of material removed (Patten et al., 2005).

The ability to characterize the mode of material removal through simulations provides an alternative approach to understanding the effect of varying machining parameters, such as rake angle, cutting edge radius, and depth of cut. A comparison of the resultant force per unit cross-sectional chip area (expressed as a pressure, GPa) can provide a measure or an indication of the mode of material removal, i.e. ductile or brittle. With this in mind, the focus of this chapter is to determine and evaluate the capability and accuracy of predicting the experimental results in the work reported by Patten et al. (2005) based on 2-D turning simulations conducted using v4.5 of the commercial machining simulation software AdvantEdge.

3.3 Experimental Procedures and Conditions

Results from three sets of experiments on single crystal SiC are considered for comparison to the simulations. The first set of experiments involved depths of cut (infeed) of 100 nm, 300 nm and 500 nm using a 2 mm round nose mono-crystalline diamond tool with a 0° rake angle. This same tool was reoriented to create an effective rake angle of -45°, and cuts were made at the same depths forming the second set of experiments. The first two sets of experimental results are reported in Patten et al. (2005). Additionally, machining at a depth of 50 nm was conducted but not reported previously. The third set of experiments involved 50 nm and 250 nm depths using a flat nose mono-crystalline diamond tool with a -45° rake angle. The
experiments were all conducted at a low speed of 3 m/min to minimize temperature rise and consequent thermal effects, such as thermal softening of the material. Dry cutting conditions allowed for collection of machining chips and provided simplified simulation boundary conditions, i.e. no coolant or cutting fluid effects were considered. Table 3.1 and Table 3.2 summarize the experimental process parameters.

<table>
<thead>
<tr>
<th>Table 3.1: Experimental Set I and II.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed (nm)</td>
</tr>
<tr>
<td>------------</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>100</td>
</tr>
<tr>
<td>300</td>
</tr>
<tr>
<td>500</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 3.2: Experimental Set III.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Feed (nm)</td>
</tr>
<tr>
<td>-----------</td>
</tr>
<tr>
<td>50</td>
</tr>
<tr>
<td>250</td>
</tr>
</tbody>
</table>

3.4 2-D Turning Simulations of 6-H Silicon Carbide

Simulations were carried out by using values that matched the experimental conditions. The simulations were conducted in 2-D and as a result a round nose tool geometry could not be simulated, therefore the simulated tool cutting edge is flat. The rake angle (α) and clearance angle (β) on the tools were varied based on the
experimental conditions. The cutting edge radius for all tools in the experiments was estimated to be between 20 nm and 50 nm. For the simulations, the cutting edge radius ($r$) was maintained at 40 nm.

The simulation process is a 2-D Lagrangian finite element-based machining model assuming plane strain conditions (Marusich et al., 2001). A typical setup for 2-D orthogonal turning with relevant parameters is shown in Table 3.3. Note that the nose radius cannot be simulated in 2-D but the approximation is valid for the small feeds for which the experiment and simulation were conducted.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Variable Definition</th>
<th>Workpiece-Tool geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>$r$</td>
<td>tool cutting edge radius</td>
<td><img src="image" alt="feed" /></td>
</tr>
<tr>
<td>$\alpha$</td>
<td>tool rake angle</td>
<td></td>
</tr>
<tr>
<td>$\beta$</td>
<td>tool clearance angle</td>
<td></td>
</tr>
<tr>
<td>feed</td>
<td>In-feed/uncut chip thickness</td>
<td></td>
</tr>
<tr>
<td>loc</td>
<td>length of cut</td>
<td></td>
</tr>
<tr>
<td>$v$</td>
<td>work piece velocity</td>
<td></td>
</tr>
<tr>
<td>$h$</td>
<td>height of workpiece</td>
<td></td>
</tr>
</tbody>
</table>

The workpiece was made long enough to ensure that the length of cut (loc) along the workpiece would allow for steady state conditions to be achieved. The height ($h$) of the workpiece was much larger (between 10 to 100 times) in comparison to the feed or uncut chip thickness. With regards to boundary conditions, the workpiece surface is assumed to be traction free and constrained in the vertical direction. The top and rear surfaces of the tool are rigidly fixed with adiabatic conditions.

The simulations were carried out using elastic properties for a 6H-SiC
polycrystalline material model, although the experiment made use of a single crystal 6H-SiC wafer, thus no crystal orientation effects (planes and directions) were included in the simulations. Additionally, the material model was set up to simulate a ductile workpiece, i.e. similar to metal machining. To reflect the ductile behavior in ceramics promoted by the HPPT, a pressure sensitive Drucker-Prager constitutive model as proposed by Ajjarapu et al. (2004) was specified as detailed in Chapter 2. The material model for the tool is polycrystalline diamond with elastic properties.

Since a slow cutting speed of 3 m/min was used during machining, the temperature rise was not expected to be significant based on simulations by Kumbera et al. (2001). As a result, thermal calculations were not enabled for the simulations in the interest of reducing computing time. A coefficient of friction (COF) of 0.4 was specified for the simulation based on the apparent COF from experimental data. The simulation matrix created to match all experimental conditions is given in Table 3.4.

Table 3.4: Simulation matrix.

<table>
<thead>
<tr>
<th>Experimental Set</th>
<th>Depth of cut*</th>
<th>Rake Angle</th>
<th>Clearance Angle</th>
<th>Tool geometry/(flat nose)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Set I</td>
<td>100</td>
<td>0</td>
<td>5</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>0</td>
<td>5</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td></td>
<td>500</td>
<td>0</td>
<td>5</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td>Set II</td>
<td>50</td>
<td>-45</td>
<td>50</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>-45</td>
<td>50</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td></td>
<td>300</td>
<td>-45</td>
<td>50</td>
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</tr>
<tr>
<td></td>
<td>500</td>
<td>-45</td>
<td>50</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td>Set III</td>
<td>50</td>
<td>-45</td>
<td>5</td>
<td><img src="image" alt="tool" /></td>
</tr>
<tr>
<td></td>
<td>250</td>
<td>-45</td>
<td>5</td>
<td><img src="image" alt="tool" /></td>
</tr>
</tbody>
</table>

*The depth of cut (doc) here refers to the in-feed or the uncut chip thickness.
3.5 Analysis of Force Data for Different Tools

In order to make a one-to-one comparison of the forces, the experimental conditions and the simulated conditions need to be considered. To conform to a 2-D orthogonal cut used during the experiments, the single crystal wafer of SiC was machined on its circumference (across the thickness) rather than the polished face. As a result, the only forces generated are cutting forces and thrust forces. Thus, a 2-D simulation of the experimental (machining) conditions is justified.

Experimental sets I and II made use of a round nose tool, while set III involved the use of a flat nose tool. The simulations were conducted in 2-D and as such, the results are directly comparable to a flat nose tool. A direct comparison of the experimental results and the simulation results for the nose radius tool is still valid. This is because the radius of curvature of the round nose tool (2 mm) used in the experiments, is much larger than the thickness of the wafer (250 µm, i.e. maximum width of the cut) over which the cuts were made (depths less than 500 nm).

The experimental cutting force and thrust force data provided in the graphs that follow are obtained from work done by Patten et al. (2005). For comparison to the simulated results, a single value of each force is reported which is representative of the average force for a given depth. However, for each depth, the crystallographic nature of the single crystal material created regions of both ductile and brittle material removal. Thus an averaged ductile force is reported when the machining operation is dominated by ductile material removal, and an averaged brittle force is reported in other cases dominated by brittle material removal. For the simulations, the force
results are always for the ductile conditions, since a ductile workpiece model was simulated. The polycrystalline material simulation model implies that orientation dependence is not accounted for. All simulated force results are based on achieving steady state conditions.

3.5.1 Cutting Force and Thrust Force Data for 0° Rake Angle with 5° Clearance Angle

Figure 3.1 shows a comparison plot of the cutting forces from the experiments and the simulations for different depths using a 0° rake angle tool with a 5° clearance. Referring to Figure 3.1, the simulation results show a steady increase in the cutting force with an increase in depth. The cutting forces from the experiments, however, do not show this trend. Note that brittle experimental cutting force values, i.e. lower values compared to purely ductile cuts, are reported in the case of 300 nm and 500 nm depths of cut, as these cuts resulted in predominantly brittle material removal. Additionally, the magnitude of the forces from the simulation are much larger than the corresponding experimental values, as the simulation represents purely ductile machining conditions, while the experiments, even at a depth of 100 nm, involve a combination of ductile and brittle cutting conditions.
In the case of the experiments, the cutting forces were dominated by brittle fracture events especially at larger depths (300 nm and 500 nm). In general it takes less energy (lower forces) to remove material in a brittle mode compared to the ductile mode of material removal (Patten et al., 2005). The decrease in the experimental cutting force from 100 nm to 300 nm is due to the transition from mostly ductile cutting at 100 nm depth to mostly brittle cutting at 300 nm, i.e. the ductile-to-brittle transition (DBT). The lower experimental cutting force at 100 nm, compared to the simulation, is also attributed to the combination of ductile and brittle material removal which occurred at this depth, i.e. it is likely that the DBT is < 100 nm, which reduces the cutting force compared to fully ductile cuts as reflected in the simulations.

The simulation material model does not account for brittle behavior and only simulates ductile material removal. The trend in the cutting forces from the simulation clearly shows this, with increasing depth requiring larger forces for
material removal. This accounts for the large difference in the comparison of force magnitudes (experiments and simulations) for the 300 nm and the 500 nm depths. For the 100 nm depth of cut, which is more ductile than the larger depths of cut, brittle material removal still occurs; but not to the extent that it does at the larger depths of cut, and thus the experimental forces are still lower than the simulated forces. A look at the pressures generated from the machining operation provides additional insight into this result. This aspect of the experimental results and simulations will be discussed next.

In order to generate a ductile cutting environment through purely applied stress (hydrostatic and shear) required that the pressures in the workpiece-chip interface need to be equal to, or higher than, the hardness of the material (O’Connor et al., 2004), which is taken to be 26 GPa for SiC. Experiments have indicated the hardness of 6H-SiC to be between 25-35 GPa (Noreyan, 2005). Table 3.5 provides the cutting forces from the experiment and the values for the force per unit cross-sectional area, i.e. cutting pressure, for the different depths of cut.

<table>
<thead>
<tr>
<th>Nose type</th>
<th>Feed (nm)</th>
<th>Cutting Force (N)</th>
<th>ChipArea (m²)</th>
<th>Cutting Pressure (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ductile Brittle</td>
<td></td>
<td>Ductile Brittle</td>
</tr>
<tr>
<td>round</td>
<td>100</td>
<td>0.45 0.15</td>
<td>24.7E-12</td>
<td>18.2 6.1</td>
</tr>
<tr>
<td>round</td>
<td>300</td>
<td>- 0.30</td>
<td>74.7E-12</td>
<td>- 4.0</td>
</tr>
<tr>
<td>round</td>
<td>500</td>
<td>- 1.00</td>
<td>124.5E-12</td>
<td>- 8.0</td>
</tr>
</tbody>
</table>

Table 3.5: Experimental cutting force and pressure data for different depths, 0° rake.
It is seen that the pressures, even in the case of the 100 nm depth of cut, do not fall within the range expected to achieve purely ductile cutting of 6H-SiC, i.e. pressures > 26 GPa. This is because the 100 nm cut, while being predominantly ductile, also produced some brittle fracture events. The reported ductile force is based on an average value of the forces obtained from the experiment, which includes a contribution (lower forces) due to some degree of brittle behavior even during the “mostly” ductile cut. Thus, a purely ductile cut would produce higher cutting forces (the partially brittle cutting conditions, even at a depth of 100 nm, would act to lower the average measured force), and thus higher pressures, would result in better agreement with the result obtained from the simulations. It is also noted that the use of a zero degree rake angle tools produces less ductile and more brittle behavior compared to a large negative rake angle tool, such as a -45° rake angle tool.

Figure 3.2 provides a plot comparing the thrust forces from the experiments and the simulations. Here both the experimental and simulated results show the general trend of increasing thrust force with increase in depth of cut. Further, the values are in much better agreement as compared to the cutting force results.
Figure 3.2: Thrust force comparison for $0^\circ$ rake.

The simulation does not account for brittle fracture and the relatively small difference in the comparison of thrust values (experiments versus simulations) can be attributed to this fact, as some brittle fracture occurred at all depths for the zero degree rake angle tool. Brittle material removal tends to affect the cutting force component, Figure 3.1, more than the thrust force, Figure 3.2. For a zero degree rake angle tool, especially at smaller depths of cut, brittle fracture is generated in front of the tool in the chip formation zone. Thus brittle fracture in the chip formation zone, which is most likely for the zero degree rake angle tool, affects the cutting force directly, whereas the thrust force is more sensitive to fracture occurring beneath the tool (Patten et al, 2004). Brittle fracture beneath the tool generally occurs either at larger depths of cut, even for a highly negative rake angle tool, or due to preexisting cracks in the workpiece surface. Brittle fracture beneath and behind the tool generally occurs during the unloading of the workpiece (in the wake of the tool) which occurs outside the force measurement loop of the sensing system. Thus the measurement
system is not sensitive to brittle fracture events of this nature.

3.5.2 Cutting Force and Thrust Force Data for -45° Rake Angle with 50° Clearance Angle

Looking at the cutting forces in Figure 3.3, the experimental cutting forces using a -45° rake angle show a trend similar to the 0° rake angle tool. The magnitudes of the cutting forces, however, are higher than the 0° case, as expected. This is due to the highly negative rake angle which is known to increase the cutting and thrust forces due to the conditions of high hydrostatic pressure generated immediately underneath the cutting tool (Patten et al., 2004), which promotes a ductile cut.

![Figure 3.3](image)

Figure 3.3: Cutting force comparison for -45° rake, 50° clearance.

The simulation software does not account for brittle fracture and assumes ductile cuts at all depths of cut. This accounts for the large difference in the experimental versus simulated results at the larger depths (300 nm and 500 nm). The experimental cutting forces at the 50 nm and 100 nm depths of cut compare favorably with the
simulated results, as these are the most ductile cuts and thus provide the most comparable conditions to the simulation. For the -45° rake angle tool, conditions throughout the chip formation zone are conducive for ductile deformation. However, as the depth of cut increases brittle fracture can occur in the wake of the tool (in the unloaded tensile stress field), which will then produce surface and subsurface cracks. These cracks will then affect the cutting conditions during chip formation, (during turning operations, the tool passes over the same region of the wafer with every revolution of the spindle) leading to a combined ductile (due to the HPPT) and brittle (due to the presence of cracks) material deformation and material removal, via formation of a chip. The effect of material removal via brittle fracture, for the case of a zero degree tool at larger depths of cut, is thus more dramatic, relative to the impact on the cutting force, compared to the more ductile conditions that are present for the -45 degree rake angle tool, even in the presence of material containing cracks (caused by the preceding pass of the tool).

The negative rake angle tool creates pressures high enough to accommodate the HPPT and the conditions generated as a result are comparable to the simulated conditions as shown in Table 3.6 (Pressures > Hardness for ductile cuts). Table 3.6 shows the average forces and the corresponding pressures that are generated for these machining conditions.

The thrust force values for this case are not reported due to large clearance angle (50 degrees), which decreases the pressure under the tool, and makes the comparison unrealistic.
Table 3.6: Experimental cutting force and pressure data for different depths, -45° rake, 50° clearance.

<table>
<thead>
<tr>
<th>Nose type</th>
<th>Feed (nm)</th>
<th>Cutting Force (N)</th>
<th>Chip Area (m^2)</th>
<th>Cutting Pressure (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ductile</td>
<td>Brittle</td>
<td>Ductile</td>
</tr>
<tr>
<td>round</td>
<td>50</td>
<td>1.70</td>
<td>-</td>
<td>12.2E-12</td>
</tr>
<tr>
<td>round</td>
<td>100</td>
<td>1.45</td>
<td>-</td>
<td>24.7E-12</td>
</tr>
<tr>
<td>round</td>
<td>300</td>
<td>-</td>
<td>1.23</td>
<td>74.7E-12</td>
</tr>
<tr>
<td>round</td>
<td>500</td>
<td>-</td>
<td>2.30</td>
<td>124.7E-12</td>
</tr>
</tbody>
</table>

3.5.3 Cutting Force and Thrust Force Data for -45° Rake Angle with 5° Clearance Angle (50 nm and 250 nm Depth of Cut)

The experimental and simulated values for the cutting forces, as shown in Figure 3.4, indicate a general trend of an increase in force with an increase in the depth of cut, for these predominantly ductile depths. While the simulated results are attributed to the ductile behavior of the model, the trend in the experimental values is due to the presence of brittle behavior at the 250 nm depth. Thus, the experimental value at 250 nm is larger but not substantially (lesser than 5x) larger than the 50 nm depth results, owing to the brittle nature of the cut at 250 nm, which reduces the corresponding cutting force, compared to the mostly or even completely ductile nature of the cut at 50 nm.
Figure 3.4: Cutting force comparison for -45° rake, 5° clearance.

The difference in the experimental and simulated values at 250 nm is again due to the completely ductile behavior of the simulated workpiece as opposed to that of the experiment conditions, which includes some brittle response. The simulated value at 50 nm depth compares most favorably with the corresponding experimental results, as the experimental conditions at 50 nm are mostly or even entirely ductile and thus more comparable to the simulation. Table 3.7 shows the values of pressure generated by the cutting force.

Table 3.7: Experimental cutting force and pressure data for different depths, -45° rake, 5° clearance.

<table>
<thead>
<tr>
<th>Nose type</th>
<th>Feed (nm)</th>
<th>Cutting Force (N)</th>
<th>Chip Area (m²2)</th>
<th>Cutting Pressure (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Ductile</td>
<td>Brittle</td>
<td>Ductile</td>
</tr>
<tr>
<td>flat</td>
<td>50</td>
<td>1.50</td>
<td>-</td>
<td>12.2E-12</td>
</tr>
<tr>
<td>flat</td>
<td>250</td>
<td>2.25</td>
<td>1.25</td>
<td>62.2E-12</td>
</tr>
</tbody>
</table>

Referring to Figure 3.5, the simulated thrust force value matches well with the experimental value at the 50 nm depth. The smaller value for the 250 nm result is due
to brittle fracture that accompanied the experiments, which reduces the overall thrust force compared to that of the simulation that is purely ductile.

Figure 3.5: Thrust force comparison for -45° rake, 5° clearance.

Figure 3.6 shows a pressure contour plot for the 50 nm depth of cut with -45° rake angle and the 5° clearance angle. Values in yellow are at the hardness of the material.

Figure 3.6: Pressure plot machining at 50 nm depth of cut.
3.6 Conclusion

The simulations were used to predict the behavior of SiC under different cutting conditions, by using the Drucker-Prager yield criterion. The simulations were able to satisfactorily predict the cutting and thrust forces generated under ductile cutting conditions. The simulations were not able to predict the forces where the experiments revealed brittle machining conditions, as expected as the software currently only includes ductile or plastic deformation and does not include a fracture criterion or brittle material removal mechanisms.
CHAPTER 4

2-D TURNING SIMULATION OF POLYCRYSTALLINE SILICON CARBIDE

4.1 Introduction

For semi-conductors and ceramics, high-pressure phase transformations (HPPT) can occur at the contact interface between the workpiece and the cutting tool. These high pressure phases are believed to be metallic in nature (Patten et al., 2005). The results from this earlier work, involving single crystal Silicon Carbide (SiC), showed that material removal was completely ductile at a depth of 50 nm using a -45° rake angle tool with a 5° clearance. Based on this information, plunge cutting experiments were conducted on a tube of polycrystalline SiC (CoorsTek SC-30) using straight edge (flat) diamond cutting tools, at two depths, 10 nm and 25 nm (Bhattacharya, 2005). The machining experiments were performed at these small depths to guarantee that material removal would take place in the ductile mode. Simulations matching the experimental process conditions and geometries were conducted, and the results were used to determine the precision with which the present model can predict the forces generated from experiments. Given the presumed metallic nature of the high pressure phase of this material, the metal machining simulation software AdvantEdge can be used for predicting cutting and thrust forces and can be used for comparison to the experiments. Thus, while brittle fracture of semi-conductors and ceramics cannot be simulated with this software at this time, machining forces generated from
experiments involving predominantly ductile material removal should be in good agreement with the simulations.

4.2 Simulation Setup for SiC

The simulation process is a 2-D Lagrangian finite-element based machining model assuming plane strain conditions. The simulations were carried out by specifying the elastic properties for polycrystalline α-6H-SiC (SC-30) provided by the manufacturer (CoorsTek). Thus, the constitutive model does not incorporate phase transformations and treats the material as elastic-plastic and ductile. To reflect the ductile behavior in ceramics, promoted by the HPPT, a pressure sensitive Drucker-Prager constitutive model as explained in section 2.2 is used.

The experiments on polycrystalline α-6H SiC were conducted at depths of 25 nm and 10 nm. The simulation software was able to simulate the larger depth of 25 nm but was not able to simulate, at this time, the depth of 10 nm due to present limitations in the code. The experiments were conducted at a low speed of 0.015m/sec, to minimize temperature rise and consequent thermal effects (such as softening of the material). Dry cutting conditions allowed for collection of chips and provided simplified simulation boundary conditions, i.e. no coolant or cutting fluid effects were considered.

The cutting edge radius for all tools in the experiments was estimated to be between 20 nm and 50 nm. For the simulations, the cutting edge radius (r) was maintained at 50 nm. Process conditions for the simulation are given in Table 4.1.
Table 4.1: Simulation tool, workpiece and process parameter listing.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cutting edge radius, $r$</td>
<td>50.0</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Rake angle, $\alpha$</td>
<td>45.0</td>
<td>deg</td>
<td></td>
</tr>
<tr>
<td>Clearance angle, $\beta$</td>
<td>11 &amp; 0</td>
<td>deg</td>
<td></td>
</tr>
<tr>
<td>Workpiece length, $l$</td>
<td>3.0</td>
<td>$\mu$m</td>
<td></td>
</tr>
<tr>
<td>Workpiece height, $h$</td>
<td>1.0</td>
<td>$\mu$m</td>
<td></td>
</tr>
<tr>
<td>(Actual) Depth of Cut, $doc$</td>
<td>24.0</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Length of Cut, $loc$</td>
<td>2.0</td>
<td>$\mu$m</td>
<td></td>
</tr>
<tr>
<td>Cutting Speed, $v$</td>
<td>5.0</td>
<td>m/s</td>
<td></td>
</tr>
<tr>
<td>coefficient of friction, COF</td>
<td>0.1</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

The width of the workpiece for simulation was set equal to the thickness of the machined cross-section of the tube (3 mm). Thus, the forces obtained from the simulation do not need to be normalized, with respect to the cross sectional area of the uncut chip or the volume of material removed, and a direct comparison of the experimental and simulation results can be made.

A clearance angle of 11°, as well as an iteration with 0°, was simulated. The 0° clearance was specified to simulate the effect of rubbing on the clearance face (as a result of significant tool wear in the experiments, mainly a result of the dry cutting conditions). A total length of 3 $\mu$m of the clearance face was in contact with the workpiece in the case of the 11° clearance angle while the contact length for the 0° clearance is not known. The experiments reported a contact length on the clearance face of 370 $\mu$m. This would require a simulation with a tool having the same contact length, and a workpiece material that is at least 1 to 2 mm in length (l). The relative
size scales of the depth of cut (nm) and the workpiece makes it difficult to perform
the simulation.

The cutting speed of the simulation was left at its default value of 5 m/s since
thermodynamic calculations were not enabled. Given the difficulty of the simulation,
the work was conducted with help from the software developers who chose to leave
the speed at the default value.

4.3 Results from Simulation of Polycrystalline SiC

Figure 4.1 shows the AdvantEdge results for the case with 11° clearance angle.
The workpiece deflection can be seen clearly, as well as the rubbing of the clearance
face on the workpiece material. Figure 4.2 shows the cutting and thrust forces from
this same simulation (as shown in Figure 4.1). These results and the force results from
the 0° clearance angle simulation are compared to the experimental results. Figure 4.3
shows a comparison chart of the results.

Figure 4.1: Pressure plot for 25 nm cut with 11° clearance angle.
The results show that there is a difference in the values obtained from the experiment compared to the simulation, especially in the case of the thrust forces. Further, it is noticed that the cutting force from the two simulations bounds the cutting force from the experiment, while the thrust force from the simulations do not
show the same trend.

4.4 Discussion of Results

The reason for the observed behavior may be due to a number of factors – the included angle (θ in Table 4.1), the material model, the force ratio, and the contact length, as further explained below.

4.4.1 Included Angle, θ

Changing the simulation clearance angle (β) from 11° to 0° led to an increase in the cutting force. The increase in the included angle of the tool effectively increased the contact area of the clearance face with the workpiece and led to increased rubbing. This increased rubbing added to the frictional force which is in the cutting direction and as a result increased the overall value of the cutting force.

The increased contact area of the tool with the workpiece also increases the resistance offered by the tool to the spring back of the workpiece material. This adds to the normal force seen by the simulation and can explain the reported increase in the thrust force value.

Post process analysis of tool edge showed significant wear on both the rake and clearance face, primarily due to dry cutting conditions. Further, there was greater wear on the clearance face compared to the rake face (Bhattacharya, 2005), due to the relative angles (11° and 45° respectively, resulting in about a 4:1 wear ratio). This would indicate that the included angle of the tool did increase similar to the setup in the simulation. However, the cutting edge itself appeared to be retained, and
maintained its sharpness.

4.4.2 Material Model

A different material model, compared to that outlined in Chapter 2, was proposed by Third Wave Systems (TWS), the developers of the simulation software. The difference in the material model lies in the manner in which the value of $\kappa$ (initial yield) is determined. The equation used in this case is

$$\kappa = \frac{H}{2.2}$$

(4.1)
as opposed to equation 2.7. In equation 4.1, $H$ is the hardness of the material. As a result (based upon equation 4.1 and using an $H$ of 26 GPa), the value of $\kappa$ is determined to be 11.82 GPa and $\alpha$ is 0.545 (as calculated using equation 2.6) as compared to a $\kappa$ value of 16.25 GPa and an $\alpha$ value of 0.38 as determined and used in the work presented in Chapter 2. The material parameters specified for this simulation are given in Appendix C-3.

A lower initial yield stress value would effectively reduce the simulation force values compared to a simulation with the higher initial yield criterion. This would mean that a harder material would result in increased values of cutting and thrust forces from the simulation. Looking again at Figure 4.3, this would move the simulated value of thrust force favorably toward the experimental value. This would however also increase the difference between the cutting force results unfavorably. To understand why this happens, it is useful to look at the force ratio and its contribution to the simulated cutting force results.
4.4.3 Force Ratio

The force ratio from the experiment is simply \( F_c/F_t \) (cutting force/thrust force), also called the apparent coefficient of friction (\( \mu_a \)), which is 0.1 from the experiment. This value is specified in the simulation as the friction coefficient (\( \mu \)). The results of the simulation however show that the force ratio is 0.23. Thus in order to achieve an apparent COF of 0.1 from the simulation, a lower value of \( \mu \) should be specified, and the cutting force values will then be in better agreement with the experiments and both the cutting and thrust forces from the simulations should show similar trends.

4.4.4 Length of Clearance Face

As explained earlier, the length of the clearance face is smaller than the value reported by the experiment. This would indicate that increasing the length of the clearance face would result in an increase in the cutting and thrust force values from the simulation.

4.5 Conclusion

Machining simulation of SiC at an actual depth of 25 nm has been achieved. This achieved depth is close to the current limit of the simulation software. A single value of cutting and thrust force obtained from the simulation agrees reasonably well (given that the software was operating at the lower limits of simulation depth) with the experimental results.

There is an increase in the cutting and thrust force values reported by the simulation by changing the clearance angle from 11° to 0°. Further, the cutting force
from the simulations bound the experimental cutting force values, but the thrust forces did not show the same trend. This is believed to be due to four factors: the included angle which increases the cutting and thrust force values, the softer material model which reduces the hardness of the simulated material, the specified friction factor, which should be smaller than the apparent coefficient of friction, and length of the clearance face.
CHAPTER 5

DETERMINATION OF THE CRITICAL DEPTH OF CUT IN 6-H SILICON CARBIDE THROUGH FLY-CUTTING

5.1 Introduction

The recent surge of interest in the research, development and testing of silicon carbide (SiC) (Zolper and Skowronski, 2005), has brought about increasing demands for higher form accuracy and better surface quality, coupled with lower costs (Tanaka et al., 2004). The machining of this hard and brittle material to achieve the required form and surface finish, is presumed to be made possible by the ductility, and the presumed metallic nature of its high pressure phase (HPP), or possibly as a result of amorphization in the material (Szulfarska, 2005). This allows SiC to behave in a ductile fashion, exhibiting plastic deformation at room temperatures (Patten et al., 2004). Since grinding and polishing are widely recognized to be slow and costly in semiconductor and optical applications, there is a continuing motivation to use single point diamond turning (SPDT) to eliminate some of these steps (O'Connor et al., 2004) to reduce production time (compared to polishing) and to reduce overall component costs.

Experiments involving SPDT performed on the edge of a single crystal wafer of SiC (6H) have demonstrated the ability to remove this material in a ductile fashion with the formation of chips similar to conventional metal machining (Patten et al., 2005). Further, this paper (Patten et al., 2005) identified a ductile to brittle transition
in accordance with the six fold symmetry of the crystal structure.

Recent published work made use of a fly-cutting operation to identify the critical chip thickness along different directions on the (001) cubic face of a Si workpiece (O'Connor, 2004). Unlike traditional SPDT, which performs multiple overlapping tool passes on the same surface, the fly–cutting operation used permits non-overlapping cuts, i.e. plunge cuts that produce scratch like features. Thus the resulting surface topography of each individual cut provides accurate information about ductile to brittle transition. However, the chip cross-section for these non-overlapping cuts is considerably different that the overlapping or feed based cuts, and therefore analysis and comparison is somewhat complicated by the resultant geometry.

5.2 Experimental Setup

The experiment was conducted by Jeremiah Couey at the Pennsylvania State University (PSU) under the supervision of Dr Eric Marsh. The fly-cutting experiment involved the use of a hydrostatic diamond turning lathe (Moore Nanotechnology Systems 150AG) consisting of two independent air bearing spindles – the fly-cutter spindle (Professional Instruments AC Foot/Flange) and the work spindle (Professional Instruments Twin-Mount). The axes of the two spindles are at right angles to each other, i.e. orthogonal, and offset. The setup has a translational resolution of 10 nm in the cutting and thrust directions for the fly-cutter spindle, and a rotational resolution of 1.6 arc-seconds on the work spindle. For reference purposes, fly-cutting setup of Si from O’Connor et al. (2004) is shown in Figure 5.1.
A 2 in. wafer of 6-H single crystal SiC from SiCrystal AG was used as the workpiece for these experiments. The workpiece was glued to a workpiece chuck (a block of aluminum) and a three axis dynamometer (Kistler MiniDyn 9256A2) was attached to the side of the workpiece chuck. The dynamometer is used to capture the forces during the experiment (not shown in figure). A fly-cutter head and diamond tool are mounted onto the fly-cutter spindle, while a capacitance probe (Lion Precision DMT-10 C1-C) placed behind the fly-cutter head triggers the data acquisition for force measurement. Since the tool-workpiece contact occurs only for a small period during a given revolution (less than 1% of a revolution) of the fly-cutter spindle, triggering the data acquisition helps to filter out a majority of the unnecessary data (while cutting air). Figure 5.2 provides a schematic of the fly-cutting operation.
The tool used for the machining experiment is a round nose monocrystalline diamond tool (Chardon Tool #3661) with a -45° rake angle (planar rake), 5° clearance angle and a 1 mm nose radius. The cutting edge radius of the tool is estimated to be 50 nm. A schematic of the tool is provided in Figure 5.3.
Figure 5.3: Schematic of diamond tip that is brazed on the tool shank.

5.3 Experimental Procedure

The experiment was conducted without the use of coolant, i.e. dry cutting conditions. The fly-cutter radius is estimated to be 110 mm. Adhesive was used to fix the workpiece to the workpiece chuck and this created an out of flatness condition. As a result, a number of preliminary passes were made on the SiC surface to ensure engagement of the workpiece. Since it is difficult to observe tool-workpiece contact given the desired depth of the cut (less than 1 µm), the data acquisition system (force dynamometer) was initially used to determine the tool-workpiece engagement or contact, indicated by a rise in the forces. Once tool-workpiece contact was established, the tool was relocated to a new position on the workpiece, and the experiment commenced. The data acquisition system was restarted now at the
commencement of the experiment. First the workpiece was fed in 250 nm from the touch-off height. In the time it took to start the workpiece spindle rotation, 6 overlapping passes (cuts at the same location collectively shown as cut 1 in Figure 5.4) had been made on the workpiece. After this, 3 more distinct (cuts 2, 3 and 4), non-overlapping passes were made on the SiC workpiece. The fly-cutter spindle was maintained at 45 RPM while the work spindle was maintained at 0.625 RPM. Thus, four distinct cuts were made with the diamond tool on the SiC workpiece, on the Si face, at a speed of 82.5 mm/sec.

5.4 Results from Flycutting of SiC

The cutting force and thrust force data for the entire duration of the experiment is plotted as shown in Figure 5.4. The first half of the data set (up to about 8000 counts) involves no contact between the tool and workpiece. This involved rotation of the fly-cutter spindle only and not of the workpiece (spindle). The subsequent rise in the cutting and thrust force values indicate the tool-workpiece contact. After 6 (six) passes (shown as cut 1 in Figure 5.4), there is an increase in the force value for cut 2, and then a gradual drop in the values for cut 3 and cut 4. The noise seen in the data is caused by the stiffness of the vacuum chuck air line hose. The slightest movement of the line caused a lot of vibration, especially during the latter part of the experiment. Cutting forces from cut 4 are within the noise from the measurement.
Figure 5.4: Cutting and thrust force data from the experiment.

The Wyko RST white light interferometer was used to collect the depth profile of each cut. Figure 5.5 shows one such image of cut 3 with varying depth for reference while the remaining images are given in Appendix B.

Figure 5.5: Wyko image of cut 3. Arrow shows direction of cut.
5.5 Discussion of Results

Looking at the forces from cut 1, there is an increase in force for the second pass as compared to the first pass. This is because the depth of cut was being increased to achieve a desired maximum depth of cut. After the second pass of cut 1, the depth was not increased any further and as a result the forces decreased with every subsequent pass, as presumably less material (and thus lower forces) was being removed in successive cuts over the same area. While the depth of cut was not increased after the second pass of cut 1, the tool still made contact with the workpiece, partly as a result of elastic spring back, and the tool probably cut slightly deeper and wider with each subsequent pass.

The second cut (cut 2) was made on a new location (after starting the rotation of the workpiece spindle) and the forces increase compared to cut 1. However, the forces from cuts 2, 3, and 4 show a progressive decrease in magnitude. This is attributed to the tilt in the workpiece setup as explained earlier, consequently leading to three different and decreasing depths for cuts 2, 3, and 4, even though the programmed depth of cut was not changed.

For analysis of the depth profile obtained using the Wyko RST, plots are made of a slice (plane) down the center of the cut along its length. The corresponding forces generated as a result of the cuts are plotted along with the depth profiles (as shown in Figure 5.6 to Figure 5.9). The forces are used to determine the ductile and brittle regions within the cut. The force data has not been filtered to eliminate the noise in the system.
Comparison of forces and scratch depth from Cut #1

![Graph of forces and scratch depth](image)

Figure 5.6: Forces generated from pass 2 of cut 1 while depth profile (lower image) is from final or resultant surface after all six passes of cut 1.

Comparison of forces and scratch depth from Cut #2

![Graph of forces and scratch depth](image)

Figure 5.7: Forces corresponding to cut 2.
Looking at the forces from the cuts, the cutting and thrust forces increase as the actual depth of cut is increased (Figure 5.7, Figure 5.8, and Figure 5.9). The cutting force from cut 4 is lost in the noise (refer to Figure 5.4) and is not shown in Figure 5.9. Since a -45° rake angle tool was used, the thrust forces are larger than the cutting
forces as expected. Figure 5.6 (cut 1 - note this surface profile resulted from six cuts at the same location) shows a catastrophic brittle fracture at depths larger than approximately 600 nm, while Figure 5.7 (cut 2) and Figure 5.8 (cut 3), show catastrophic fracture all along the length of the cut. Fracture in the workpiece material, with the brittle material coming out of the surface is indicative of fracture occurring behind or in the wake (trailing tensile stress field) of the tool (Patten et al., 2004). The resultant depth profile of cut 1 may be due to multiple (overlapped) passes of the tool on the same cut area, i.e. previously generated brittle fracture may be removed in subsequent passes. Figure 5.10 gives an optical image of cut 1 collected using the Nikon optical microscope. It can be noted that the image was combined from two separate images. The ends of the cut clearly show ductile surfaces as opposed to the center of the cut which shows brittle fracture.

Figure 5.10: Optical image of cut 1 showing ductile regions at either ends of the cut.

Looking at cut 4 in Figure 5.9, the profile of the cut varies smoothly up to a depth of approximately 70 nm, after which there is an abrupt change in the depth profile
indicative of brittle fracture of the material. Again, the material coming up out of the surface is indicative of fracture taking place in the wake of the tool. The profile resumes to a smooth transition as the depth of cut drops back to 70 nm and below, as the tool leaves the workpiece. An example of a very catastrophic brittle fracture that tool place during initial depth adjustments (not part of the experimental results) is provided in Figure B5 in Appendix B.

5.6 Conclusions

Four, distinct flycuts were made using a single crystal diamond tool (1 mm nose radius) on single crystal 6H SiC. The forces from the flycuts were plotted along with the corresponding depth profiles. It is seen that the forces rise as the depth of cut is increased, with the thrust forces being larger than the cutting forces due to the negative rake angle (-45°). Completely ductile material removal is observed from a single pass, up to depths of 70 nm, establishing approximately 70 nm as the ductile-to-brittle transition (DBT) for the non-overlapping (non cross feed) cuts. The DBT depth is consistent with work reported by Patten et al. (2005). The average force ratio (apparent coefficient of friction) was determined to be 0.22.
CHAPTER 6

NUMERICAL SIMULATIONS ON FLY-CUTTING OF SINGLE CRYSTAL SILICON CARBIDE

6.1 Introduction

The fly-cutting experiments discussed in chapter 5 indicated a ductile-to-brittle transition takes place in single crystal silicon carbide (SiC) at depths below 70 nm. This is consistent with the edge turning work reported by Patten et al. (2005), on the a wafer, where the DBT was established to occur between 50 nm and 100 nm. Among the four fly-cuts on the SiC workpiece, cut 4 shows ductile surfaces for a single pass of the tool and contains force values corresponding to the ductile depths. Simulations were conducted to match the conditions of this flycut. The resulting forces from the simulations were then compared with the experimental forces to determine how well they agree for depths at or below the critical depth of cut, i.e. in the ductile regime.

The flycut operation is inherently a 3-D operation and ideally should be simulated in 3-D for comparison purposes. However, relative size scales of the operation (nanometer dimensions of the cut compared to millimeter workpiece and tool nose radius), make it difficult to simulate the operation under release 4.5 and 4.6 of the AdvantEdge software. As a result, 2-D simulations are presently used to approximate the experimental conditions.

For a given cut, the flycutting operation creates a path that incrementally varies both the depth of cut (due to in-feed), and the width of cut (due to the nose radius), up
to a maximum set depth at the center of the cut. After this point, the depth and width continuously decrease in size until the tool exits the workpiece. Figure 6.1 shows a typical profile for a flycut, as taken from a white light interferometer surface measuring instrument (Wyko RST). The three-dimensional nature of the profile (depth and width are a function of length or distance along the cut) makes it difficult to perform a 2-D orthogonal cutting condition simulation while re-creating the 3-D machining conditions and geometry.

Figure 6.1: Typical profile of a fly-cut from machining obtained using a Wyko RST.

One approach (Method A) adopted herein, to approximate the 3-D cut with a 2-D simulation, is to obtain the machining forces at specific depths along the length of the cut, i.e. at specific cross sections. Separate simulations for each specific depth (constant workpiece thickness and depth of cut) can then be conducted. The resulting cutting and thrust forces can be compared to the values from the experiment based on a normalized force per unit cross-section of the chip calculation.
A second approach (Method B) is to simulate the height profile of the cut in 2-D. The 2-D simulation will however, limit the width of cut to a constant value. Now, if the tool in the simulation can trace out the curved tool path similar to the experiment (i.e. mimicking the radius of curvature of the cut path as seen in Figure 5.2), a comparable simulation can be conducted. However, the 2-D orthogonal simulations maintain the tool in a stationary location while the workpiece moves at a given velocity towards the tool in an orthogonal manner, i.e. the Lagrangian model. One way to overcome this limitation is to take advantage of the software’s capability to model a workpiece geometry with varying size or shape. By presenting the tool with a chip cross-section similar to what exists in machining experiments, the desired 2-D height profile similar to that seen in the experiment (as a depth) can be generated. Figure 6.2 shows a schematic of the simulation setup where the workpiece has been provided with a curvature similar to that seen in the experiment (the radius of curvature is similar, but the workpiece is convex whereas for the experiments the cut is concave). Note that the height profile (curvature of the workpiece) in the figure has been exaggerated for clarity.

Figure 6.2: Schematic of tool and workpiece setup. (doc = maximum depth of cut)
6.2 Method A: Constant Workpiece Thickness and Machining Depth

6.2.1 Simulation setup for Method A

This approach requires multiple simulations, each conducted at a specific depth for which a cutting and thrust force data point is available from the experiment. The material model for the simulation is single crystal SiC as explained in Chapter 2 with the parameters for the material model being outlined in Appendix C-2. As explained earlier, the profile from cut 4 is simulated as there are force values from ductile material removal present in this cut. The other cuts (cuts 1-3) contain forces resulting from mostly brittle fracture of the material in the wake of the tool, during machining.

Only thrust force results are available in the case of cut 4 as the cutting force was within the noise of the measurement (Figure 5.4). The thrust forces along with the depth profile for the case of cut 4 are shown in Figure 6.3 for reference. Also in this figure is a curve of what a completely ductile profile would look like. This is plotted on top of the actual (original) depth profile. The experimental depth profile of the cut contains a combination of ductile and brittle material removal. Further, the brittle material removal is believed to be fracture taking place in the wake of the tool and not in front of the tool.
Figure 6.3: Thrust forces and depth profile from cut 4. Direction of cut L to R.

The workpiece material in these simulations is very hard (26 GPa), and as a result it resists penetration by the tool, thereby reducing the effective depth of the cut to a value less than the programmed depth (in-feed). As a result, it is not possible to determine a-priori what the required programmed feed should be to achieve the desired actual feed after workpiece material spring back. Currently no equation or analytical expression exists to determine the required programmed depth of cut for a given material so as to achieve the desired actual depth of cut, although such an equation can be determined in the future. Simulations were conducted at different depths. The cutting and thrust forces obtained from the simulations are then interpolated to determine force values for the desired depths, i.e. to match the experimental conditions. The 61 nm depth had exact cutting and thrust force values, while the 75 nm results were obtained through interpolation. The tool, workpiece and process conditions for this set of simulations are summarized in Table 6.1.
Table 6.1: Tool, workpiece and process parameter listing.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cutting edge radius, ( r )</td>
<td>40.0</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Rake angle, ( \alpha )</td>
<td>-45.0</td>
<td>deg</td>
<td></td>
</tr>
<tr>
<td>Clearance angle, ( \beta )</td>
<td>5</td>
<td>deg</td>
<td></td>
</tr>
<tr>
<td>Workpiece length, ( l )</td>
<td>20.0</td>
<td>( \mu )m</td>
<td></td>
</tr>
<tr>
<td>Workpiece height, ( h )</td>
<td>7.5</td>
<td>( \mu )m</td>
<td></td>
</tr>
<tr>
<td>In-Feed, feed</td>
<td>variable</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Length of Cut, ( l_{oc} )</td>
<td>15.0</td>
<td>( \mu )m</td>
<td></td>
</tr>
<tr>
<td>Cutting Speed, ( v )</td>
<td>0.518</td>
<td>m/s</td>
<td></td>
</tr>
<tr>
<td>Friction factor</td>
<td>0.1</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

6.2.2 Results from Method A

In order to compare the forces from the simulation with the forces from the experiment, it is necessary to normalize the forces. This is done by dividing the force by the contact area of the tool with the workpiece. It is very difficult to estimate the tool-workpiece contact area for thrust force normalization. The calculations are complicated by the error in estimating the actual cutting edge radius (usually assumed to be 50 nm), and the length of the clearance face in contact with the workpiece. The contact area for the cutting force is more straightforward and is the actual chip cross-section in each case. In the case of the experiments, the chip cross-section is a sector of a circular cross section created by the tool’s nose radius, while the simulated chip cross-sections are rectangular due to the 2-D orthogonal machining (constant width of workpiece).

To normalize using the chip cross-sectional area, it is necessary to use the cutting
force and not the thrust force. Given the thrust force and the apparent coefficient of friction ($\mu_a$) from the experiment, it is possible to estimate the cutting force. Using this approach, the estimated cutting force at each desired depth, based on a $\mu_a$ of 0.22 as reported in Chapter 5, is given below in Table 6.2.

<table>
<thead>
<tr>
<th></th>
<th>61 nm</th>
<th>75 nm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thrust force (N)</td>
<td>0.1031</td>
<td>0.1247</td>
</tr>
<tr>
<td>Estimated Cutting force (N)</td>
<td>0.0227</td>
<td>0.0274</td>
</tr>
</tbody>
</table>

Figure 6.4: Variation in normalized cutting force with depth of cut, Method A.

Figure 6.4 shows the variation in the normalized cutting force ($N/m^2$) for two different depths of cut from the experiment and from the simulation. The graph shows the force per unit chip cross-sectional area, which is a normalized force value in units of pressure (Pa). From the plot it can be seen that the normalized cutting force for the
experiment at 61 nm is larger than the value for 75 nm. While the values from the simulation show the same trend as the experiment, the simulation values do not show a significant difference between the force values for the two depths. The depth of 75 nm shows a difference between the normalized value of thrust force for the experiment and the simulation.

6.2.3 Discussion of Results from Method A

The ductile-to-brittle transition depth for the material is believed to be 70 nm as explained in Chapter 5. At the smaller depth of 61 nm, the experimental (normalized) cutting force value is larger than the value at 75 nm. This is because the 61 nm depth is ductile (smaller than DBT depth) and as a result requires more energy to remove the material compared to material removal in a brittle mode (Patten et al., 2005). The normalized cutting force for the two depths in the case of the simulations however, is comparable. This is because the simulation does not account for brittle material removal and assumes ductile material removal even at the larger depth. Further, this reasoning also accounts for the difference between the values of the experiment and the simulation at the depth of 75 nm, where the experiment represents a partially brittle cut, while the simulation represents a purely ductile cut.

6.3 Method B: Variable (curved) Workpiece Thickness and Constant Machining Depth

6.3.1 Simulation setup for Method B

This approach, as mentioned previously, attempts to mimic the fly cutting
operation and the geometry of the cut surface, i.e. replicate the shape of the cutting path. This is achieved by providing a curvature in the workpiece material (an inverse or mirror image of the actual experimental cutting path), thereby presenting the tool with an effective chip thickness equal to what it would see during the fly-cutting operation as it traces out a curved path in the workpiece (Figure 6.2). As the tool engages the workpiece, the depth of cut (doc) increases from a value of zero at the beginning of the cut to a maximum (at the center along its length), and then reduces back to zero at the end of the cut.

The tool parameters and process conditions for this simulation are the same as that outlined in Table 6.1 except for the length of cut, and the feed. The length of cut (loc) was set to 140 µm, to equal the actual length of material removal from experiment. The length of cut parameter is usually set to a value so as to ensure that a sufficiently long cut is produced such that steady state conditions are achieved in the simulation. In this particular case, the depth of cut continuously varies and as such, steady state conditions are not achieved. The initial feed (depth) was set to be 250 nm as suggested by the software developers, since the desired (ideal) feed of zero was not supported under the current release.

6.3.2 Results from Method B

To simulate this condition, the curvature of the workpiece will provide the desired depth of cut (refer to Figure 6.2). Figure 6.5 shows a plot of the cutting forces collected from the simulation plotted along with the depth profile of cut 4. A third order fit was applied to the curve of the cutting forces from the simulation to obtain a
smooth curve.

Figure 6.5: Simulation cutting force variation with depth of cut for cut 4.

The simulation stops about 70% of the complete length of cut. This is because of a numerical error in the computations. To compare these forces to the experiment, the cutting forces need to be normalized. The normalized values from the experiment and simulation, for the two depths of interest (61 nm and 75 nm) are shown in Figure 6.6. The two cutting forces for the two depths from the simulation can be obtained by interpolating between existing force values in the plot or by directly extracting from the simulation results after determining the required locations along the cut. Here it can be seen that the normalized cutting force values from the simulation are much larger than the experimental values. Further, the normalized values from the simulation show the same trend as the experiments.
6.3.3 Discussion of Results from Method B

The simulation forces show a significant difference from the experimental values, and this has to do with the initial (tool) depth of cut specified for the simulation. As explained before, the simulation does not permit a zero initial depth of cut for the tool with respect to the workpiece. An initial tool depth of 250 nm, as suggested by the software company, was used for the simulation. This explains the significant difference between the normalized force values as the simulated force results are from a much larger depth.

One problem with this simulation approach is that the desired depth is not what is actually being simulated when the tool moves over the workpiece. This comes back to the problem of the workpiece spring back when the tool moves over it, given the hardness of the SiC material. The workpiece is provided with the depth profile of cut
4 with the intention that when the tool moves over it, it will take off this desired depth. However, given the spring back problem, the resultant depth that is being removed (for the simulation) is smaller than the intended/desired depth.

6.4 Conclusion

To overcome the current limitation of the AdvantEdge software in 3-D, namely the difficulty with the relative size scale difference between the tool’s nose radius (mm) and cutting edge radii (nm), and the depth of cut (nm), two approaches were investigated to simulate the 3-D fly-cutting operation in 2-D. The first approach (Method A) involved performing machining simulations at specific depths of cut for which comparable experimental force data were available. A comparison of the normalized cutting forces showed that the simulation is in good agreement for the depth of cut (61 nm) that is smaller than the ductile-to-brittle transition depth. At the larger depth (75 nm), the results show a significant difference between the simulated and experimental normalized cutting force values, because the simulation does not account for brittle fracture of the material and the experiments involve brittle material removal.

The second approach (Method B), which used a curved workpiece to approximate the fly cutting geometry, showed a significant difference in normalized cutting force values at both depths. This is because the initial depth of cut for the tool was 250 nm due to the limitation of the software. Ideally, a zero initial depth of cut should have been supplied.
Perhaps a better agreement of results will be achieved by reducing the initial depth of cut to (say) 25 nm, which is a lot closer to the initial desired depth. Future improvements in the software will perhaps provide for variation in tool position in the y-direction as a function of length/time. This will eliminate the need to create a curved workpiece, and the tool motion alone will create the desired cut profile. Additionally, overcoming the current software limitations with respect to the relative size of the tool (specifically the millimeter nose radius and the nanometer cutting edge radius) compared to the depth of cut (in nanometers) may allow such a simulation to be performed in 3-D in the future.
CHAPTER 7

3-D SCRATCHING (GROOVING) SIMULATIONS OF SILICON AND SILICON CARBIDE

7.1 Introduction

Material removal in hard brittle materials, such as ceramics and semiconductors, leads to brittle fracture of the workpiece unless material removal is performed in a ductile regime. The high pressure phase transformation (HPPT) created at the tool-workpiece interface requires pressures greater than, or equal to its hardness. These high pressure phases (HPPs) are believed to be metallic in nature and chip formation is seen similar to metal machining. The ductile nature of the material is a consequence of the HPPT or amorphization induced by the tool-workpiece interaction at small (nm) depths. The HPPs have been clearly demonstrated in silicon (Si) (Dominich et al., 2004), and preliminary studies on silicon carbide (SiC) also reveal a ductile response and phase transformation induced by machining (Patten et al., 2005).

Scratch,ing with a diamond stylus or cutting tool provides a method of determining the ductile-to-brittle transition (DBT) depth in nominally brittle materials, such as semiconductors and ceramics. The recently developed 3-D grooving module in AdvantEdge provides an alternative means of studying the mechanics of the plastic deformation and material removal during scratching. The grooving/scratching experiments can also be used to simulate a single point cutting edge or grit, such as a grinding grit or polishing particle. In this paper, scratching
simulations of Si based on experimental values from Dong (2004), and SiC using experimental results from Bhattacharya (2005) are presented.

7.2 Silicon Simulation

7.2.1 Simulation Setup for Si

The simulation involves scratching a Si workpiece using a diamond conical tool tip. The tool moves through the workpiece material at a constant penetration depth. The tool is a custom tool, generated using a CAD software program in the STL file format. As per the experiment, the diamond tool is provided with a 5 µm tip radius. The tool was initially designed to allow scratching at a depth of 100 nm. To help minimize the number of elements in the mesh, a maximum allowable depth of 300 nm was specified. Beyond this depth (300 nm), the cylindrical surfaces of the tool will interfere or make contact with the workpiece material and affect the simulation in an undesirable or unrealistic manner. The tool used in the simulation is shown in Figure 7.1.

![Tool model used for simulation.](image)

Experimental data for a depth of 71 nm at a speed of 0.305 mm/s indicated ductile material deformation (Dong, 2004). Initial attempts at using the grooving module
were restricted by the simulation software to a minimum depth of approximately 100 nm, and so a programmed depth of 125 nm was used (even though this is larger than the experimental data available). The actual depth achieved after elastic spring back, due to the hardness of the material, was 115 nm, which is still larger than the experimental value of 71 nm used for comparison. The process setup parameters are summarized in Table 7.1.

Table 7.1: Process parameter listing for simulation of Si simulation. (programmed depth 125 nm).

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
<th>Geometry</th>
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</thead>
<tbody>
<tr>
<td>Programmed Depth (feed)</td>
<td>125</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>(Actual) Depth of Cut, doc</td>
<td>115</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Length of Cut, loc</td>
<td>10.0</td>
<td>µm</td>
<td></td>
</tr>
<tr>
<td>Cutting Speed, v</td>
<td>0.305</td>
<td>mm/s</td>
<td></td>
</tr>
<tr>
<td>Friction factor</td>
<td>0.1</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

Figure 7.2: Progress of 3-D scratching simulation showing mesh refinement.

A typical simulation would progress as shown in Figure 7.2. The tool obscures the
pressures at the tool-workpiece interface and usually the tool is removed from the window, as shown in Figure 7.3, when presenting the results. This provides a clear view of the pressures, which gives an idea of the interactions taking place at the tool-workpiece interface, i.e. the potential for a HPPT and a ductile material response.

7.2.2 Results from Simulation of Si

An initial estimate of the success of the simulation is obtained by determining the pressures generated at the tool-workpiece contact area. Under steady state conditions, this value is expected to be greater than, or equal to, the hardness of the material for ductile material response of brittle materials (Patten et al., 2005). Figure 7.3 shows a view of the pressure contours generated at the tool-workpiece interface in the simulation, shown with the tool removed. The pressures in red are equal to or higher than 12 GPa, which is the generally accepted hardness of the single crystal Si material (Dong, 2004).

Figure 7.3: Pressure plot of workpiece showing values greater than 12 GPa.
The highest pressures (in red) shown in Figure 7.3 indicate that there is significant pressure build up at the interface of the tool and the workpiece. These highest pressures occur at the contact interface between the tool and the workpiece, and are of sufficient magnitude to cause the HPPT and thus achieve ductile material deformation. The pressures are lower in the wake of the tool, i.e. in the trailing stress field.

7.2.3 Discussion of results

At present, the only way to compare the experimental results and the simulations is in terms of the force values. In the case of the experiment, a desired gram weight (dead load) is placed on the diamond stylus and scratching leads to material deformation at a certain depth, i.e. the force/load is applied and the resultant depth of penetration is subsequently measured. This achieved depth is determined using Atomic Force Microscopy (AFM) as shown in Figure 7.4.

Figure 7.4: AFM groove depth measurement (Dong, 2004).
AdvantEdge does not allow for specifying a load, but allows the user to specify a depth (feed) for penetration of the tool into the workpiece material. Thus, the achieved depth from the experiment is entered into the simulation. However, due to the elastic response of the hard materials simulated (Si workpiece and diamond tool), the actual depth of the material displaced in the simulation (measured after the simulation has completed) is less than the programmed feed. Post processing of the simulation results provides machining forces, and the actual depth of the material deformation, which are compared to the experimental loads and used to validate the simulation.

The Si scratching experiment did not measure cutting forces (transverse or horizontal force component) and as such only the thrust force (normal loading) is available. This value is compared with the thrust forces achieved from the simulation. The result of the comparison is shown in Figure 7.5.

![Figure 7.5: Thrust force values comparison from simulation and experiment.](image)

In the case of Si, the thrust force from the simulation result is comparable, but
slightly smaller, than the experimental result, although the simulated depth is larger (115 nm) than the experiment (75 nm). This difference may be due to the material model used for the simulation and/or due to the limitations in the numerical analysis at the nanometer range for 3-D scratching (grooving). But, for a first attempt at using the 3-D grooving module to simulate scratching at the nanoscale in a nominally brittle material, the results are encouraging.

7.3 Simulation of CVD SiC

7.3.1 Simulation Setup for CVD Coated SiC

The tool used for simulating the scratching of CVD (Chemical Vapor Deposition) coated SiC is the same 5 µm tip diamond tool used in the Si scratching simulations. The process conditions for the simulations are summarized in Table 7.2.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Value</th>
<th>Unit</th>
<th>Geometry</th>
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<tbody>
<tr>
<td>Programmed Depth (feed)</td>
<td>125</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Actual depth, doc</td>
<td>103</td>
<td>nm</td>
<td></td>
</tr>
<tr>
<td>Length of Cut, loc</td>
<td>10.0</td>
<td>µm</td>
<td></td>
</tr>
<tr>
<td>Cutting Speed, v</td>
<td>0.305</td>
<td>mm/s</td>
<td></td>
</tr>
<tr>
<td>Friction factor, µ</td>
<td>0.1, 0.26, 0.6</td>
<td>-</td>
<td></td>
</tr>
</tbody>
</table>

Three simulations were conducted; one with a friction factor (µ) of 0.1, a second with a value of 0.6, and lastly an intermediate value of 0.26. The value of 0.1 was based on the apparent coefficient of friction (Fc/Ft) results obtained from plunge cutting experiments conducted on polycrystalline SiC (Bhattacharya, 2005), and as
such does not correlate directly to an actual friction factor. The value of 0.6 was used as an upper bound. The apparent COF of 0.26 was also determined from experiments, where the thrust force was 50 mN and the cutting force was 13 mN (Bhattacharya, 2005). The slow cutting speed of 0.305 mm/s was based on previous experiments on Si (Dong, 2004), and matched the experimental conditions used for scratching SiC (Bhattacharya, 2005).

7.3.2 Results from Simulation of CVD SiC

A quick estimate of the usefulness of the simulation is obtained by determining the pressures at the tool-workpiece interface compared to the material’s hardness (relative to a possible HPPT or stress induced amorphization). For this SiC material, the hardness value is given to be 26 GPa. The plot generated from the simulation with the COF of 0.1 indicates pressures greater than this hardness value, as shown in Figure 7.6 (with the tool removed). The zone comprising the severe material plastic deformation (red contours) corresponds to areas where the tool-workpiece contact pressures are comparable to the material’s hardness (26 GPa) as shown in Figure 7.6. A similar plot was obtained for the simulation with COF of 0.6 and 0.26.
Figure 7.6: Pressure contour for scratching simulation of SiC with $\mu$ of 0.1.

In the case of the scratching experiments involving CVD SiC both thrust forces and cutting forces are available, along with the achieved depth for material deformation (Bhattacharya, 2005). The results of the comparison of the experimental values with the simulated forces are given in Figure 7.7.

Figure 7.7: Cutting and thrust force comparison for an approximate depth of 100 nm.
The simulated thrust forces show a gradual drop as the value of $\mu$ is increased and all values are in reasonably good agreement with the experimental value. The cutting forces show a gradual increase with increasing $\mu$, as expected. In all cases, the simulated "cutting" forces are lower than the actual measured forces. However, the trend in the data is consistent for the simulations and experimental values, in that lower thrust forces correspond to higher cutting forces for all the data. Further research and experimentation is needed to resolve these apparent discrepancies.

7.3.3 Discussion of Results from SiC Scratching

For scratching simulations of CVD SiC, the thrust forces decrease with an increase in COF. The thrust force from the frictional case of $\mu=0.26$ (which matches the experimental force ratio, i.e. the apparent coefficient of friction) shows good agreement with the experimental value, but not in the case of the cutting force, i.e. the experimental cutting (frictional) force is higher than the simulation cutting force. The latter condition is partially due to the fact that the achieved simulation depth is approximately 105 nm, while the experimental results are closer to 120 nm, which would yield a higher cutting force as found. If the simulation had achieved a larger actual depth, or if experimental data was available for a smaller depth, the comparison between the simulation and experimental cutting forces would be improved, but still different. As both the simulation and experimental depths were ductile, the force should be higher in the case of the 120 nm experimental cut, compared to a depth of 105 nm from the simulation, which is consistent with the results.
7.4 Conclusions

The simulation software AdvantEdge release 4.6 was used to simulate scratching of single crystal Si and CVD coated SiC using the newly developed scratching (grooving) module. The pressures generated by the software at the tool-workpiece interface indicate that pressures are comparable to the material's hardness, for both Si and SiC, which would provide for a HPPT and a ductile material response.

As a first attempt at simulating a 3-D scratching and plastic deformation of nominally hard and brittle materials (Si and SiC) at the nanoscale, the comparison with limited experimental data is quite encouraging and shows promise. Future work will concentrate on investigating the difference in the magnitudes of the cutting force data (comparing the experiments and simulations) and improvements or modifications to the software and material model to improve the correlation between the force results from the experiment and simulation.
CHAPTER 8

CONCLUSIONS AND FUTURE WORK

The science of HPPT relating to ceramics and semiconductors has made significant progress in the last decade (Gogotsi and Domnich, 2004). While this phenomenon has been reasonably documented and explained in materials like silicon (Si) and germanium (Ge), the science of room temperature plastic deformation and phase transformations in silicon carbide (SiC) have not been satisfactorily or fully explained. Ongoing experiments are aimed at answering these questions.

Given the relatively short history behind the science of HPPT, it is not surprising that simulation software have not been fully developed, characterized and validated to accurately predict the mode of material removal (via plastic deformation such as occurs during machining) in ceramics and semiconductors for a given set of process conditions. Using AdvantEdge, two types of SiC simulations SiC have been presented in this thesis: 2-D simulations of orthogonal machining and 3-D simulations of cone (stylus) scratching. The 2-D orthogonal simulations have been conducted on SiC, while the recently developed 3-D scratching module was used to simulate scratching of Si and SiC. The DP yield criterion is used to differentiate the yield in tension versus the yield in compression, under ductile machining conditions, in an attempt to capture the characteristic ductile behavior of these materials under high pressures, via a pressure induced phase transformation (HPPT) to a more ductile material state.
Using this approach, 2-D orthogonal machining simulations were conducted from 500 nm down to a depth of 25 nm. The simulations showed that the cutting and thrust forces agree reasonably well for depths of cut where the material removal during the experiments is dominated by ductile cutting conditions (for example where depths of cut are less than 100 nm). Under brittle machining conditions (for depths of cut > 100 nm), the cutting and thrust forces from the simulation do not agree with the experimental values since the simulation presently does not account for fracture in the material which occurs during the experiments for the larger depths of cut (> 100 nm).

The new scratching module was used to simulate scratches in Si and SiC at depths close to 100 nm. For the first attempt at simulating a 3-D scratch and plastic deformation of hard and brittle materials (Si and SiC) at the nanoscale, the comparison with limited experimental data is quite encouraging.

Future work includes validation of material models used in the simulations similar to the work presented in Appendix A. Further, given the difference in the models based on this study, it is necessary to revisit the simulations on single crystal SiC in Chapter 3 to determine if better agreement between simulations and experiments (under the ductile mode) can be achieved. Other future work includes developing an analytical model to help predict the actual depth for a given programmed depth of cut. This will help achieve desired depths in the simulations with little need for multiple iterations or force interpolation.

However, all of these simulations will be limited by the software’s ability to accurately model the brittle and ductile behavior of ceramics. Thus, while present
simulation results are limited to the ductile mode of material removal (and these results compare favorably to experiments conducted in the ductile regime), future improvements in the model will hopefully allow for simulations under both ductile and brittle modes of machining.

In closing, it must be said that it is quite impressive that AdvantEdge can simultaneously be used to optimize process parameters in machining of titanium for aircraft (large) components and for predicting forces during machining of ceramics in the ductile regime down to the nanometer scale.
REFERENCES


Ceramic Property database, [www.ceramics.org](http://www.ceramics.org).


Appendix A

Comparison of Stress-Strain Curves for Silicon Carbide
Summary of studies

For the study at the University of Tennessee (UT), Tabor’s (Tabor, 1970) model was used to determine the strain values, for a given cone indenter angle (included angle of the indenter), and the corresponding stress from the hardness (load versus displacement, or pressure) values obtained experimentally (Shim et al., 2005). From this information an iterative procedure is used to determine a plastic stress-strain curve of SiC, based upon convergence of the solution.

Using the constitutive material model in AdvantEdge and material properties, the plastic part of the stress-strain curve was developed and compared with the UT curve as shown in Figure A1 using available data points and in Figure A2 using the given equation from the study for values of strain up to 8.

![Figure A1: Comparison plot of flow stress vs. plastic strain.](image-url)
Figure A2: Comparison plot of flow stress vs. plastic strain for strains up to 8.

The limited data points in Figure A1 in the case of the experiment are obtained directly from the work presented by Shim et al. (2005) and the corresponding values for the simulation material model were determined and plotted for comparison. To determine how the curves compare at high values of strain as was seen in 2-D simulations of SiC, the curves were extrapolated as shown in Figure A2.

The plots show a significant difference. The first difference lies in the value of initial yield stress. The study at UT determined the initial yield stress to be 10 GPa while the material model in AdvantEdge uses an initial yield of 16.25 GPa determined using the Drucker-Prager material model. The difference in the slope of the curve is due to the work (strain) hardening coefficient used in the two models. The UT work is based on a model with strain hardening of 0.21, while the WMU work uses a work hardening coefficient of 50. The value of 50 was used to diminish any work hardening effects as explained previously.
Appendix B

Images of Flycuts Using WYKO RST
Note: Arrows indicate direction of cut.

Figure B1: WYKO image of fly-cut 1 (image altered to remove other cuts). Refer to Figure B5 for original image.

Figure B2: WYKO image of fly-cut 2.
Figure B3: WYKO image of fly-cut 3.

Figure B4: WYKO image of fly-cut 4.
Figure B5: Brittle cuts in the vicinity of cut 1.
Appendix C

Material Property Listing for Various Ceramic Materials
C-1: Material Property listing for single crystal silicon

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<th>Simulation Symbol</th>
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C-2: Material Property listing for single crystal silicon carbide

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C-3: Material Property listing for polycrystalline silicon carbide

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### C-4: Material Property listing for CVD coated silicon carbide

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