euspen's 24th International Conference &
Exhibition, Dublin, IE, June 2024
www.euspen.eu

Relationship between phase transformation pressure and shear stress in the machining of semiconductor crystals

Marcel Henrique Militão Dib[1], Alessandro Roger Rodrigues[2], Renato Goulart Jasinevicius[2]

[1]*Inst. Federal de Educ. Ciência e Tecnologia de São Paulo, CEP 14801-600 Araraquara – SP, Brazil*

[2]*Depto Eng. Mecânica, EESC, USP, C.P. 359, CEP 13566-590, São Carlos, São Paulo, Brazil*

marceldib@ifsp.edu.br

Abstract

In diamond tool turning of semiconductor crystals, the phenomenon of ductility emerges at submicrometric cutting thickness. This is attributed to the complex tool-material interaction, where the pressure in the contact region between the cutting edge and the material can reach levels comparable to the phase transformation pressure of the machined material. Ductile removal varies with the crystallographic orientation and negative rake angle tools, particularly around -37.5°, enhance the ductile response during cutting. Cutting forces decrease as the machining direction transitions from the harder [100] to the softer [110]. This study investigates the shear stress variation with different rake angles in machining semiconductor crystals (Si) oriented along the (001) plane. Results show a clear correlation between increased shear stress and improved material removal efficiency, providing clear-sightedness on the effect of ductility for precision machining in semiconductor manufacturing.

Monocrystalline Silicon; Diamond tool; Transition pressure; Rake angle

1. Introduction

Transition pressure plays an important role in addressing the issue of fragile to ductile behavior in monocrystalline semiconductor materials under loading [1]. Indentation is a commonly employed technique to illustrate pressure-induced phase transformations. It relies on the interaction between the indenter and the material, controlling the dynamic displacement of the indenter into the surface [2]. In materials such as Si and GaAs, specifically on the (100) orientation plane, the [100] direction is anticipated to be the hardest, in contrast to the softer [110] direction [3]. During indentation, the [100] direction exhibits brittle behavior, while the [110] direction demonstrates ductile behavior [4]. However, under the influence of loads from the cutting process, there is an inversion in the brittle and ductile behavior. The [100] direction becomes ductile, while the [110] direction becomes brittle [5]. One explanation for this phenomenon concerning cutting is related to the compression of the tool on the material, which increases the shear stress. This increase in shear stress may be responsible for the inversion of behavior, changing from brittle and ductile during indentation to ductile and brittle during cutting. To clarify this, the specific objective of this study was to demonstrate the effect of shear stress on monocrystalline Si (100) during ultraprecision turning with a diamond tool for different rake angles.

2. Material and Methods

We used single crystal silicon in ultra-precision machining with a circular tip diamond tool. The specimens (20 × 20 mm) were cut from silicon wafers with (100) surface orientation, 1 – 10 Ω.cm resistivity, P-type (Boron concentrations: 10^{15} - 10^{16} atoms cm^{-3}), 55 mm diameter and 500 µm thick.

Commercial diamond tools were used for the experiment with monocrystalline diamond with a nose radius of 762 µm and 100 µm, cutting edge radius of 40 nm, clearance angles of 10º and rake angles of 0º.

Single point diamond turning experiments were carried out on a commercially available diamond turning machine, the Aspheric Surface Generator Rank Pneumo ASG 2500. This is a very rigid system with a T-base carriage configuration and carriages (hydrostatic bearing, driven with pulse-width-modulated DC servomotors, rotary-to-linear motion through 5 mm pitch ballscrews and position feedback using laser interferometer) that had a 10 nm positioning accuracy.

We used cutting forces data to determine the value of shear stress during machining. An acquisition system was assembled to measure the machining forces, consisting of an acquisition plate (400 kHz), a multi-channel load amplifier, and a piezoelectric dynamometer Kistler, model 9652C2 (0 to 250 N; natural frequency of 2 kHz), all commercial. The forces were recorded at a sampling frequency of 130 kHz for each force. The positioning of the dynamometer was established in such a way that the x-axis provided the thrust force (Ft), and the y-axis provided the cutting force (Fc). A device with rotating capability was designed and manufactured to vary the tool's rake angle (Figure 1). This device consisted of an angled base and a tool holder. The angular base was attached to the dynamometer, and the tool holder was attached to the angular base in the position corresponding to the desired rake angle.

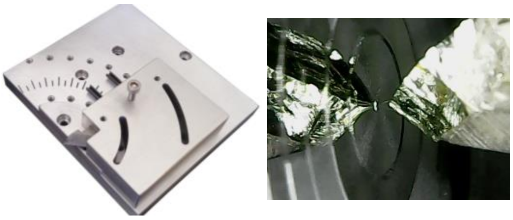


Figure 1. Device for changing rake angle.

The shear stress (τ_s) was estimated using measured cutting forces, as proposed by Merchant [6]. It was determined by the decomposition of thrust and cutting forces into the normal and friction forces to the tool face (F and N), as well as the friction force (F_s) in the shear plane. These forces are distributed in the shear plane (As), which is related to the shear angle (φ) and friction angle (β), expressed by the following equations:

$$F = Fc.\sin(\alpha) + Ft.\cos(\alpha)$$
$$N = Fc.\cos(\alpha) - Ft.\sin(\alpha) \tag{1}$$
$$F_s = F_c.cos(\varphi) - F_t.sin(\varphi)$$

$$\varphi = 45 + \frac{\gamma}{2} - \frac{\beta}{2}\ ; \quad \beta = \tan^{-1}\left(\frac{F}{N}\right) \tag{2}$$

$$\tau_s = \frac{F_s}{A_s}\ ; \quad A_s = \frac{f.ap}{\sin|\varphi|} \tag{3}$$

f: tool feedrate per revolution; ap: depth of cut; α: tool rake angle.

To determine the Vickers Hardness in each direction, we employed a durometer with loads ranging from 1 gf to 2 kgf for indentation tests on silicon (100).

3. Results and Discussion

Figure 1 presented the results of Vickers hardness testing, revealing a notable brittleness along the [100] direction, characterized by more pronounced fractures and propagation of cracks.

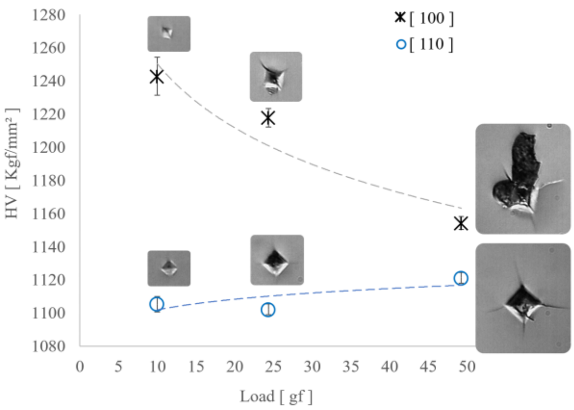
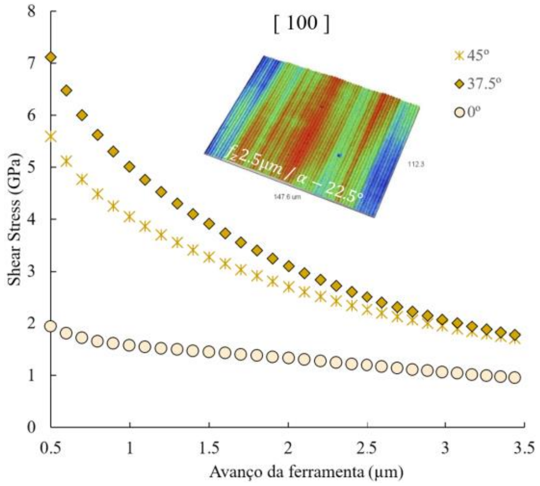


Figure 2. Vicker Hardness on silicon (100).

Figure 3 shows the shear stress results in turning and the influence of tool angle rake, demonstrating an increase in shear stress as it becomes more negative, thereby improving ductile response.



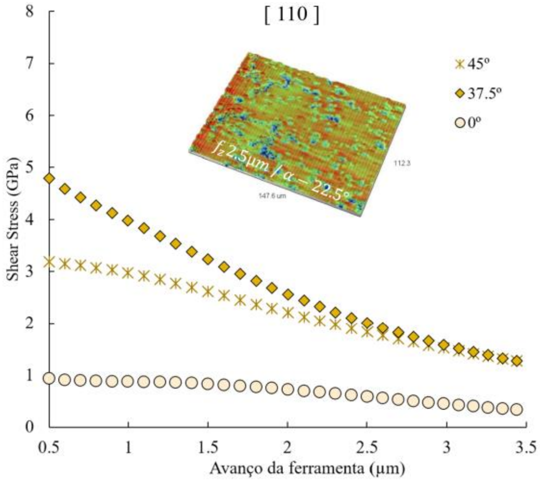


Figure 3. Shear stress in (100) silicon cutting.

However, the peak performance occurs around -37.5°; beyond this angle, the shear stress diminishes once again. This phenomenon was also noted by Lai et al. [7].

In the context of machining, there is a reversal in the brittle and ductile behavior compared to indentation. Unlike in indentation, where the [100] direction shows greater fragility, machining reveals that the [110] direction exhibits more pronounced fractures and crack propagation. This characterizes the beneficial effect of the increased shear stress generated during machining, particularly when the [100] direction attains higher shear stress values, promoting a more ductile behavior.

4. Conclusions

This study evaluated the ductile response of single crystal silicon, considering the influence of shear stress in ultraprecision turning. Contrary to the expected brittleness in the [100] direction of silicon (100) under loading, the turning process reveals a reversal in behavior as shear stress increases, promoting a more ductile behavior of the [100] direction during the cutting.

References

[1] Budnitzki M, Kuna M. Stress induced phase transitions in silicon. Journal of the Mechanics and Physics of Solids 2016;**95**:64–91.

[2] Domnich V, Gogotsi Y. Pressure-Induced Phase Transformations In Semiconductors Under Contact Loading. Frontiers of High Pressure Research II: Application of High Pressure to Low-Dimensional Novel Electronic Materials 2001:291–302.

[3] O'Connor BP, Marsh ER, Couey JA. On the effect of crystallographic orientation on ductile material removal in silicon. Precision Engineering 2005;**29**:124–32.

[4] Gao R, Jiang C, Dong K, Lang X, Jiang J, Huang P. Anisotropy mechanical behavior of crystals based on gallium arsenide cleavage processing. Ceramics International 2021;**47**:22138–46.

[5] Mukaida M, Yan J. Ductile machining of single-crystal silicon for microlens arrays by ultraprecision diamond turning using a slow tool servo. International Journal of Machine Tools and Manufacture 2017;**115**:2–14.

[6] Merchant ME. Mechanics of the Metal Cutting Process. II. Plasticity Conditions in Orthogonal Cutting. Journal of Applied Physics 1945;**16**:318–24.

[7] Lai M, Zhang X, Fang F, Bi M. Effects of crystallographic orientation and negative rake angle on the brittle-ductile transition and subsurface deformation in machining of monocrystalline germanium. Precision Engineering 2019;**56**:164–71.