Effects of grain size on removal mechanism of brittle polycrystalline materials in laser assisted diamond turning

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KEYWORDS: Machining mechanism, Laser assisted turning, Grain size, Numerical simulation

The nano-cutting performance of brittle polycrystalline materials is greatly influenced by their grain size. In the present work, a finite element model of laser assisted diamond turning of polycrystalline tungsten carbide (WC) was developed, aiming to evaluate the influence of grain size on the material deformation and removal mechanism in laser assisted diamond turning. The thermal effect of laser in-situ radiation on the workpiece is implemented in a user subroutine. The simulation results show that the grain boundary density and intergranular bonding strength decrease significantly with the increase of grain size. Therefore, cutting energy cannot be absorbed through material plastic deformation and tends to be released through intergranular fractures, causing grain spalling on the machined surface. Thermal softening effect of laser can reduce the grain spalling by reducing the grain strength, but it cannot be avoided, thereby compromising the finish surface integrity inevitably.

1. Introduction

With the rapid development of materials science and metallurgy, brittle polycrystalline materials, such as tungsten carbide (WC), are now widely used in the field of advanced manufacturing, optical engineering, biomedicine, and laser technology [1, 2]. These materials possess high hardness and low fracture toughness at room temperature. This makes them prone to leave crack on the machined surface after tradition diamond turning [3]. Laser-assisted diamond turning (LADT) method can improve the machinability of brittle materials by laser heating, thereby prolonging the diamond tool life, and ensuring the optical finish quality.

Grain size plays a crucial role in determining the surface integrity during the laser-assisted machining of WC. Finer grains in tungsten carbide result in better surface morphology due to the reduced occurrence of grain spalling and lower sub-surface damage. In contrast, larger grains can lead to increased voids and gaps, contributing to grain spalling and necessitating extensive post-processing to achieve a better surface morphology. The correlation between grain size and surface morphology has been demonstrated in several studies, where finer grain structures in binderless WC alloys have shown superior machinability and are more suitable for achieving mirror-like surfaces with minimal post-polishing [4]. Therefore, optimizing grain size is essential for enhancing surface integrity.

Despite extensive experimental research, there remain gaps in understanding how grain size affects surface quality during machining. Most existing studies have relied on experimental approaches, which lack the precision and control needed to isolate specific variables like grain size.

Given the significant influence of grain size on the nano-cutting performance of brittle polycrystalline materials, this study develops a finite element model to investigate laser-assisted diamond turning of polycrystalline tungsten carbide (WC). This model evaluates the impact of grain size on material deformation and removal mechanisms, incorporating real-time thermal effects via the VDFLUX subroutine. An improved Johnson-Cook model describes the plastic response of grains at high temperatures, and cohesive elements simulate damage at grain boundaries.

2. Numerical simulation model setup

To evaluate the influence of grain size on the material deformation and removal mechanism in laser assisted diamond turning. The 2D orthogonal cutting finite element analysis (FEA) model was established. The polycrystalline WC workpieces with 20, 40 grains were generated using the Voronoi algorithm as illustrated in Fig. 1. And the WC material removal process was compared with and without laser assistance.

The polycrystalline WC workpiece and the diamond tool were assembled in the model as illustrated in Fig. 1. The size of workpiece is $2 \times 1\ \mu m^2$. The tool edge radius was configured to 30 nm. During the diamond cutting process, the tool moves along the negative X-axis, with a depth of cutting (DOC) of 200 nm. The bottom of workpiece was fully fixed to simulate the supporting effect of surrounding materials.

For the workpiece with 20 grains, meshing was done with CPE4RT elements for the grains and COH2D4 elements for the grain boundaries, with an overall element size of 20 nm. For the specimen with 40 grains, the meshing used CPE4RT elements for the grains and COH2D4 elements for the grain boundaries, with a finer element size of 10 nm. The diamond tool, utilized for different grain size models, was uniformly meshed with CPE3T elements.

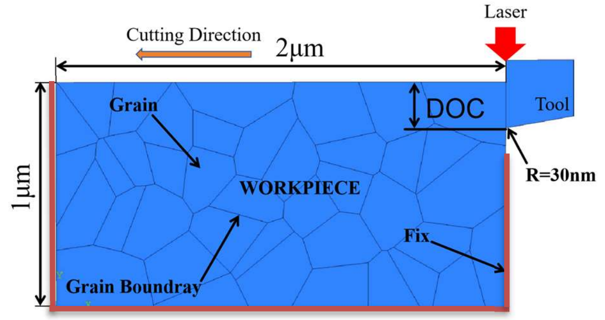

Fig.1. 2D orthogonal cutting model: Polycrystalline tungsten carbide (WC) specimen and diamond tool

This study employs Johnson-Cook model to describe the plastic response of the WC material at high temperatures. Additionally, the Johnson-Cook failure model was used in this study. To simulate damage behavior at grain boundaries, cohesive elements were incorporated into the model [5]. These cohesive elements follow a traction-separation law, where bilinear functions are used to describe tensile-separation failure.

Given that the hardness of the diamond tool exceeds that of the WC workpiece, the tool was modeled as rigid body. The friction coefficient between the tungsten carbide chips and the tool was set to 0.2, referring to the study of Zhao et al. [6]. A 1064 nm near-infrared continuous laser was employed for the laser-assisted diamond turning process, with predefined field temperatures of 273 K for both the workpiece and the tool. To minimize the heat-affected zone and ensure machining quality, a Gaussian beam was utilized. The laser spot was modeled as a surface heat flux in the simulation. The VDFLUX subroutine for laser heating was developed in Fortran to simulate the laser conditions during the LADT process. The laser heat flux distribution was defined based on the energy pattern of a 170 μm Gaussian laser spot, with the laser spot center aligned with the diamond tool tip. For clarity, the simulation parameters have been summarized in Table 1.

Table 1 Finite element simulation model parameters

Parameters	Values
Workpiece material	Tungsten Carbide
Cutting tool material	Diamond
Depth of cutting	200 nm
Tool edge radius	30 nm
Grain numbers	20, 40
Element size	20nm, 10nm
Laser power (P)	0, 3 W
Initial temperature	273K
Laser beam diameter	170 μm
Material emissivity (ε)	0.75
Material absorptivity (δ)	0.23
Convective heat transfer coefficient (h)	$300 W/(m^2 \cdot K)$[7]

3. Results and Discussion

3.1 Effects of laser in-situ heating

The machinability of polycrystalline WC can be effectively improved with the laser in-situ heating assistance. The study investigates the impact of laser in-situ heating on the machinability of polycrystalline tungsten carbide (WC), focusing on cutting force, and surface quality. The comprehensive comparison aims to elucidate the material removal mechanisms during the laser-assisted diamond turning (LADT) process.

3.1.1 Cutting force

Cutting force is a crucial parameter that reflects both the stability of the machining process and the wear on the diamond tool. The cutting force data were obtained from simulations, with and without laser assistance, to assess the impact of laser heating on cutting efficiency. As illustrated in Fig.2(a), the cutting force was monitored over varying cutting distances. The data indicate significant fluctuations in the cutting force without laser assistance, as shown in the raw data and in the low-pass FFT filtered curve (Fig.2b). These fluctuations correspond to noticeable grain spalling observed in the stress contour plots, indicating a strong correlation between cutting force variance and material removal discontinuities. In contrast, with laser assistance, the cutting force curve shows reduced fluctuations and a lower average force. This reduction is attributed to the localized heating effect of the laser, which softens the material near the cutting point, thereby reducing its hardness and strength and making it easier to cut. Despite these improvements, the cutting force curve still exhibits peaks, indicating that while laser assistance mitigates grain spalling, it does not entirely eliminate it.

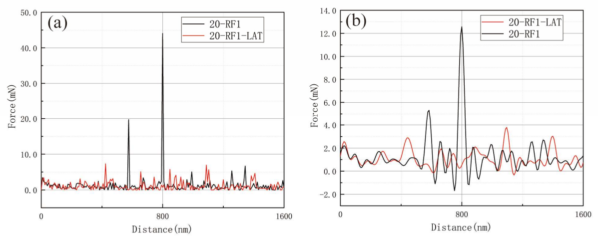

Fig.2. Effects of laser-assisted heating on (a) the cutting force (RF1) with cutting distance, (b) the filtered cutting force after low-pass FFT processing

3.1.2 Surface quality

Surface quality is a critical measure of machining performance, significantly influenced by cutting forces and residual stress distribution. The stress contour diagrams in Fig. 3 illustrate the impact of laser assistance on the surface quality of polycrystalline tungsten carbide.

Fig 3(a) presents the stress distribution for a 20-grain sample without laser assistance, highlighting high stress concentrations along grain boundaries and evident grain spalling. The magnified view emphasizes surface defects, such as disrupted grain boundaries and voids, which compromise surface integrity. These defects arise from localized stress concentrations that weaken intergranular bonding, leading to grain dislodgement and poor surface texture.

The magnified region of Fig 3(a) further reveals areas of grain spalling, marked by the partial removal of grains and void formation along the grain boundaries. Without laser assistance, the material remains in a harder, more brittle state, causing stress to accumulate at grain boundaries and exceed their fracture strength. This results in significant surface damage and roughness, which are detrimental to overall machining quality.

In contrast, Fig. 3(b) displays the stress distribution in the same sample when laser assistance is applied. Notably, there is no grain spalling at the same cutting distance, and the overall surface quality is significantly improved. The localized stress distribution is further magnified in magnified region of Fig 3(b), revealing that the surface is more uniform, with reduced grain boundary dislocations and minimal grain torsion. The laser's localized heating effect facilitates material softening, allowing for smoother cutting and reducing the likelihood of defects caused by grain dislodgement.

Additionally, it is evident from Figs. 3(a) and 3(b) that laser assistance also minimizes dislocation along grain boundaries and reduces grain torsion, contributing to the overall enhancement of surface quality. The reduction in stress concentration and the improved distribution of compressive stress across the machined surface result in fewer defects and a more uniform finish.

These observations underscore the efficacy of laser-assisted machining in producing higher-quality surfaces with fewer defects by mitigating stress-induced grain spalling and promoting better material behavior under cutting forces.

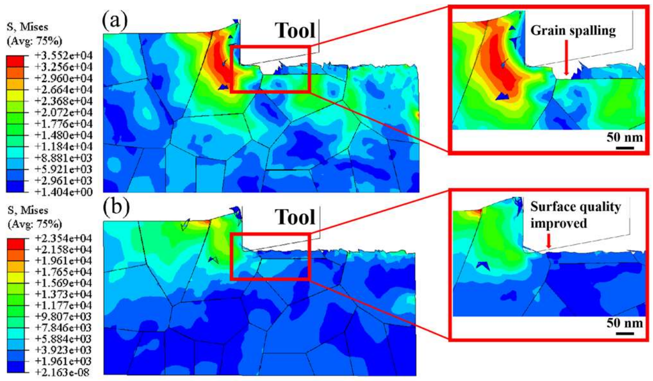

Fig.3. Stress contour and surface quality during the cutting process: (a) Grain spalling observed without laser assistance, (b) Improved surface quality with laser assistance.

3.2 Effects of grain size

Although LADT method can effectively improve the finish quality of brittle polycrystalline materials. The nano-cutting performance of polycrystalline WC materials is also greatly influenced by their grain size. This section systematically examines how varying grain sizes influence cutting force, and surface quality, based on simulation results from models with different numbers of grains.

3.2.1 Cutting force

Cutting force is a crucial parameter that reflects both the stability of the machining process and the wear of the diamond tool. Understanding how grain size affects cutting force under laser-assisted conditions is essential for optimizing machining performance and tool longevity. This subsection analyzes the cutting force behavior in polycrystalline tungsten carbide samples with different grain sizes during LADT.

Fig 4(a) illustrates the variation in cutting force (RF1) with cutting distance for two polycrystalline tungsten carbide models: a 20-grain model and a 40-grain model, representing larger and smaller grain sizes, respectively. Fig 4(b) presents the cutting force curves after applying low-pass Fast Fourier Transform (FFT) filtering to smooth out high-frequency noise.

The 40-grain model (40-RF1-LAT) exhibits more frequent fluctuations and higher peak values compared to the 20-grain model (20-RF1-LAT). This behavior indicates that smaller grain sizes, corresponding to a higher number of grains, result in the cutting tool encountering grain boundaries more frequently. Each grain boundary interaction induces localized stress concentrations, leading to sudden increases in cutting force and more pronounced fluctuations. These fluctuations are a direct consequence of the increased grain boundary density in smaller grain-sized materials, which disrupts the continuity of material removal and introduces variability in the cutting process.

In contrast, the 20-grain model, with larger grains, experiences fewer interactions with grain boundaries, resulting in a more stable cutting force profile with lower peak values. However, larger grains absorb cutting energy less effectively through plastic deformation, often leading to energy release via intergranular fracture. This manifests as higher peak cutting forces when the tool interacts with larger grains, potentially increasing tool wear and reducing machining stability.

Overall, the grain size plays a pivotal role in determining the cutting force dynamics during LADT. Smaller grain sizes lead to increased variability and higher peak forces due to more frequent grain boundary interactions, which can impact machining stability and tool wear. Conversely, larger grain sizes result in more stable cutting forces but may compromise energy absorption and lead to higher stress concentrations during intergranular fractures.

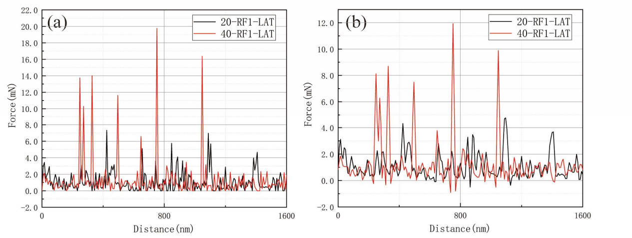

Fig. 4. Grain size impact on cutting force: (a) Cutting force vs. distance, (b) Filtered cutting force after FFT.

3.2.2 Surface quality

Surface quality is a critical indicator of machining performance, affected by cutting forces, residual stresses, and microstructural features. This section examines how grain size influences the surface quality of polycrystalline WC during laser-assisted cutting, focusing on stress distribution and surface morphology, as highlighted in the magnified views of Figs 5(a) and 5(b).

Fig 5(a) illustrates the stress contour of a 20-grain WC model under laser-assisted cutting, where the magnified view reveals deteriorated surface quality due to larger grain sizes. In contrast, Fig 5(b) shows the

40-grain model with significantly improved surface characteristics, as highlighted in its corresponding magnified view.

In the 20-grain model (Fig. 5(a)), the larger grain size leads to fewer, sparsely distributed grain boundaries, causing uneven stress distribution. The magnified view shows disrupted grain boundaries marked as dashed lines, indicating material removal due to localized boundary failure. This boundary damage reflects weakened intergranular bonding, resulting in significant surface irregularities, including grain spalling and dislocations, contributing to poor surface integrity.

Conversely, the 40-grain model (Fig. 5(b)) exhibits a higher density of grain boundaries, which improves stress distribution and mitigates boundary failure. The magnified view displays a smoother, more continuous surface with minimal defects, highlighting the ability of smaller grains to effectively absorb and distribute machining stresses. This enhanced grain boundary network ensures uniform material removal, markedly improving surface quality.

The comparison of the magnified views emphasizes the significant impact of grain size on surface quality. The 20-grain model's disrupted boundaries, marked as dashed lines, indicate compromised integrity and rough texture. In contrast, the 40-grain model maintains intact boundaries, promoting intergranular cohesion and yielding a smoother, defect-free surface.

In summary, smaller grain sizes with denser grain boundaries significantly enhance surface quality during laser-assisted machining. The higher boundary density effectively redistributes cutting stresses and strengthens intergranular connections, reducing boundary failures. The combination of smaller grains and laser heating synergistically enhances surface integrity, highlighting this approach as optimal for improving the machinability of brittle polycrystalline materials.

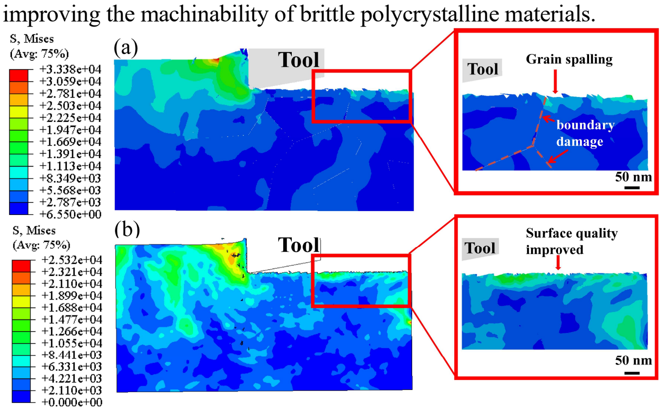

Fig. 5. Grain size impact on stress and morphology: (a) 20-grain stress contour and Magnified view, (b) 40-grain stress contour and Magnified view.

3. Conclusion

In this article, a FEA numerical simulation model was developed to investigate laser-assisted diamond turning of polycrystalline WC. The study focused on the effects of grain size and laser in-situ heating on material deformation and the removal mechanism. The main conclusions are as follows:

1. Laser-assisted cutting performance: FEA simulation results demonstrate that laser-assisted cutting method significantly reduces the variance in cutting forces and improves surface integrity by minimizing grain spalling, resulting in enhanced overall surface quality.

2. Impact of Grain Size on Stress Concentration and Surface Defects: Larger grain sizes correlate with higher stress concentrations and more pronounced surface defects. This occurs due to the increased likelihood of encountering weak grain boundaries, leading to higher cutting forces and more noticeable surface irregularities.

3. Importance of Grain Size Optimization: The study emphasizes that optimizing grain size is critical for enhancing machining performance, particularly under laser-assisted conditions. Smaller grains are more effective in reducing stress concentrations and improving surface integrity, making them ideal for achieving high-quality machining results.

ACKNOWLEDGEMENT

This work was supported by the National Key Research and Development Program of China (2023YFB3407200); the Sichuan Natural Science Foundation (2024NSFSC0896); the National Natural Science Foundation of China (52035009); the China Postdoctoral Science Foundation (2023M730502, 2024T170103).

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