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Analysis of effects of mechanical properties on ductile-to-brittle transitions at nano-scale mechanical machining

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Abstract

Single-crystal materials, characterized by their uniform atomic structures and properties, find extensive applications across various industrial sectors, including electronics, optics, and displays. While lapping or polishing of single-crystal materials is a widely employed technique in industries, mechanical machining for patterning is not commonly applied due to their brittle fracture characteristics. Although some previous research has demonstrated the possibility of mechanically machining these materials at ultra-low forces on the nano-scale, estimating the critical thrust force at the ductile-to-brittle transition remains challenging. Furthermore, it is unclear how much plastic deformation affects ductile machining on the nano-scale, as analysing nano-sized chips is inherently difficult. To address these issues, our research focuses on analysing how mechanical properties influence the critical thrust force at the ductile-to-brittle transition during nano-scale mechanical machining using a few single-crystal materials. We also proposed a quantitative method for determining plastic deformation by measuring volume changes in this study. We utilized a nanoscratch tester equipped with a diamond machining tool, which closely resembles an ultra-fine machining system, to measure ultra-low thrust forces during nano-scale machining. We successfully created V-grooved nano-patterns on silicon, germanium, and gallium arsenide and determined the critical thrust force. Our analysis, considering several mechanical properties, revealed that the critical thrust force correlates with hardness and elastic modulus, which are key mechanical parameters influencing plastic deformation and material fracture. The volume change was measured by AFM(Atomic Force Microscope) after machining, the amount of plastic deformation could be successfully calculated without observation of chips.

Ductile-to-brittle transition, Mechanical machining, Nano-scale, Critical thrust force, Plastic deformation

1. Introduction

Single-crystal materials are commonly perceived as difficult-to-cut due to their brittle characteristics. However, previous studies [1,2] have demonstrated that these materials can be mechanically machined with ultra-low forces, exhibiting a phenomenon known as 'ductile machining.' This occurs at forces lower than the critical thrust force determined in earlier research. The ductile machining of single-crystal materials by diamond turning was investigated in previous researches, however, there was limited research on quantitative analysis of thrust force of nano-scale planing. Recent research [3] has revealed that the critical thrust force for single-crystal silicon varies with the applied force per unit, indicating it is an experimental parameter rather than an inherent material property. Moreover, distinguishing whether ductile machining is based on cutting or plastic deformation remains challenging due to the inherent difficulty in analyzing nano-sized chips. Therefore, this study investigates the variation in material mechanical properties affecting the critical thrust forces for selected single-crystal materials and proposes a quantitative method for elucidating the mechanism of ductile machining by measuring volume changes.

2. Experimental methods

We selected three types of single-crystal materials—silicon(001), GaAs(001), and Ge(001). The critical thrust force for each material was determined following the methodology proposed in recent research [3]. A nanoscratch tester (Anton Paar) equipped with a diamond machining tool with a 90-degree shape angle, resembling an ultra-fine machining system, was employed as shown in Fig. 1. All scratching experiments were performed along [110] crystallographic direction on the three single-crystal materials. The critical thrust force, marking the ductile-to-brittle transition, was confirmed by SEM (Scanning Electron Microscope) observation. Mechanical properties were measured using the nanoindentation method [4]. Volume changes after ductile machining were measured using an AFM (Atomic Force Microscope), calculating changes in the volumes of the machined V-groove and pile-ups.

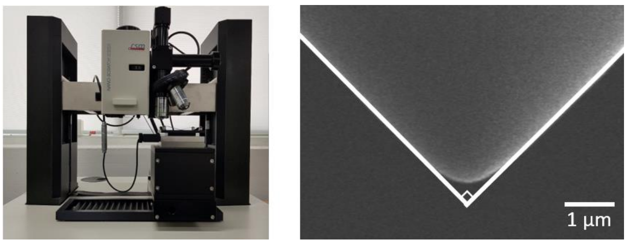

Figure 1. A nanoscratch system(left) and a diamond machining tool(right)

3. Results and discussion

Figure 2 presents ductile machining and brittle fracture of a single-crystal silicon. The ductile machining was observed at much low force as previous researches, and then the ductile-to-brittle transition was observed. The critical thrust force was defined as the force at which the first brittle fracture occurred. To ensure the reliability of our findings, we conducted five repetitions of the same experiments on a single material, demonstrating high repeatability. The critical thrust forces for silicon, GaAs, and Ge were approximately 17 mN, 27 mN, and 8 mN, respectively. The critical forces showed a similar tendency to the results of the previous research [5]. Minomura et al. found that the ratios of the pressure to make phase transition of silicon, GaAs and Ge are about 1:1.25:0.62,respectively. The exact pressure values and further crystallographic analysis are needed in a future study.

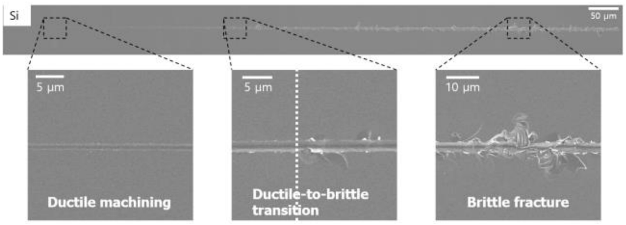

Figure 2. Ductile machining and brittle fracture occurred in a single-crystal silicon

Since ductile and brittle characteristics are clearly related to elastic and plasitic properties of a material, we chose elastic modulus (E) and hardness (H) as representative mechanical properties for studying the ductile-to-brittle transition. Among several combitions of E and H, Tsui et al. [6] proposed that H^3 over E^2 was a parameter of the critical force of plastic deformation in nanoscratch tests. H^3 over E^2 exhibited a robust positive relationship with the critical thrust forces in this study. Though the physical meaning of H^3 over E^2 should be addressed in further study, it can be used for predicting the critical thrust force of a machined material.

Figure 3 shows AFM profiles of silicon and GaAs. The profiles were measured at five machined V-grooves, and they were overlapped much well. We calculated the decresed area of a V-groove and the increased area of pile-ups around the surface of a V-groove. Since we could assume that the V-groove and the pile-ups had the same length, the ratio between the two calculated area should be same to the ratio of the volumes. If the ductile machining is based on plastic deformation, the volume change would be zero theoretically, which means the decreased volume and the increased volume would be same or their ratio would be one. Conversely, if the ductile machining is based on cutting, the decreased volume would be significantly larger than the increased volume, or the volume of the pile-ups would be considerably smaller. Examination of Fig. 3 reveals similar volumes for two V-grooves, yet differing volumes for pile-ups. The volume ratios of pile-ups over V-groove of silicon and GaAs were approximately 0.36 and 1.05, respectively. This allows us to infer that the ductile machining of silicon is based on cutting, while GaAs exhibits characteristics indicative of plastic deformation. Hokkirigawa et al. [7] proposed that the parameters which could predict ploughing(plastic deformation) and cutting in scratch tests Our calculations using these parameters placed GaAs closer to ploughing than silicon, corroborating our experimental findings.

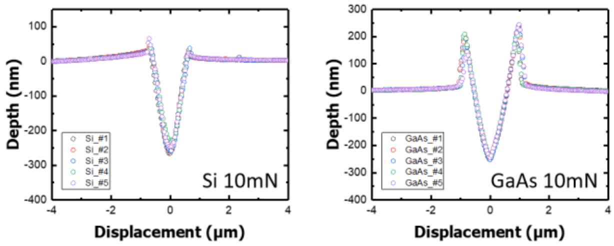

Figure 3. AFM profiles of V-groove of silicon and GaAs

4. Conclusions

We analysed the relationship of material mechanical properties and the the critical thrust forces of three single-crystal materials, and suggested a quantitative parameter for determining the mechanism of ductile machining in this study. The details are written below.

1) The critical thrust force which makes the first brittle fracture was largest in GaAs(001)[110], followed by silicon(001)[110] and Ge(001)[110]. .

2) H^3 over E^2 exhibited a strong positive correlation with critical thrust forces (H: Hardness, E: Elastic modulus).

3) The volume ratio of the V-groove and the pile-ups can be used as a parameter for determining the mechanism of ductile machining of each single-crystal materials.

Acknowledment

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