

High-precision machining behavior of the single crystal scintillator, bismuth germanate (Bi₄Ge₅O₁₂)

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ABSTRACT

This study focuses on understanding the machinability of a single-crystal scintillator, Bismuth Germanate (BGO), a material widely used in Time-of-Flight Positron Emission Tomography (ToF-PET). The micromachining process of such a hard, brittle material presents several challenges, particularly in maintaining surface integrity without inducing fractures or microcracks. In this work, we employed the Johnson-Holmquist 2 (JH-2) material model to simulate the micro-milling process of BGO. Experimental data from quasi-static uniaxial compression and split tests were used to estimate the key parameters for the JH-2 model. The simulation results closely aligned with experimental outcomes, confirming the reliability of the model in capturing the mechanical behavior of BGO under stress. Simulations were conducted with different machining parameters, successfully replicating the conditions observed in practical machining tests. Our findings demonstrate the impact of feed rate and depth of cut on the machinability of BGO, validating the use of the JH-2 model of this material. Looking ahead, this robust computational framework offers the potential to further optimize the machining process, ultimately enabling the production of high-performance heterostructures for scintillator applications in TOF-PET.

1. Introduction

The medical imaging sector has undergone substantial scientific progress, especially in the area of Time-of-Flight Positron Emission Tomography (ToF-PET). ToF-PET enhances spatial resolution by measuring the time it takes for emitted photons to reach the detectors, allowing for the localization of the point of annihilation along the line of response compared to traditional PET imaging, which relies intrinsically on coincident photon detection [1–3]. A critical factor in this process is the coincidence timing resolution, which defines how precisely the time difference between detected photon pairs is measured, directly affecting the accuracy of image reconstruction.

Recently, the concept of heterostructured scintillation detectors, where two scintillator materials work in synergy to achieve unparalleled performance (sub-nanosecond timing and short attenuation length) [4], was proposed to bypass the intrinsic limitations of the current ToF-PET detector technology [5,6]. Various crystalline materials are used in scintillator-based imaging techniques, such as Bismuth Germanate

(BGO) and Lutetium Yttrium Orthosilicate (LYSO) [7]. However, these typically show relatively slow timing performance. Integrating heterostructure scintillation detectors into ToF-PET markedly reduces the coincidence timing resolution. This reduction enhances the precision of gamma-ray detection timing, which is crucial for producing more accurate images.

Various research groups have explored different scintillation detector designs. A PET simulation showed that a BGO-plastic (EJ232) heterostructure achieved a coincidence time resolution of (204 ± 49) ps, compared to 276 ps for bulk BGO [8], marking progress toward sub-nanosecond resolution. Further advancements led to a layered nanocomposite polystyrene matrix with scintillating dyes and high-density nanoparticles combined with single-crystal BGO, achieving an even better resolution of 180 ps [9]. In order to achieve the desired performance, a recent study evaluated a figure of merit for various heterostructures [10], leading to the proposal of a filled matrix design requiring micromachining for pixel manufacturing [11]. However, machining such a hard, brittle material presents significant challenges,

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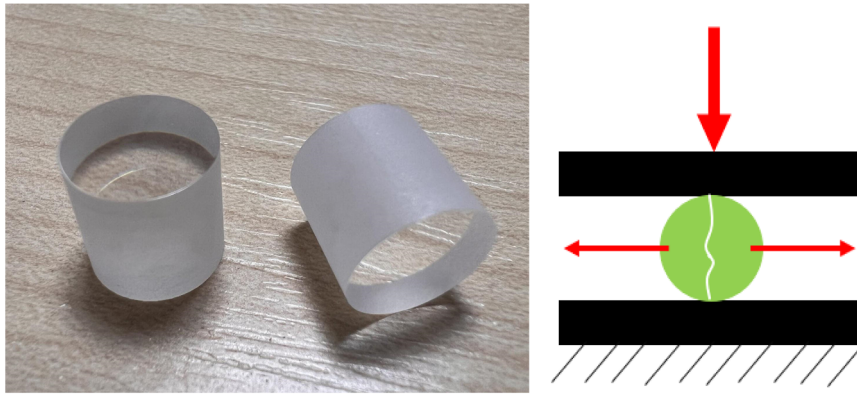


Fig. 1. (left). BGO specimens used for compression tests, (right). Diagram of the split test method.



Fig. 2. BGO slices used for micromachining tests.

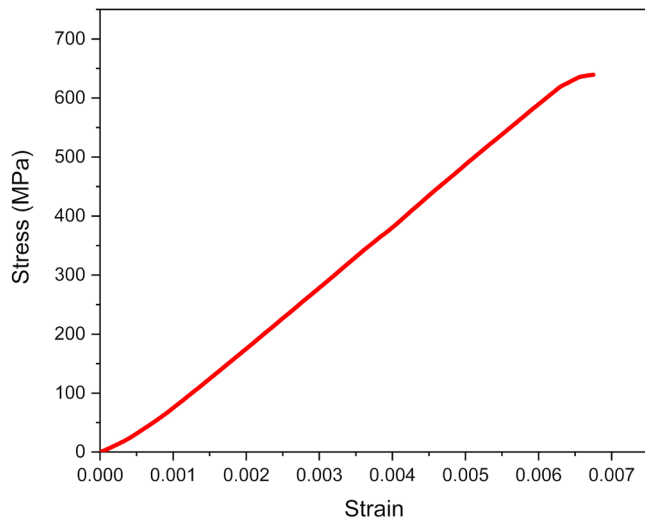


Fig. 3. Mean quasi static uniaxial compression testing stress–strain curve.

Table 1

Quasi-static uniaxial compression testing results.

No.	Compressive strength (MPa)	Young's Module (GPa)	Average (GPa)	Standard Deviation (GPa)
C1	612.71	104.59	102.60	1.6349
C2	605.63	101.18		
C3	630.53	104.18		
C4	578.95	102.69		
C5	668.23	100.39		

as these materials are highly prone to fracturing under conventional machining conditions. This tendency to fracture results in poor surface finishes, as even minor cracks can propagate rapidly when the applied stress surpasses the material's fracture toughness, resulting in poor surface finishes, chipping, and catastrophic damage [12].

In this context, achieving an optimal surface finish is critical for improving the coincidence timing resolution in ToF-PET systems, as smoother surfaces reduce photon scattering and enhance light collection efficiency, thereby improving timing precision. Studies have shown that minimizing surface roughness improves scintillator performance [13].

Advancements in micromachining technology, coupled with a deeper understanding of material behavior, have significantly enhanced the ability to machine brittle materials with greater precision. One key innovation is the development of the ductile-mode cutting technique, which enables controlled material removal by maintaining the machining process within a regime where the material exhibits ductile behavior [14]. This approach minimizes fracture and improves surface finish, thereby overcoming many of the inherent challenges associated with brittle materials. Among the various constitutive models used to describe the behavior of brittle materials, the Johnson-Holmquist 2 (JH-2) model has been shown to effectively capture cracking, fracturing, and material removal, outperforming alternatives such as the Johnson-Holmquist Concrete (JHC) and Karagozian and Case Concrete (KCC) models [15]. Given its ability to accurately represent brittle material behavior under different stress conditions, JH-2 model provides a strong framework for analyzing micromachining processes. Building on this, the present study focuses on the machinability of BGO by employing the JH-2 material model [16]. We simulate the micro-milling process for BGO, using experimental results from quasi-static tests to calibrate key material parameters. Through a comparative analysis of simulated and experimental machining outcomes, we address the critical challenge of optimizing machining parameters to enhance material integrity and precision. This work demonstrates the effectiveness of parameter control in mitigating damage during the micromachining of brittle materials and also establishes a numerical model for the production of high-performance scintillator materials for future ToF-PET applications.

2. Materials and methods

To investigate the impact of cutting parameters on material removal behavior, we used the JH-2 constitutive model, developed by Johnson and Holmquist to simulate the behavior of brittle materials, such as single-crystal BGO, under different strain rates. Under loading, the material initially exhibits elastic behavior. At the point where the material achieves its maximum tensile strength, the damage begins and accumulates until failure [17–21]. Simulations were carried out using Abaqus/Explicit as a platform for JH2 modeling in the numerical

Table 2
Split test tensile strength results.

No.	Failure Force (N)	Specimen Diameter (mm)	Specimen Length (mm)	Tensile Strength (MPa)	Average (MPa)	Standard Deviation (MPa)
S1	3450.7	10	10	21.97	20.82	1.35
S2	2970.8	10	10	18.92		
S3	3388.8	10	10	21.58		

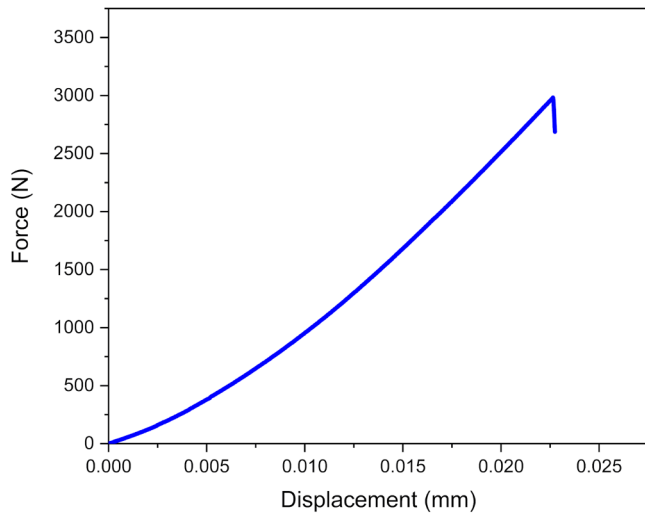


Fig. 4. Mean split testing force-displacement curve.

simulations of both quasi-static and micromachining tests.

2.1. Determination of BGO material properties

The BGO specimens used for the quasi-static test are 10 mm diameter and 10 mm height cylinders sourced from Hilger Crystals Ltd. (UK), see Fig. 1. (left). Quasi-static uniaxial compression tests were performed using an INSTRON 68FM-100 testing machine, operating at a crosshead speed of 0.12 mm/min, resulting in a strain rate of $2 \times 10^{-4} \text{ s}^{-1}$. The top and bottom surfaces of the specimens were lubricated with silicone grease (RS Pro) to reduce the friction effect. The specimens were compressed until failure.

To determine the ultimate tensile strength of BGO, a split test was conducted using the same machine. The loading rate during the test was maintained at 0.12 mm/min, and the peak pressure corresponding to failure was recorded. The splitting method is illustrated in Fig. 1. (right).

2.2. Micromachining of BGO

The BGO samples used for the micromachining study, as described in Sections 2–1, consisted of rectangular slices with dimensions of 20 mm $\times$ 3 mm $\times$ 0.3 mm, see Fig. 2. Machining of the samples was performed using a Kern Evo Ultra Precision CNC Machining Centre equipped with a 3-axis stage. The tools employed for the micro-milling process were Union Tools UDCBF Diamond-coated ball nose end mills. Two different tool diameters were used: 0.2 mm and 0.4 mm, each with a precision of ± 0.01 mm. The spindle speed was maintained at a constant 30,000 revolutions per minute (RPM) throughout the machining process. Additionally, two feed rates were tested during the milling operation: 10 mm/min and 100 mm/min. These parameters were chosen to explore their impact on the surface quality and overall machinability of BGO during micromachining. Optical inspection of the samples was performed using a Keyence VHX-6000 Digital 3D microscope at 20 $\times$ magnification. Scanning electron microscopy (SEM) was carried out on gold-coated samples using a TESCAN Vega 3 microscope, with fields of view set at 50 μm and 500 μm . Roughness measurements were taken using a Taylor Hobson Talysurf CCI white light interferometer at 20 $\times$ magnification and were subsequently processed using Talymap Gold 7.4.

3. Results and discussion

3.1. Determination of BGO material properties

3.1.1. Quasi-static uniaxial compression test

Fig. 3 represents the mean stress–strain curve obtained from the five tests conducted, numbered C1–C5. The curve reveals that under quasi-static uniaxial compression loading, BGO shows an almost linear stress–strain relationship until reaching its ultimate compressive strength, showing that BGO exhibits a highly brittle nature. Table 1 shows the results of the compressive strength tests.

The average Young's modulus is 102.6 GPa, with a standard deviation of 1.6349 GPa. This is comparable to the 105.4 GPa reported by Majorana et al. [22]. C1 and C3 fluctuate within one Young's modulus value (104 GPa). These are normal fluctuations. The mean compressive strength of BGO is 619.2 MPa, with a standard deviation of 21.3672 MPa. The high fluctuation among these five sets may be due

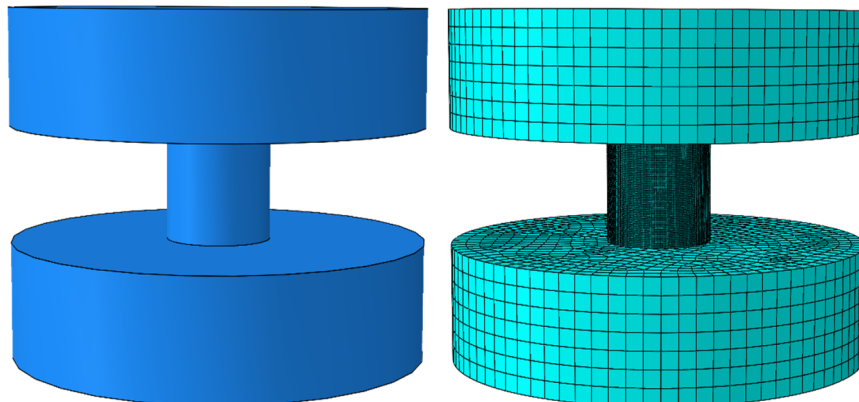


Fig. 5. The geometric structure and boundary condition of the three-dimensional (3D) finite element model (FEM) of quasi static compression test.

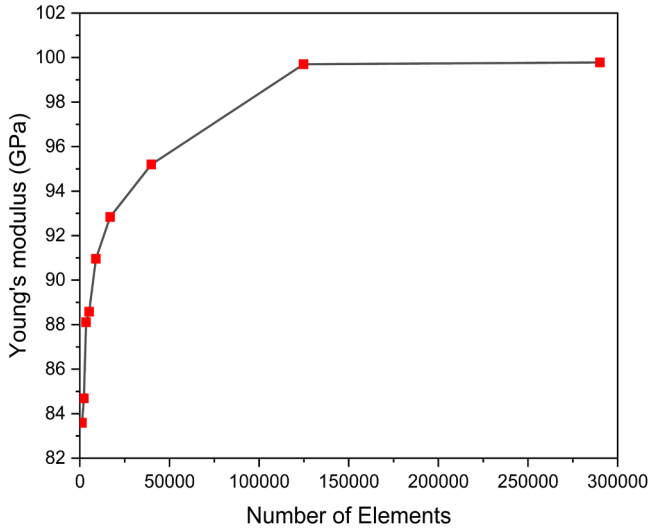


Fig. 6. Mesh convergence.

Table-3
Abaqus JH-II model material parameters of the BGO.

Density (g cm ⁻³)	7.13 [22]
Strength Constants	
A	0.97
B	0.31
C	0
M	0.6
N	0.52
Tensile strength (MPa)	9.88
Pressure at HEL (GPa)	2.84
HEL strength (GPa)	4.44
Shear modulus (GPa)	43.65
Damage constants	
D ₁	0.045
D ₂	0.85
Equation Of State	
K ₁ (GPa)	52.61
K ₂	0
K ₃	0
Bulk	1
FS	0.2

to internal defects, microcracks, and localized porosity, which can lead to variations in compressive strength. Additionally, the distribution and severity of inherent defects within each sample can cause significant deviations in the measured failure forces. Samples that fail around 650 MPa likely represent those with minimal defects and optimal microstructural integrity. In contrast, those failing around 590 MPa may contain significant stress concentrators, which drastically reduce their load-bearing capacity. These results underscore the importance of considering microstructural and defect analysis when interpreting the compressive strength of brittle materials. If a specimen already contains many defects, its strength decreases rapidly, leading to material failure.

3.1.2. Split test

The ultimate tensile strength of the BGO was indirectly estimated by determining the peak pressure at which the material failed. The tensile stress can be calculated as follows:

$$\sigma_t = \frac{2p}{\pi dl} \quad (1)$$

In the given formula, σ_t represents the maximum tensile stress in the specimen's center, in MPa; p signifies the load at failure, in N; d and l are the specimen's diameter and length, respectively, in mm.

The tensile strength results, shown in Table 2, indicate that BGO had

an average ultimate tensile strength of 20.82 MPa, with a standard deviation of 1.35 MPa.

The mean split testing force displacement curve is presented in Fig. 4.

3.2. Determination of Johnson-Holmquist 2 model parameters

As previously introduced in Section 2, the JH-2 model is employed in this study to characterize the mechanical response of BGO. It accounts for both intact and fractured material states, incorporating strain rate dependency, damage evolution, and pressure-dependent strength. This section details the specific methodology used to determine the parameters governing the model, which are derived from experimental quasi-static uniaxial compression and split tests. The proposed model is divided into three groups of parameters describing the behavior of the brittle material.

From the results of the experiments above, the average Young's modulus of the material was $E = 102.60$ GPa. The Poisson ratio was taken from literature to be $\nu = 0.175$ [22].

$$\text{The bulk modulus was } K_1 = \frac{E}{3(1-2\nu)} = 52.61 \text{ GPa} \quad (2)$$

$$\text{and the shear modulus was } G = \frac{E}{2(1+\nu)} = 43.65 \text{ GPa} \quad (3)$$

3.2.1. Parameters of the equation of state

The equation of state characterizes the relationship between hydrostatic pressure and volumetric strain in a material. At low pressures, the hydrostatic pressure tensor is relatively minor, allowing for a straightforward linear expression of the equation of state. In the JH-2 model, the equation of state of the material can be expressed by the following equation:

$$P = K_1 \mu + K_2 \mu^2 + K_3 \mu^3 \quad (4)$$

Where: K_1 is the bulk modulus of the material previously calculated. K_2 , K_3 are material constants, P is the hydrostatic pressure, μ is the volumetric strain, ($\mu = \rho/\rho_0 - 1$), ρ_0 is the material's initial density and ρ is the current density.

A plate impact test is used to obtain the P - μ curve of the brittle material under high pressure. As no plate impact test was found in the literature for BGO, based on other similar material properties [23,24], in this case it was taken that $K_2 = K_3 = 0$ GPa.

3.2.2. Parameters of the strength model

The JH2 strength model accounts for both the intact strength and the material strength at fracture. To represent the transition from the intact state to the fractured state, a damage scalar is introduced. The normalized equivalent stress σ^* is given as:

$$\sigma^* = \sigma_i - D (\sigma_i - \sigma_f) \quad (5)$$

The behavior of the material is modeled based on its damage state. When no damage is present, the scale damage parameter D is ($D=0$), the equivalent dimensionless stress is given by the following equation:

$$\sigma_i = A (P^* + T^*)^N [1 + C \ln(\dot{\epsilon} + \dot{\epsilon}_0)] \quad (6)$$

For a complete material failure, the scale damage parameter is ($D=1$), the dimensionless equivalent stress can be represented by:

$$\sigma_f = B(P^*)^M [1 + C \ln(\dot{\epsilon} + \dot{\epsilon}_0)] \quad (7)$$

In these equations, the material dimensionless constants are A , B , C , M and N . The dimensionless hydrostatic pressure is represented by P^* , where: $P^* = P/P_{HEL}$, while the maximum hydrostatic tensile stress and the equivalent stress are normalized by the general form: $T^* = T/P_{HEL}$, $\sigma^* = \sigma/\sigma_{HEL}$, respectively. The parameter P_{HEL} refers to the pressure of the brittle material at the equivalent stress (σ_{HEL}) at Hugoniot elastic

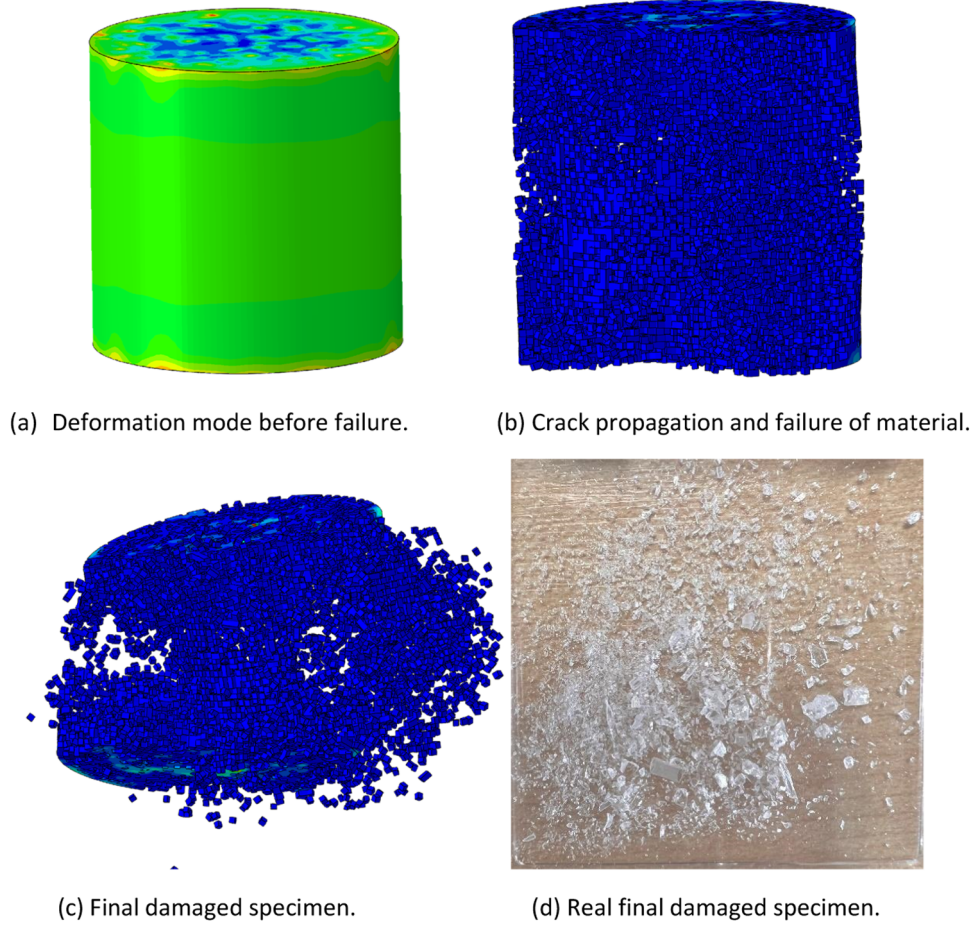


Fig. 7. Damage propagation until failure in simulation and experimental for uniaxial quasi-static compression test.

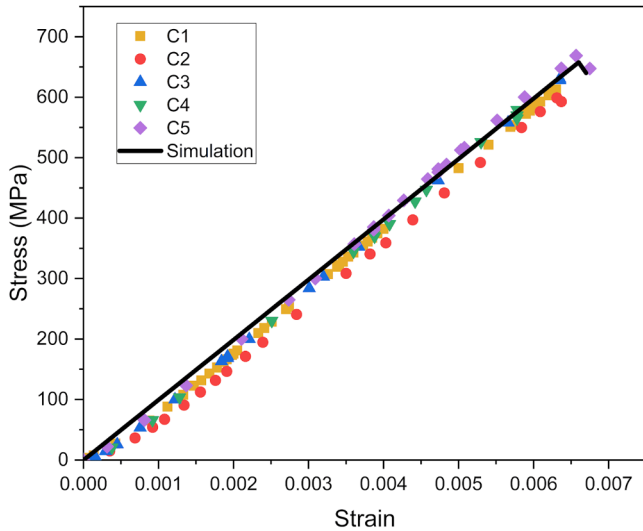


Fig. 8. Simulation and experimental stress-strain curve of quasi static compression tests.

limit (HEL). T refers to the maximum tensile pressure of the brittle material before failure. The dimensionless strain rate is the real strain rate $\dot{\epsilon}$ and $\dot{\epsilon}_0$ is the reference strain rate.

The Hugoniot elastic limit, HEL in the JH-2 model, is calculated using the plate impact test. In this paper, we will take as a reference two single crystal hard brittle materials, single-crystal quartz and sapphire,

which are similar to BGO [25].

For safety when machining bismuth germanate (BGO), it is better to take the HEL value of quartz rather than sapphire. Specifically, using the lower HEL range of quartz (5.5–8.5 GPa) would be the most conservative and safest approach, given BGO's material properties and the need to prevent failure during machining. Through a sensitivity analysis, the chosen Hugoniot elastic limit will therefore be $HEL = 5.8$ GPa in this paper. The HEL value can be described by the following formula:

$$HEL = K_1 \mu_{HEL} + K_2 \mu_{HEL} + K_3 \mu_{HEL} + \frac{4}{3} G \frac{\mu_{HEL}}{1 + \mu_{HEL}} \quad (8)$$

Where u_{HEL} is the volumetric strain at Hugoniot Limit.

By replacing the estimated HEL value, and the values obtained from Eqs. (2) and (3) in (8): $u_{HEL} = 0.054$, then we can obtain the value of P_{HEL} from Eq. (4): $P_{HEL} = 2.84$ GPa.

The tensile strength is derived from the ultimate tensile strength obtained from split from Eq. (1) by the formula:

$$T = \frac{\sigma_t}{3} \left(\frac{1+\nu}{1-\nu} \right) = 9.88 \text{ MPa} \quad (9)$$

Finally, the value of σ_{HEL} is given by the following equation:

$$\sigma_{HEL} = \frac{3}{2} (HEL - P_{HEL}) = 4.44 \text{ GPa} \quad (10)$$

For the remaining parameters A , B , M , N and C , the values were determined based on the range typically observed for brittle materials and further refined through simulations. [23,24]

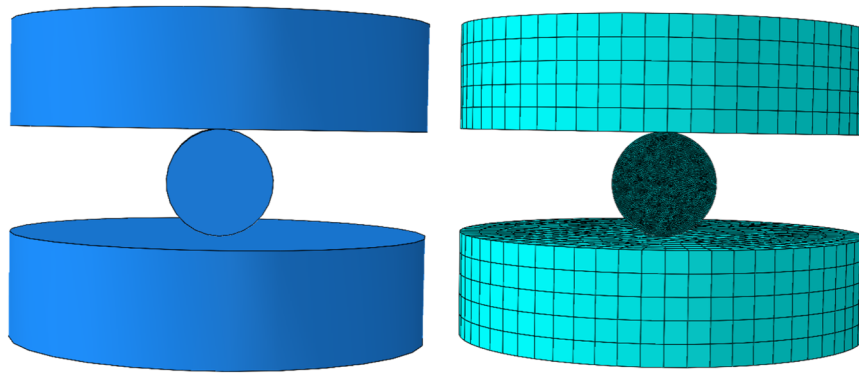


Fig. 9. The geometric structure and boundary condition of the three-dimensional (3D) finite element model (FEM) of split test.

3.2.3. Parameters for the damage model

The JH-2 model employs a damage formulation similar to the Johnson-Cook model [17]. The damage parameter, D , is defined using the following equation.

$$D = \sum (\Delta \epsilon_p / \epsilon_p^f) \quad (11)$$

$\Delta \epsilon_p$ refers to the integral of the effective plastic strain, ϵ_p^f represents the equivalent plastic strain of the material at fracture under a given pressure.

$$\epsilon_p^f = D_1 (P^* + T^*) / D_2 \quad (12)$$

In the JH-2 damage model, the parameters D_1 and D_2 are two dimensionless damage parameters used to describe material damage. Since BGO fractures under very small strains, it is challenging to determine D_1 and D_2 experimentally. These parameters can be estimated through numerical simulations to achieve realistic damage predictions. Based on experimental data comparative view of the failure mechanisms [18], numerical simulations from prior studies [23,24], and iterative comparisons with our real compression test results, the values of $D_1 = 0.045$ and $D_2 = 0.85$ were selected as the initial damage parameters in this paper.

3.3. Application of the model

In our study, we implemented the Johnson-Holmquist 2 (JH-2) model in Abaqus by using the User-defined mechanical material behavior feature, which allowed us to incorporate the JH-2 constitutive model into the Abaqus library. The model includes 32 mechanical constants and 8 solution-dependent state variables such as equivalent plastic strain (PEEQ), ductile damage initiation criterion (DUCTCRT), pressure increment due to bulking (DELTAP), and damage (D). We used the VUMAT subroutine in Abaqus/Explicit, which requires a constitutive model to be defined within the user's subroutine.

3.3.1. Quasi static uniaxial compression test simulation

The dimensions of the specimen in the simulation are the same as that used in the Quasi-static uniaxial compression test and split experiments (10 mm × 10 mm) as shown in Fig. 5. The material was considered homogeneous. Due to the larger cross-sectional area of the plates in the tests compared to the specimen, a uniform compressive load was assumed to act on the BGO surface in JH2 modeling. During the compressive test, a constant velocity was applied to the top face along the Y compression direction, allowing it to compress while deforming freely. The boundary conditions were adjusted so that the bottom face remained fixed. General contact with a defined coefficient of friction ($\mu = 0.3$) was applied based on iterative testing for specimen stability. The mesh type size was chosen to be C3D8R with a size of 0.2 mm in this study based on a mesh convergence as shown in Fig. 6. The plates were

set as rigid, and the constitutive material model for the BGO specimen was defined based on the JH-2 damage model with the parameters listed in Table 3.

In the presented quasi-static compression test, the simulation results from Abaqus, shown in Fig. 7(a to c), demonstrate a close correlation with the experimental results of the real damaged specimen (Fig. 7.d). The simulation initially captures the deformation mode before failure (Fig. 7.a), where the material exhibits a gradual build-up of internal stresses. As loading progresses, the material undergoes crack initiation and propagation (Fig. 7.b), leading to its eventual failure, depicted in Fig. 7.c.

The final state of the simulated specimen (Fig. 7.c) reveals a disintegration pattern characterized by dispersed material fragments, which closely mimics the observed behavior in the real damaged specimen (Fig. 7.d). Both the simulation and the experimental results show a similar fragmentation pattern, indicating that the implemented material model in Abaqus provides an accurate representation of the physical behavior of the material under uniaxial quasi-static compression.

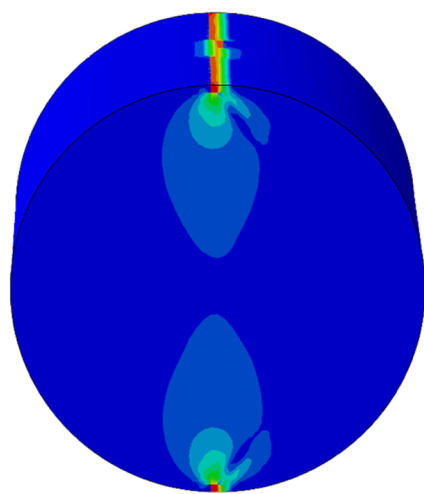
The stress-strain curves presented in Fig. 8 illustrate a comparative analysis between the experimental results from five different samples (C1, C2, C3, C4, and C5) and the simulation data. The graph reveals a remarkable consistency between the experimental data points and the numerical simulation. Each experimental curve demonstrates a similar trend of linear elastic behavior, followed by a slight nonlinearity as the strain increases. This behavior aligns closely with the simulated curve, which follows the same trajectory as the experimental data, particularly in the elastic regime up to strains of approximately 0.0067.

Notably, the dispersion observed between the experimental curves is minimal, with all curves clustering closely around the simulation curve. This suggests a high degree of repeatability and reliability in both the experimental procedure and the simulation model. The simulation slightly underestimates the stress values in the lower strain regions that can be attributed to inherent imperfections, such as microstructural defects (porosity and microcracks), but captures the overall stiffness and the material's response to increased loading with high precision.

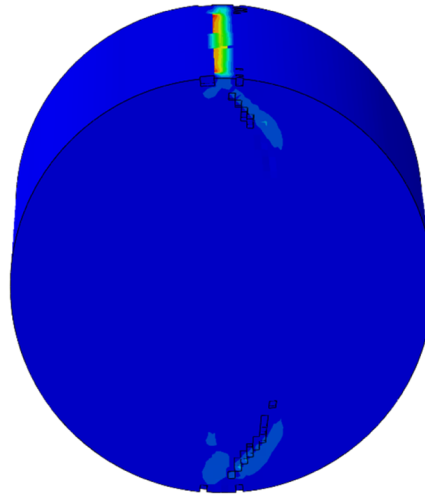
The correlation between the experimental and simulated results provides strong evidence that the simulation model is valid for predicting material behavior under similar quasi-static conditions. This accurate alignment between experimental and simulated stress-strain curves is critical for validating the mechanical model used in the finite element analysis.

3.3.2. Split test simulation

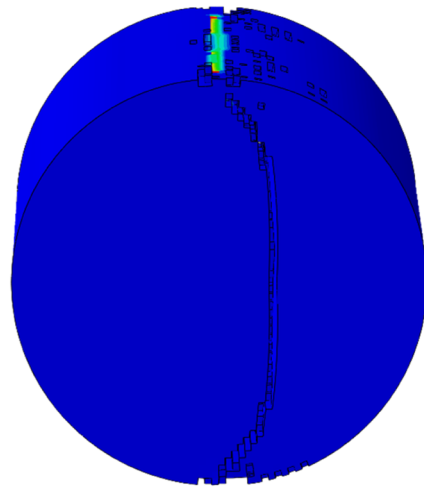
To accurately model the fracture behavior of BGO, a finite element simulation of the split test was also conducted in Abaqus. The boundary conditions and loading conditions were replicated from the experimental setup to ensure consistency in stress distribution and failure prediction. Fig. 9 illustrates the 3D finite element model (FEM) used for the split test simulation, where the lower plate was constrained while a



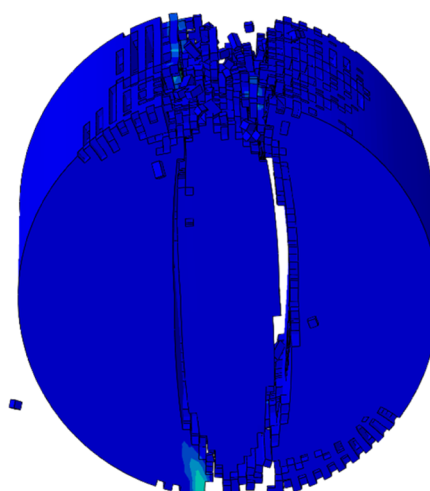
(a) Deformation mode before failure.



(b) First crack generation.



(c) Crack propagation and failure of material.



(d) Final damaged specimen.



(e) Real failure of material.

(f) Final real damaged specimen.

Fig. 10. Damage propagation until failure in simulation and experimental for quasi-static split compression test.

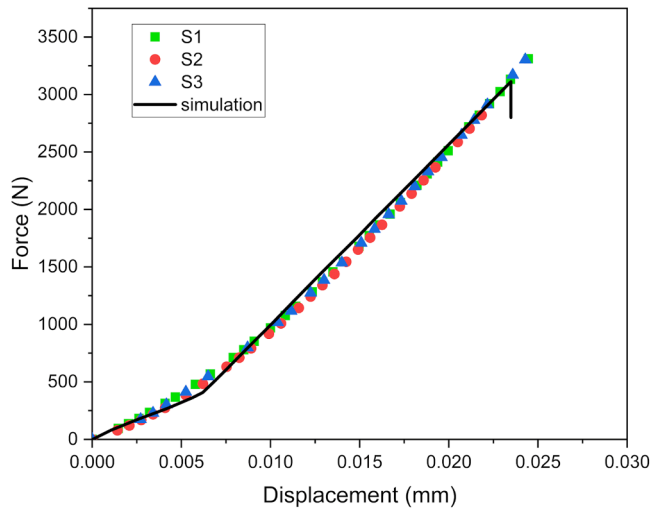


Fig. 11. Simulation and experimental stress strain curve of split tests.

compressive force was applied at the top plate to induce tensile stresses.

In the simulation results depicted in Fig. 10.a, the material undergoes a deformation before failure. The stress distribution is concentrated along the axis of loading, with stress propagating symmetrically. This behavior is consistent with brittle materials, which tend to accumulate stress at localized points before sudden failure. The large stress

concentration at the loading point indicates that the material experiences tensile stresses, leading to eventual failure. The symmetric stress propagation suggests that the loading conditions are uniform, confirming the accuracy of the simulation setup. The first visible crack in Fig. 10. b appears at the point of highest stress concentration. The model accurately predicts the onset of failure, capturing the initial fracture at the location where the material's strength is exceeded. This early-stage crack generation is critical in brittle materials, where cracks form and propagate rapidly once the material's tensile strength is reached. The initiation of this crack aligns with the experimental results in Fig. 10.e, where the crack begins at the same location, further validating the simulation model. As shown in Fig. 10.c, the simulation successfully captures the propagation of the crack throughout the material. The crack follows a predictable path, growing along the plane of maximum stress. This behavior is typical in brittle materials where failure occurs through crack extension rather than plastic deformation. The accurate depiction of crack propagation highlights the model's ability to simulate brittle fracture mechanics. In comparison to Fig. 10.e, the real-world material exhibits a similar crack path, confirming that the model closely mirrors the physical behavior of the material under load. The final damaged specimen in the simulation, shown in Fig. 10.d, demonstrates the complete fracture of the material. The material splits into two distinct sections, with visible fragmentation occurring along the crack path. This fragmentation pattern is consistent with the brittle failure mode, where the material does not undergo a big plastic deformation but instead fractures immediately. In the experimental results (Fig. 10.f), the material also fractures into similar fragments, further validating the

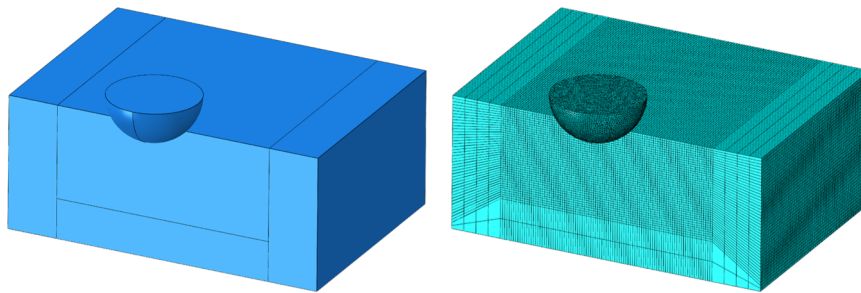


Fig. 12. The geometric structure and boundary condition of the three-dimensional (3D) finite element model (FEM) of the milling process.

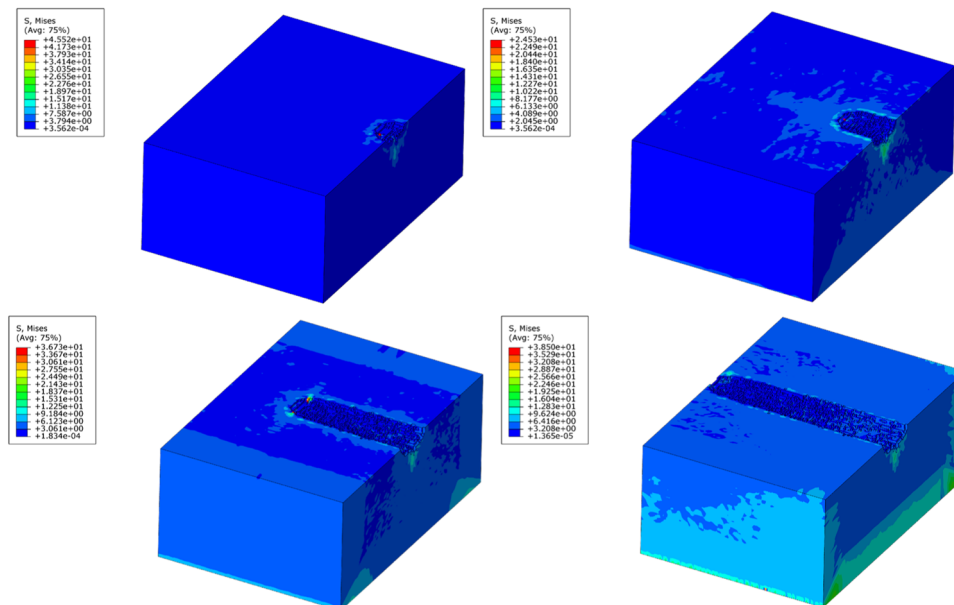


Fig. 13. Von mises variation during milling process at different times during machining.

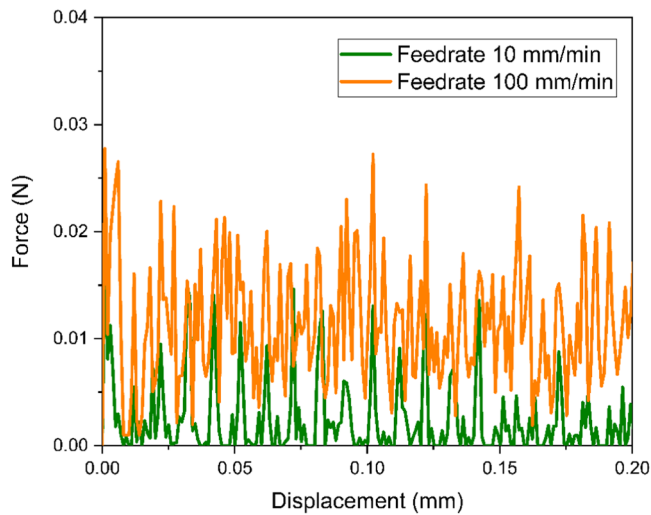


Fig. 14. Cutting force displacement curve of milling process using two different feed rates.

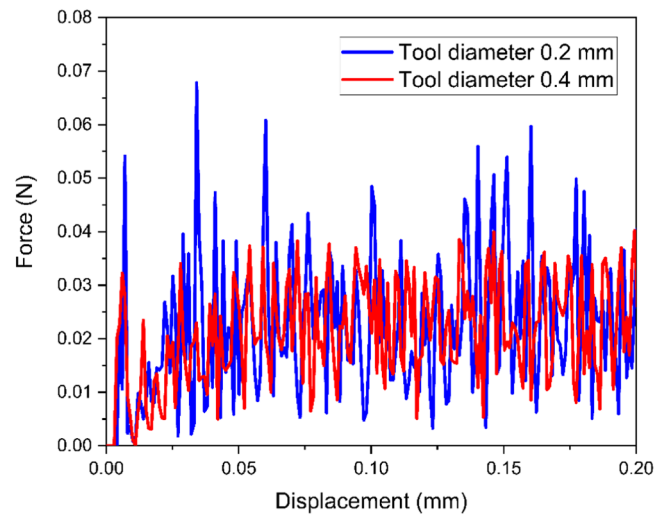


Fig. 16. Cutting force displacement curve of milling process using two different tool diameters.

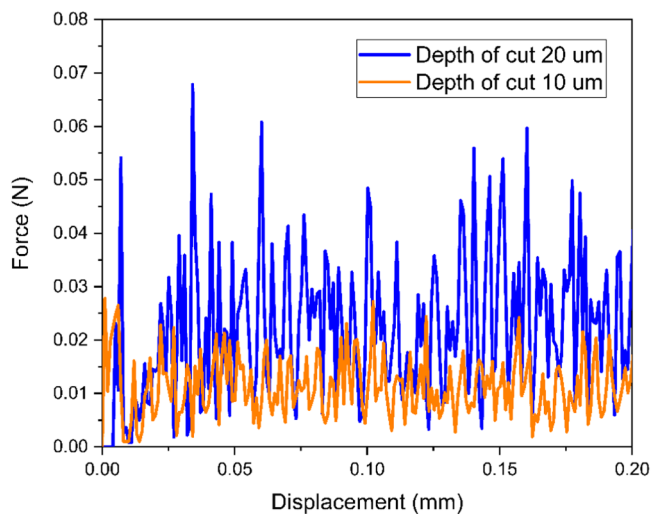


Fig. 15. Cutting force displacement curve of milling process using two different depth of cuts.

accuracy of the Abaqus model.

The stress-strain curve in Fig. 11 presents a comparison between the experimental results (S1, S2, and S3) and the simulation data for the same material under tensile loading. The plot effectively illustrates the material's response to increasing displacement, showing how the force builds up as the material is stretched, ultimately leading to failure.

The experimental data points (S1, S2, and S3) and the simulation curve closely align up to the maximum displacement of approximately 0.024 mm, with very small deviations between the curves. This close agreement suggests that the JH2 material model used in Abaqus accurately captures the tensile behavior of the material up to failure. The model reproduces both the elastic response and the linear behavior as the material approaches its strength limit. From 0–0.005 mm of displacement, the force increases linearly with displacement. This linear relationship indicates that both the simulation and experiments remain in the elastic region. The nearly perfect overlap of the simulation curve with the experimental data in this region validates the accuracy of the elastic modulus defined in the simulation model. Beyond 0.005 mm, the curve begins to deviate from linearity, signifying the onset of plastic deformation. At this stage, the material undergoes permanent deformation, and the force required to continue the deformation increases at

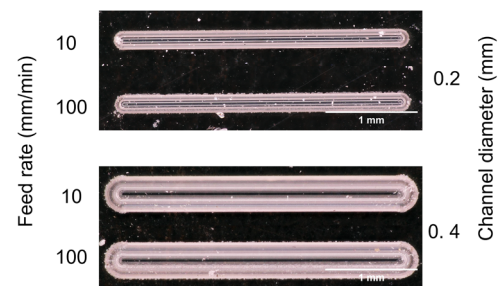


Fig. 17. 3D Microscopic view of Milled BGO (a) 0.2 mm (b) 0.4 mm in function of the feed rate.

a lower rate. The simulated curve captures this nonlinear behavior precisely, with excellent correlation to the experimental data (S1, S2, S3). This agreement indicates that the plasticity model in the simulation is well-calibrated, likely using appropriate yield stress and strain hardening parameters that reflect the actual material behavior.

Near the maximum displacement of 0.024 mm, the force peaks at around 3100 N. The experimental data points (S1, S2, S3) and the simulation both show similar peak force values, indicating that the simulation accurately predicts the material's tensile strength. Following the peak, the simulation indicates a rapid drop in force, represented by the sharp downward trend, which corresponds to material failure. This drop is typical of brittle materials, where failure occurs suddenly after reaching the maximum load. The consistency of the peak force values between the simulation and experiment is a strong indicator of the model's accuracy in predicting the failure behavior of the material.

3.3.3. Numerical and experimental investigation of micromachining

In the second phase of the numerical simulation, the JH-2 model was applied to simulate the micro-milling process using Abaqus/Explicit. The workpiece was modeled with dimensions of 0.5 mm × 0.5 mm × 0.3 mm, with two different tool diameters, each performing a cutting depth of 10 μm. As illustrated in Fig. 12, a simplified 3D conception of the milling tool was used, focusing on its lower section. A refined mesh size of 0.005 mm was applied to the deformable region to capture fine details of the material behavior. Tool wear was considered to ensure consistency with experimental conditions. The wear was observed only after extended cutting lengths, remaining negligible within the tested machining range. The tool was treated as a rigid body to reduce computational cost. The boundary conditions were set to fully constrain

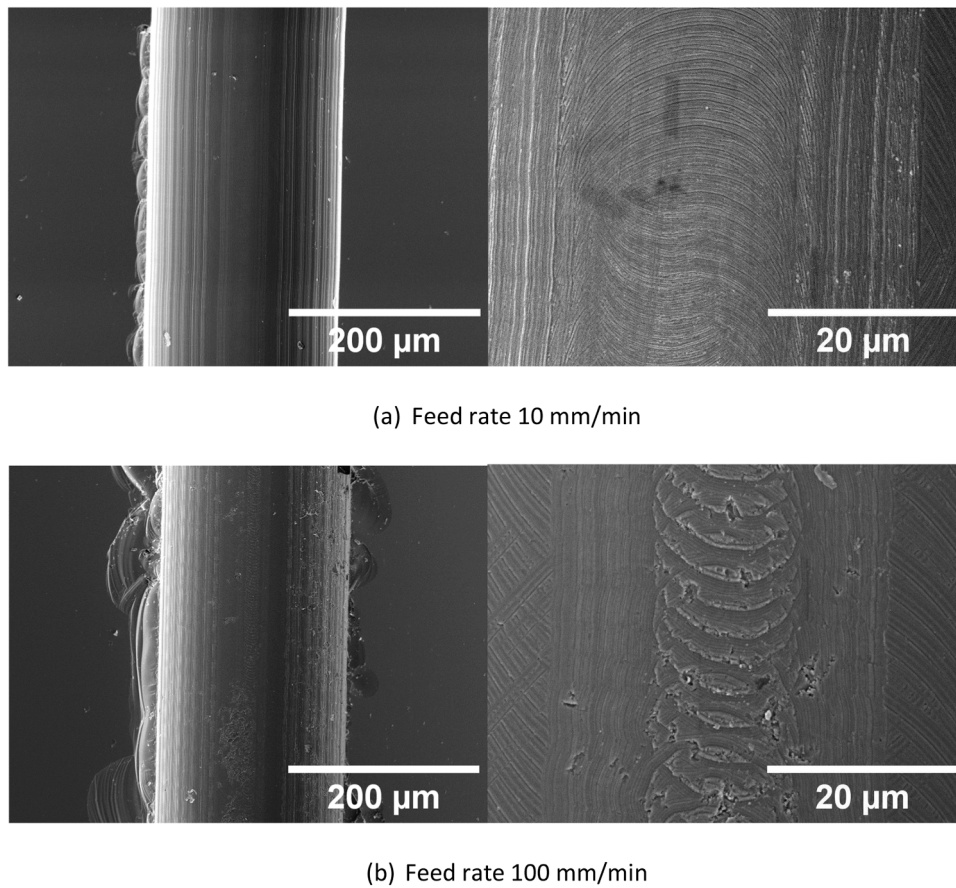


Fig. 18. SEM images of milling process using 0.2 mm tool diameter for different feed rates.

the bottom surface of the workpiece, preventing any movement in the X and Y directions, while allowing free displacement in the active milling direction, Z. A constant angular velocity of 30,000 RPM was applied to the tool to simulate the dynamic cutting motion along the specified path. This parameter was kept constant across all tests to eliminate any variability in tool speed. Additionally, an explicit dynamic analysis was employed to model the high-speed surface-to-surface interaction between the rigid tool and the workpiece, capturing the cutting forces and deformation behavior while incorporating the JH-2 material model to simulate damage evolution and fracture in the hard, brittle material. This setup provided a highly detailed representation of the micro-milling process, ensuring a balance between computational efficiency and accuracy while facilitating the validation of the model with the known behavior of brittle materials. To evaluate the accuracy and effectiveness of the JH-2 model in simulating the micro-milling process, we performed simulations using different milling parameters, starting by varying the feed rates (10 mm/min and 100 mm/min), the depth of cut (10 μm and 20 μm), and then the tool diameter ($D=0.2$ mm and 0.4 mm). These varying parameters allowed us to assess the model's response to different cutting conditions, providing insight into how well the simulation captured the cutting forces, material deformation, and overall behavior under different machining scenarios.

Fig. 13 presents the evolution of the Von Mises stress distribution during the micro-milling process. The sequence of images captures the material response at different time steps, highlighting the development of localized stress concentrations at the tool-workpiece interface. As the tool advances, the stress levels increase near the cutting edge, particularly along the shear zones where material removal occurs. At later stages, stress redistribution is observed, leading to crack initiation within the brittle material. This visualization demonstrates the interplay between cutting forces and stress accumulation, providing insight into

the material removal mechanisms governing the machining of BGO.

Fig. 14 illustrates the impact of feed rate during the milling of BGO. At a lower feed rate of 10 mm/min, the milling process demonstrates enhanced stability, characterized by reduced cutting forces and minimal disturbance to the brittle material. As the feed rate increases to 100 mm/min, while maintaining constant milling conditions, there is a noticeable rise in dynamic force fluctuations, despite the overall cutting forces remaining low (below 0.03 N). This behavior aligns with established findings on machining brittle materials, where the feed rate plays a critical role in determining the quality of the finished surface. Lower feed rates tend to produce finer surfaces by maintaining force stability, reducing crack propagation, and minimizing surface roughness, thus yielding a higher quality finish. Higher feed rates often introduce instability, adversely affecting surface integrity and increasing subsurface stress, and elevate the potential for defect propagation of structural damage to the brittle material [26–28].

Fig. 15 shows the impact of depth of cut during the milling of BGO. Increasing the depth of cut to 20 μm results in a significant rise in cutting forces. Deeper cuts generally produce higher forces, which in turn elevates the risk of fractures. The high fluctuations suggest that the material encounters localized stress concentrations exceeding its fracture toughness threshold, which can precipitate crack initiation and propagation within the machined surface. These findings align with prior studies on brittle materials, where maintaining a controlled depth of cut is essential to minimize subsurface damage, reduce crack formation, and achieve superior surface finish [26].

The use of a larger tool diameter (0.4 mm) results in more stable cutting forces compared to a smaller tool diameter (0.2 mm) under identical conditions. As shown in Fig. 16, Simulation results reveal that the 0.4 mm tool produces smoother force-displacement curves with fewer fluctuations, indicating a more consistent cutting process. This

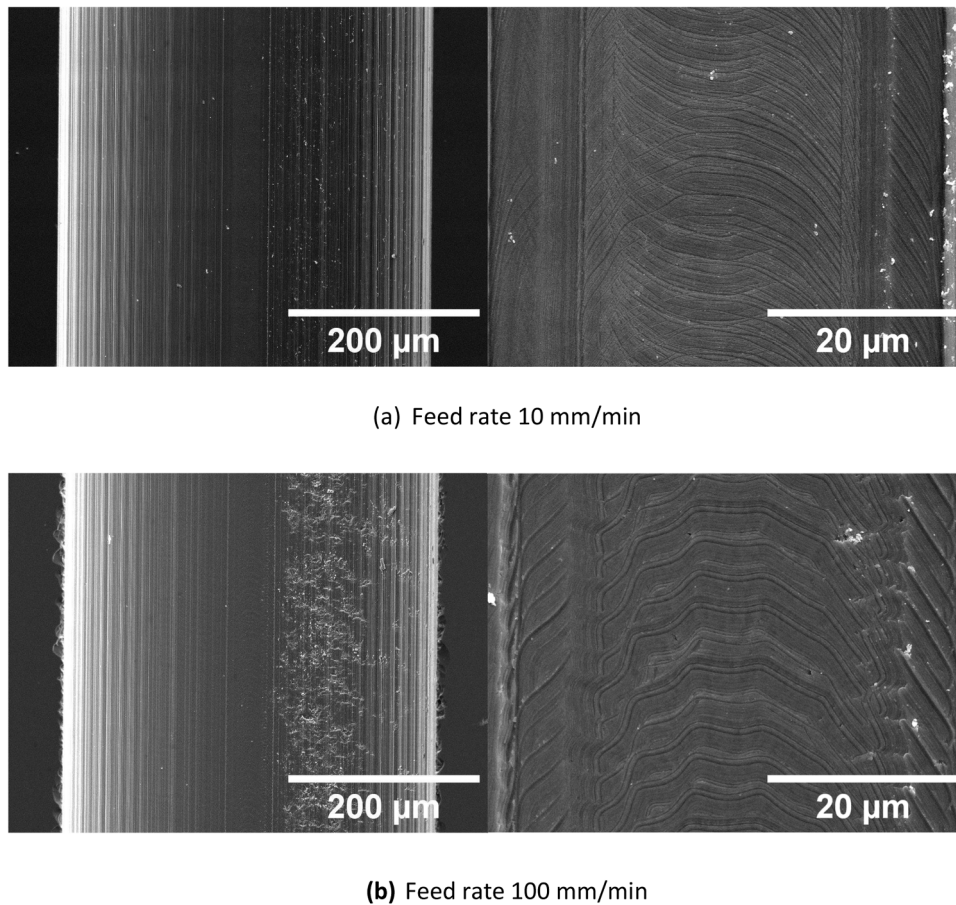


Fig. 19. SEM images of milling process using 0.4 mm tool diameter for different feed rates.

Table-4

Technological parameters for the milling process.

Diameter (μm)	Feed Rate (mm/min)	rms (nm)
0.2	10	17
	100	60.6
0.4	10	10.7
	100	41

suggests that the larger diameter facilitates better force distribution under the given conditions, reducing the risk of sudden force spikes and potential brittle fractures. In contrast, the 0.2 mm tool diameter exhibits more force fluctuations and instability, increasing the risk of micro-cracking and surface roughness during milling. Overall, the larger tool diameter maintains a more stable interaction with the material, thereby minimizing the risk of force-induced damage [29,30].

To validate the simulation findings, a series of experimental tests were performed using two feed rates (10 mm/min and 100 mm/min) combined with two tool diameters (0.2 mm and 0.4 mm), resulting in four distinct test scenarios.

Fig. 17 presents 3D microscopy analysis showing the effects of tool diameter (0.2 mm and 0.4 mm) and feed rate (10 mm/min and 100 mm/min) on the surface topography of BGO under different milling conditions. At the lowest feed rate (10 mm/min), the smaller tool (0.2 mm) achieves precise cuts with minimal chipping and a smooth surface. This suggests stable material removal, where cutting forces remain controlled, preventing severe fracture. In contrast, a high feed rate (100 mm/min) results in more chipping and surface roughness. The larger tool (0.4 mm) performs better at higher feed rates, producing

smoother surfaces with less chipping compared to the 0.2 mm tool. Nevertheless, at the highest feed rate (100 mm/min), both tools experience noticeable surface degradation, with the 0.4 mm tool showing a slight advantage.

The SEM images in Figs. 18 and 19, along with data from Table 4, further support the findings. The analysis reveals that the channel surface quality remains high, with minimal damage or brittle fracture, even at the higher feed rate of 100 mm/min. Surface roughness is relatively low, ranging from 17 to 60.6 nm. At a lower feed rate of 10 mm/min, both tool diameters produce smooth surfaces with distinct machining marks and minimal roughness, indicating efficient material removal with limited stress. Conversely, at 100 mm/min, surface quality degrades for both tool sizes, marked by increased roughness and the presence of chipping, indicating greater stress and material damage.

This degradation in surface quality at higher feed rates can be attributed to the transition from ductile-mode cutting to brittle fracture mode, as clearly evidenced by the SEM images. At 10 mm/min, the machining process results in well-defined parallel cutting tracks with a smooth, continuous surface and edges, indicating stable material removal. The 0.4 mm tool produces a more uniform and consistent pattern, while the 0.2 mm tool exhibits slightly deeper and more pronounced machining marks, though still maintaining a relatively smooth finish. However, at 100 mm/min, excessive cutting forces cause material removal to shift toward brittle fracture, leading to irregular tool marks, fragmented edges, and visible chipping. The SEM images show microcracks along the machined path, particularly in the 0.2 mm tool, where the smaller diameter results in high irregularities in surface morphology and random fracture lines. In contrast, the 0.4 mm tool, while also showing signs of increased roughness, maintains a more controlled and structured machining pattern with fewer irregularities.

These observations confirm that optimizing feed rate and tool geometry is crucial for achieving precise surface integrity in BGO machining.

Overall, the findings confirm that the lowest feed rate consistently delivers superior surface quality for both tool diameters, reflecting the direct relationship between reduced cutting forces and improved surface finish [31,32].

4. Conclusions

This study has thoroughly explored the machinability of single-crystal Bismuth Germanate (BGO) under diverse micro-machining conditions, providing critical insights into its behavior as a brittle material used in high-precision applications. By varying key process parameters in the micro-milling process, we observed the material's response to different machining environments, confirming BGO's machinability across a range of conditions. Detailed material characterization through quasi-static compression tests allowed for the accurate determination of the mechanical properties necessary for defining the Johnson-Holmquist 2 (JH-2) material model, which was subsequently integrated into finite element analysis (FEA) simulations using Abaqus. These simulations, designed to replicate quasi-static compression, splitting, and micro-machining tests, were systematically compared with experimental data, leading to a robust validation of the JH-2 model for BGO.

The close agreement between the simulated and experimental results confirms the validity of the JH-2 model in capturing the key aspects of BGO's mechanical behavior under different machining regimes. The FEM model for BGO, validated through both literature and experimental results, confirms its reliability in predicting the effects of tool diameter, feed rate, and depth of cut during micro-milling. The investigation of surface integrity confirmed that machining parameters critically influence surface morphology in BGO. Lower feed rates (10 mm/min) and larger tool diameters (0.4 mm) produced smooth, continuous machining tracks with minimal defects, while higher feed rates (100 mm/min) led to brittle fracture, chipping, and irregular tool marks, especially with the 0.2 mm tool. SEM analysis showed that controlled cutting conditions resulted in better surface quality, whereas excessive cutting forces caused surface damage and irregular machining patterns. These findings emphasize the importance of optimized micro-milling parameters to achieve precision machining with minimal surface damage in BGO. The computational framework developed in this study can serve as a reference for exploring the machinability of other brittle scintillator materials, aiming to enhance the manufacturing of high-precision components for PET imaging and similar applications.

CRediT authorship contribution statement

bizarri gregory: Writing – review & editing, Project administration, Methodology, Investigation, Funding acquisition, Conceptualization. **Taieb Kahina:** Writing – original draft, Validation, Methodology, Investigation, Formal analysis. **Belkhir Nabil:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Khennab Abdelghani:** Writing – review & editing, Software, Methodology, Investigation, Formal analysis. **Rogers Edith:** Writing – review & editing, Supervision, Methodology, Investigation, Formal analysis, Data curation. **Giusca Claudiu:** Writing – review & editing, Supervision, Methodology, Formal analysis.

Declaration of Competing Interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Gregory bizarri reports financial support was provided by Engineering and Physical Sciences Research Council. If there are other authors, they declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

All the data can be found in DOI: <https://doi.org/10.57996/cran.ceres-2699> and Handle: <https://dspace.lib.cranfield.ac.uk/handle/1826/23386>

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