Key Engineering Materials Vol. 329 (2007) pp. 397-402
online at http://www.scientific.net

Numerical Simulation and Prediction of Surface Heterogeneity in Diamond Turning of Single-Crystalline Germanium

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Keywords: Numerical Simulation, Single-Crystalline Germanium, Crystallographic Orientation, Diamond Turning, Ductile Machining, Precision Machining

Abstract. This paper deals with the mechanism of surface heterogeneity due to crystallographic anisotropy effects in diamond turning of single-crystalline germanium. A microplasticity-based numerical simulation model was proposed, in which the effects of tool geometry and machining conditions can be involved. Two coefficients were introduced to compensate the Schmid factors of two different types of symmetrical slip systems. Simulation of ductile machinability was conducted on two crystallographic planes (100) and (111), and the simulation results were consistent with the experimental results. It was indicated that the simulation model can be used to predict the brittle-ductile boundary change with machining conditions and crystal orientations of germanium.

Introduction

Single-crystalline germanium (Ge) is used in infrared spectroscopes and other optical equipment which requires extremely sensitive infrared detectors. Unlike most other semiconductors, germanium has a small band gap, allowing it to efficiently respond to infrared light. Therefore, precision machining of germanium, to obtain super smooth optical surfaces, has become a very improtant research area. A number of works have been reported on the ductile machining of germanium [1-5]. In a previous paper [3], the ultraprecision machining characteristics of various crystallographic planes of single-crystal germanium were examined. The machined surface quality sometimes showed strong nonuniformity due to the crystallographic anisotropy, and the brittle-ductile transition boundary varied significantly with the crystal orientation angle. Although under specific optimal conditions, smooth ductile-machined surfaces with nanometric roughness can be obtained on all crystal planes, the understanding and prediction of the surface heterogeneity is essentially important for optimizing the ductile machining process.

In the previous studies [1-3, 6, 7], the surface heterogeneity phenomena of silicon, germanium and other crystalline materials, during diamond turning, have been noticed and some of the authors attempted to explain this phenomenon through the cleavage fracture theory [1, 2]. Using the cleavage theory, one can explain some experimental results under rough machining conditions, but cannot give satisfactory explanations to the changes of surface features when the machining conditions and tool geometries changes in the brittle-ductile transition region. Shibata et al proposed a plasticity parameter, namely, slip orientation factor and successfully explained some surface features in diamond turning of silicon in the brittle-ductile transition region [6].

In this paper, an improved model based on Shibata's model was used to simulate the ductile machinability and surface heterogeneity of germanium in diamond turning. In the model, the cutting force direction to simulate the effects of machining parameters such as tool rake angle, edge radius and undeformed chip thickness, was changed. This method enabled the simulation of both brittle and brittle-ductile transition modes using one model. The slip orientation factor, proposed by Shibata, et al by introducing two correction coefficients to correct the Schmid factors of symmetrical slip systems, was also improved. By comparing the simulation results and the experimental results, an approach to predict the ductile machinability and optimum machining conditions for various crystalline systems, was found.

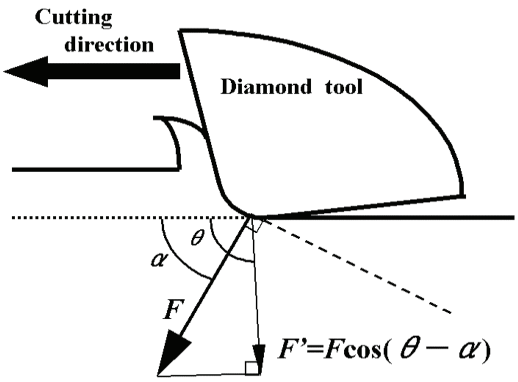


Fig.1 Schematic of the two-dimensional cutting force model used for simulation

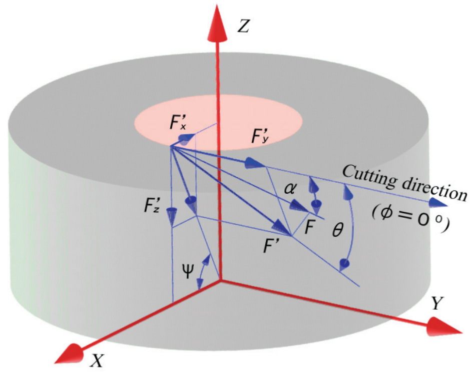


Fig.2 Schematic of a three-dimensional cutting force model in diamond turning flat surface

Simulation Models

Cutting force model. To analyze the deformation behavior of a crystalline material during machining, the direction and distribution of the cutting forces needed to be defined. Here, for simplicity, a two dimensional orthogonal cutting model as schematically shown in Fig.1 is considered. It was assumed that the total cutting force F acts on the workpiece material in a direction inclined at an angle α to the cut surface. The total cutting force F is equivalent to its force components F' in a direction whose angle from the cut plane is θ, and F' can be given by the following equation.

$$F' = F\cos(\theta - \alpha) \tag{1}$$

Shibata, et al found the cutting force angle was α=65º, and used this angle in the simulation [6]. In the present paper, the cutting force angle is not fixed. The cutting force angle is dealt with as a variable which depends on tool geometry and cutting conditions [4]. Generally, the bigger the edge radius and the higher the negative rake angle, the larger the cutting force angle α, and this angle will also change as the tool wears. The force direction is also affected by the undeformed chip thickness: the smaller the undeformed chip thickness, the larger the cutting force angle α. Therefore, by characterizing the relationship between the cutting force direction and the above cutting parameters, it might be possible to simulate various machining modes using the same simulation model.

In diamond turning, the cutting force direction is always changing with respect to the circumferential direction of the workpiece as the spindle rotates, as shown in Fig.2. In an actual cutting process, the workpiece rotates along the Z-axis of the machine. In this paper, in order to simplify the simulation process, the workpiece was fixed and the cutting force rotated along the Z-axis in a reverse direction. As an initial situation, the cutting position is located on the X, Z plane, the angle between the X-axis and the cutting point is ψ and the cutting direction is parallel with the Y-axis. Then the components F' (F'_x, F'_y, F'_z) of the cutting force F can be obtained by:

$$\begin{aligned} F'_x &= F\cos(\theta - a)(-\sin\theta\cos\psi) \\ F'_y &= F\cos(\theta - a)\cos\theta \\ F'_z &= F\cos(\theta - a)(-\sin\theta\sin\psi) \end{aligned} \tag{2}$$

As the workpiece rotates (the cutting force rotates in the reverse direction), the components *F'* of the cutting force changes with the rotation angle ϕ, and can be given by:

$$\begin{aligned} F'_x &= F\cos(\theta - a)(-\sin\theta\cos\psi\cos\phi - \cos\theta\sin\phi) \\ F'_y &= F\cos(\theta - a)(-\sin\theta\cos\psi\sin\phi + \cos\theta\cos\phi) \\ F'_z &= F\cos(\theta - a)(-\sin\theta\sin\psi) \end{aligned} \quad (3)$$

Slip system model. As known from plasticity, when a single crystal is deformed under an external force, slip occurs when the shear stress acting in the slip direction on the slip plane reaches a critical value. This critical shear stress is related to the stress required to move dislocations across the slip plane. Usually the ease of slip deformation can be determined by the Schmid factor, $\cos\chi\cos\lambda$, where χ is the angle between the tensile axis and the slip plane normal; λ is the angle between the external force and the slip direction. For machining brittle materials, the Schmid factor can be used to evaluate the ductile machinability for a certain combination of crystal structure and an external force. The greater the Schmid factor, the higher the ductile machinability.

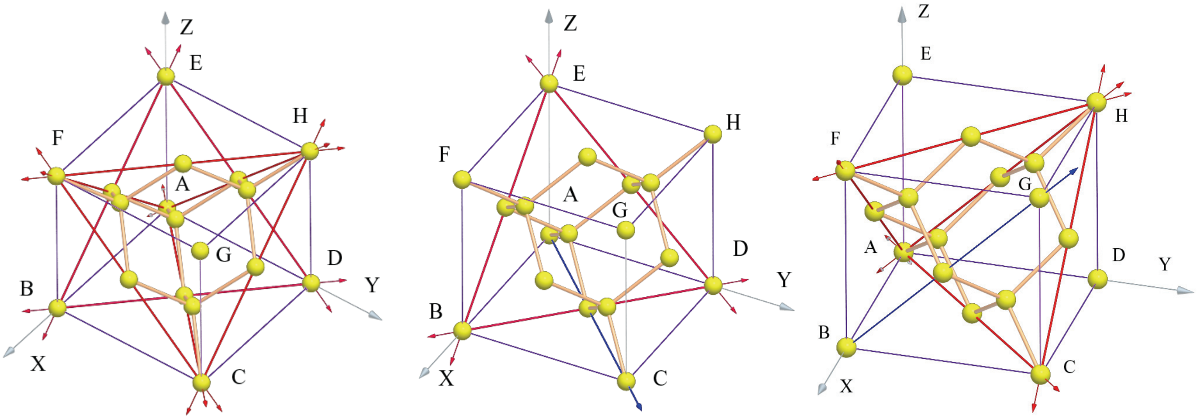


Fig.3 (a) Primary slip systems of germanium single crystal; (b) Symmetrical slip systems in the same slip plane; (c) Symmetrical slip systems in different slip planes

For a single-crystalline material, there are always primary slip systems which have the greatest Schmid factor under a specific external force. In the case of germanium, the primary slip system includes four slip planes, namely $(\bar{1}11)/(1\bar{1}1)/(11\bar{1})/(111)$, and twenty-four <111> slip directions, as shown in Fig.3 (a). During the diamond turning operation, the orientation of the primary slip systems always changes with the cutting force direction, accordingly the Schmid factor also changes, causing the variation in machinability and the surface heterogeneity.

The Schmid factor η for a given slip system and a force component can be calculated by:

$$\eta = \frac{F'}{F}\cos\chi\cos\lambda = \cos(\theta - \alpha)\cos\chi\cos\lambda \quad (4)$$

The maximum Schmid factor in a given slip system for all the component force *F'* is defined by:

$$\eta_{ij} = \max\{\frac{F'}{F}\cos\chi_i \times \cos\lambda_{ij}\} = \max\{\cos(\theta - \alpha)\frac{F'\cdot N_i}{|F'||N_i|}\frac{F'\cdot S_{ij}}{|F'||S_{ij}|}\} \quad (5)$$

Where N_i and S_{ij} is the normal vector of slip plane and the orientation vector of a slip plane, respectively.

Symmetrical modification coefficient. In diamond turning, there exist situations where two slip systems are symmetrical to the cutting force direction. On these occasions, the interference between the symmetrical slip systems probably restricts the slip in both individual systems; as a result, the effective Schmid factor will be smaller than the sum of their respective values [6]. This symmetrical effect must be compensated for in simulation. Shibata, et al used a coefficient γ to modify the Schmid factor and the modified parameter was termed the "slip orientation factor" [6]. However, the value of γ (=0.40) was determined from experimental observation results which might involve singularities. Another problem is that it is difficult for one to determine the angle range where the symmetric compensation should be performed.

In this paper, a new compensation method is proposed to correct the Schmid factor as described below. The modified parameter is simply termed the "slip factor", and is used to present the effective Schmid factors for all active slip systems.

At first, the slip system symmetries of germanium were divided into two types: one is that two slip directions in the same slip plane are symmetrical to the cutting direction; the other is that two symmetrical slip directions are in different slip planes. Fig. 3 (a) shows the first type of symmetry: two slip systems $(111)[01\bar{1}]$ and $(111)[10\bar{1}]$ are in the same slip plane (111), and both slip systems are symmetrical to the cutting direction [110]. For this case, the modification coefficient β is given by:

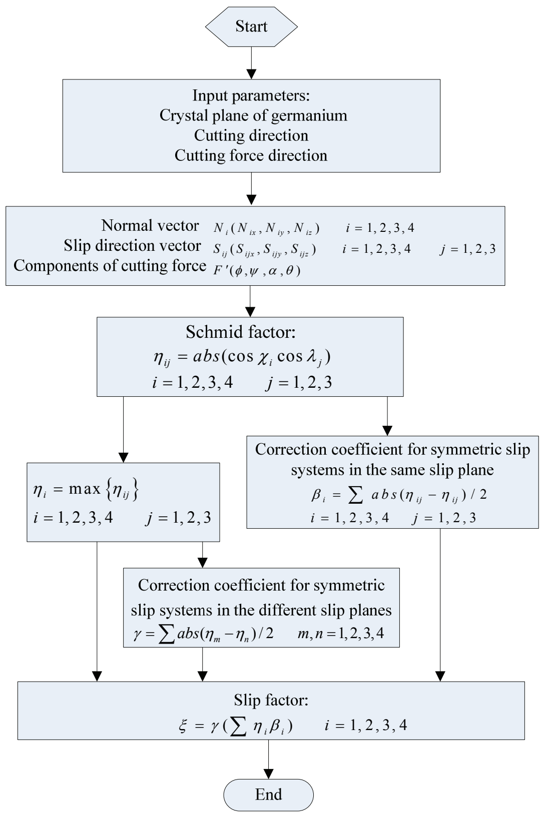


Fig.4 Simulation procedures

$$\beta_i = abs(\eta_{i1} - \eta_{i2}) + abs(\eta_{i2} - \eta_{i3}) + abs(\eta_{i3} - \eta_{i1}) \tag{6}$$

Where $\eta_{i1}, \eta_{i2}, \eta_{i3}$ are the Schmid factors in the same plane calculated by Eq. (5). Therefore, the slip factor ξ is given by:

$$\xi = \eta_1\beta_1 + \eta_2\beta_2 + \eta_3\beta_3 + \eta_4\beta_4 \tag{7}$$

Where η_i and β_i (i=1, 2, 3, 4) are the maximum slip factors and the correction coefficients for four slip planes, respectively.

Fig. 3 (b) shows the second symmetrical slip: two slip systems $(11\bar{1})[\bar{1}0\bar{1}]$ and $(1\bar{1}1)[\bar{1}\bar{1}0]$ are in different slip planes, but both of them are symmetrical to the cutting direction [011]. A new correction coefficient γ was used here to correct the values of the Schmid factor, and γ is given by:

$$\gamma = abs(\eta_1 - \eta_2) + abs(\eta_1 - \eta_3) + abs(\eta_1 - \eta_4) + abs(\eta_2 - \eta_3) + abs(\eta_2 - \eta_4) + abs(\eta_3 - \eta_4) \tag{8}$$

Where $\eta_1, \eta_2, \eta_3, \eta_4$ are the maximum Schmid factors on the four slip planes.

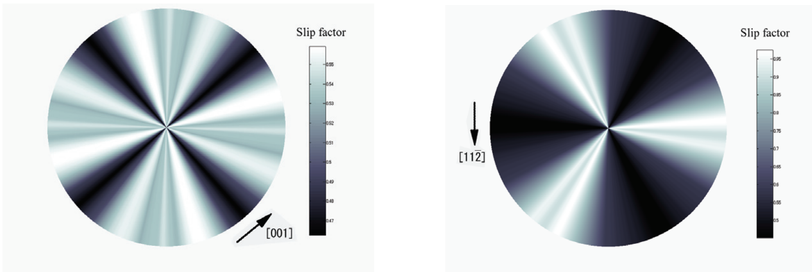
By means of the correction with coefficients β and γ, the final slip factor is given by:

$$\xi = \gamma(\eta_1\beta_1 + \eta_2\beta_2 + \eta_3\beta_3 + \eta_4\beta_4) \tag{9}$$

In the above compensation method, the coefficients β and γ are automatically derived from the symmetry extent of the slip systems. Therefore they are self-defined in the simulation and need not be input subjectively. This can avoid singularity due to experimental errors.

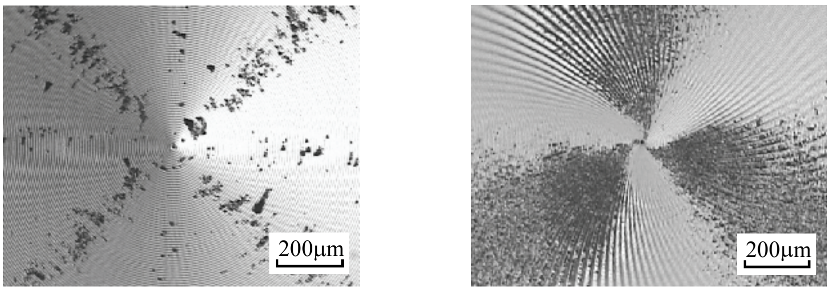
Simulation Procedures

Based on the above models, a simulation process for evaluating the slip factors during diamond turning germanium was developed as shown in Fig.4. First, the initial parameters of the cutting planes, cutting direction and the direction of cutting force are input. Then, the normal vector N_i and the slip direction vector S_{ij} of the cutting plane, and the components of the cutting force F' are calculated. These vectors were used to calculate the slip factor for the four slip planes and the three couples of slip directions on a slip planes. Next, three values of the Schmid factors in same slip plane are used to calculate the correction coefficient β. The maximum value of the Schmid factors in the same slip plane was taken as the effective Schmid factor for this slip plane, and the four values are used to calculate the correction coefficient γ for symmetrical slip systems in different planes. Finally, the slip factor ξ was calculated using the correction coefficients. By calculating the slip factors for all the orientation angles, the surface heterogeneity of single-crystalline germanium can be obtained.



(a) (100) plane (b) (111) plane

Fig.5 Slip factor distribution when cutting force angle is 60º



(a) (100) plane (b) (111) plane

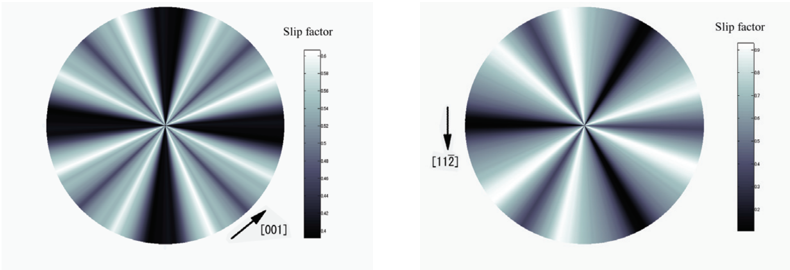
Fig.6 Surface features at workpiece center in diamond turning of germanium [3]

Results and Discussion

As known from previous experimental results, the thrust force is higher than the principal force in ductile and brittle-ductile transition regimes of brittle materials, and the cutting force angle is larger than 45º; whereas in the brittle regime at large undeformed chip thickness, the thrust force is lower than the principal force and the cutting force angle is smaller than 45º. Here, as examples, simulation was first performed by setting the cutting force angle to 60º and 30º respectively.

Fig.5 shows simulation results of slip factor distribution on Ge (100) and (111) planes at a cutting force angle of α=60° which corresponds to machining conditions of small undeformed chip thickness, high negative rake angle, and cutting tools with certain edge radius. Dark areas in the figure have small slip factors thus are easy to be brittle-fractured, while the bright areas having large slip factors are easy to be ductile-cut. Fig.6 shows the micrographs of the workpiece center of Ge (100) and (111) planes after diamond turning at an undeformed chip thickness of 163 nm (brittle-ductile regime) [3]. It is evident that the simulation results are generally consistent with the experimental results.

Fig.7 shows simulation results of slip factor distribution at a cutting force angle of α=30°. This cutting force angle corresponds to machining conditions of large undeformed chip thickness, low negative rake angle, and extremely sharp cutting tools. The surface heterogeneity features in this figure are distinctly different from those in Fig.5. These surface patterns agree with the experimental results of previous studies [1, 2].



(a) (100) plane (b) (111) plane

Fig.7 Slip factor distribution when cutting force angle is 30º

Conclusions

A numerical simulation model based on the Schmid factor in microplasticity was proposed to simulate the surface heterogeneity in diamond turning of germanium. In this model, the effects of tool geometry and machining conditions are concerned by varying the cutting force angle. Two correction coefficients were introduced to modify the Schmid factors of symmetrical slip systems. Simulation of ductile machinability was conducted on Ge (100) and (111) planes, and the simulation results were compared with experimental results. It was confirmed that the simulation model can be used to predict the surface feature and its changes with machining conditions and crystal orientations of germanium. This method may be extended to other brittle single crystalline materials.

Acknowledgments

We would like to thank the Japan New Energy and Industrial Technology Development Organization (NEDO) for their support as an industrial technology research grant program (04A31508).

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