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EFFECT OF CRYSTALLOGRAPHIC ORIENTATION ON MATERIAL REMOVAL BEHAVIOR DURING HIGH SPEED SCRATCHING OF MONOCRYSTALLINE SILICON

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Abstract

Monocrystalline silicon has anisotropic attributes due to asymmetric and non-uniform interatomic lattice structures, which affects its deformation and fracture properties. This paper aims to investigate the effect of crystallographic orientation on the material deformation and removal behavior during high speed scratching of monocrystalline silicon. A high-speed scratching setup is developed which can achieve the highest scratching speed of 40 m/s. Inclined scratching experiments are conducted on (001), (110) and (111) crystallographic planes over the speed range of 1 m/s to 30 m/s. As the scratching depth increases, the ductile-to-brittle transition of silicon at different crystallographic orientations are analyzed. The experimental results suggest that scratching in the direction of [$\bar{1}$10] on (111) plane presents the largest critical residual depth of ductile-to-brittle transition. Phase transformation from Si-I to the phases of Si-IV and a-Si dominates ductile deformation of silicon during scratching process, while scratching tests in [$\bar{1}$10] direction on (111) plane demonstrates the largest degree of material amorphization. This study can provide guidance for optimizing processing parameters of monocrystalline silicon components with different crystallographic orientations.

Keywords:

Crystallographic orientation, High speed scratching, Monocrystalline silicon, Material removal behavior

1 INTRODUCTION

Monocrystalline silicon, as one of the most common semiconductor materials, is widely used in solar cells, micro-electromechanical systems, and integrated circuits. High-quality silicon wafers without surface and subsurface damage are the basis for the production of silicon devices. However, damage-free machining of silicon is challenged due to its high brittleness and associated poor machinability. The common processing processes for silicon wafer such as slicing and grinding have common characteristics that the elementary abrasive event is scratching of silicon wafer with diamond grit. Consequently, scratching tests with diamond scriber can be used to investigate the material removal behavior of silicon [Pala 2018; Zhang 2019].

Although silicon is a typically brittle material, the material removal mode of silicon under specific processing conditions can be ductile deformation instead of brittle fracture [Choi 2017]. The ductile regime machining of silicon has been reported in many studies [Li 2022; Wang 2022; Zheng 2022]. Ductile removal mode for silicon can minimize surface and subsurface damage during machining to obtain high surface quality [Yan 2003]. Moreover, suppressing machining damage formation is beneficial for cutting down subsequent grinding/polishing chains and improving material utilization rate. Motivated by these factors, the critical scratching depth of ductile-to-brittle transition for silicon becomes an essential data that has been widely focused on.

Available studies show that the machining mode of silicon is affected by such factors as processing parameters, the shape and size of abrasive grains, and the material properties of silicon [Kumar 2017]. Due to asymmetric and non-uniform interatomic lattice structures, the mechanical properties of monocrystalline silicon present anisotropic features. Different research has investigated the fracture toughness of different crystallographic planes of monocrystalline silicon with experimental or simulation methods [Gallo 2019; Shiroki 2019]. As fracture toughness characterizes the ability of a material to prevent crack expansion, larger fracture toughness values would be beneficial for ductile deformation mode under certain loading conditions. The variation of material deformation and removal behavior caused by monocrystalline silicon anisotropy has also been reported. It has been found that (111) plane exhibit greater ductile machinability [Wu 2012]. The ductile-to-brittle transition characteristics vary with crystallographic orientation even on the same wafer [Yan 2002]. However, most studies about the effect of monocrystalline silicon anisotropy on material mechanical properties have been limited to low speed (i.e., 1 μm/s – 0.167 mm/s) scratching tests, which are far below the relative speeds (5 m/s – 20 m/s) between the abrasive grains and machined surface during actual processing

[Wang 2020]. Fundamental understanding of the effect of crystallographic orientation on material removal behavior during high speed processing is still lacked.

In this study, high speed scratching tests with a maximum speed of 30 m/s are conducted to investigate the effect of crystallographic orientation on material removal behavior and surface damage formation of monocrystalline silicon. The characteristics of scratched surface morphology and surface damage at different crystallographic orientations are studied with microscopic analyses. Furthermore, the effect of different scratching conditions on the ductile-to-brittle transition behavior of monocrystalline silicon are revealed.

2 EXPERIMENT PROCEDURES

The setup of high speed scratching test used in this study is as shown in Fig. 1. Micro-electronic grade (001), (110) and (111) monocrystalline silicon wafers were used in the experiments. The silicon wafers were cut into 10 mm × 10 mm samples and fixed on the force dynamometer (Kistler 9109AA), which can detect the initial contact between the silicon sample and diamond scriber. The force dynamometer was mounted rigidly on X-Y-Z motion stage (Aerotech ANT130V-5), which has a positioning resolution of 1 nm in the Z direction (Fig. 1(a)). As shown in Fig. 1(b), the diamond scriber was fixed on the customized scratching disk, which was attached to a high speed spindle (NAKANISHI BMS-4020RA) with a speed range of 1000-20000 RPM. Conical tipped diamond scribers with a tip angle of 120° and a tip radius of 30 μm were used as shown in Fig. 1(c) and Fig. 1(d). High speed scratching tests were achieved by the combination of rotation of the spindle-driven scriber and the horizontal movement of the motion stage.

Firstly, scratching tests with a constant scratching depth of 300 nm were performed to investigate the effect of crystallographic orientation on material removal behavior. In addition, inclined scratching tests with consecutively increasing depth for all crystallographic orientations were conducted. All scratching tests for different crystallographic orientations were performed with three speeds of 1mm/s, 1 m/s and 30 m/s. Afterwards, the morphologies of the scratched grooves were observed with scanning electron microscope (TESCAN MIRA LMS). Meanwhile, Raman spectra were obtained for selected positions with Raman spectrometer (Nanobase XperRam S) to detect the phase transformations in the scribed grooves. The critical residual depth of ductile-to-brittle transition during inclined scratching tests was determined through microscopic observation with confocal laser scanning microscope (Keyence VK-X250). Four repetitive tests were performed for each scratching condition to ensure the reproducibility of the results.

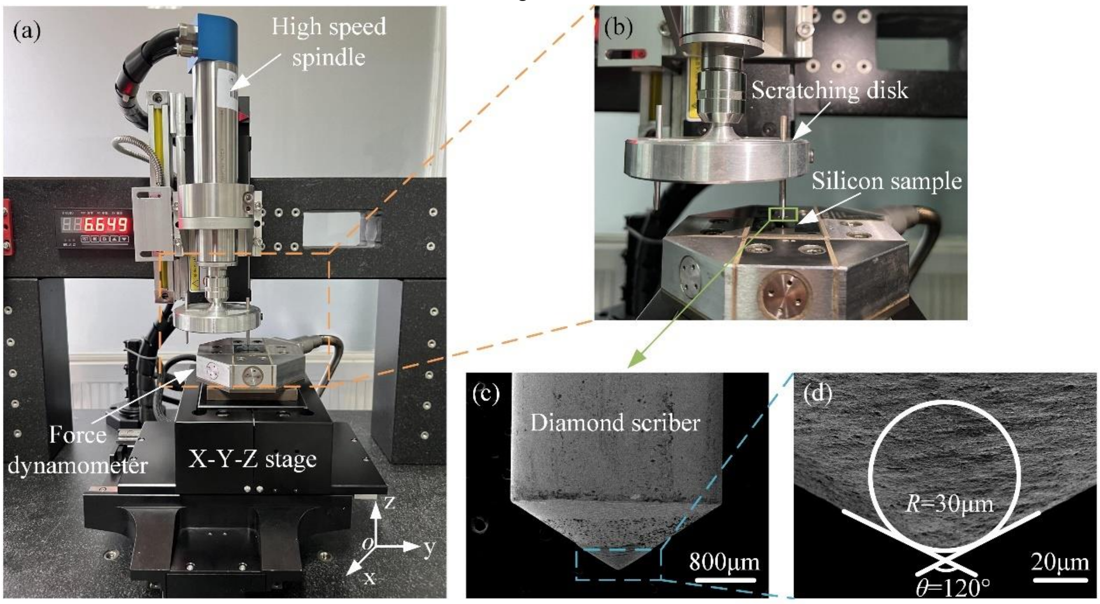

Fig. 1: High speed scratching test setup (a) overall setup, (b) scratching disk, (c, d) diamond scriber.

3 RESULTS AND DISCUSSION

3.1 Surface morphology of scratched grooves

Fig 2 shows the morphologies of scratched grooves generated with a constant scratching depth of 300 nm in different monocrystalline orientations with speeds of 1 mm/s, 1 m/s and 30 m/s. As shown in the images, the scratching direction present significant effect on the scratched surface morphology. At all scratching speed conditions, significant radial cracks occurred during scratching along [110] and [010] directions on (001) plane, which indicates that brittle fracture occurred during material removal process. Similarly, at the speed of 30 m/s, brittle fracture was dominant material removal mode at the scratching direction of [1$\bar{1}$0] on (110) plane. Comparatively, no brittle fracture characteristics were found at all test conditions on (111) plane, and material removal mode was dominated by ductile deformation. Therefore, it can be concluded that (111) plane exhibit greater ductile machinability than (001) and (110) planes. In addition, there is a significant correlation between the surface characteristics of scratched grooves and scratching speed. Higher scratching speeds tend to produce more severe surface defects.

Raman spectroscopy is achieved by Raman scattering effect that can efficiently characterize phase transformations during material deformation process. Fig. 3 shows the Raman spectra of chips produced at high scratching speed of 30 m/s. As shown in Fig. 3(a-c), phase transformation from Si-I to the phases of Si-IV and a-Si

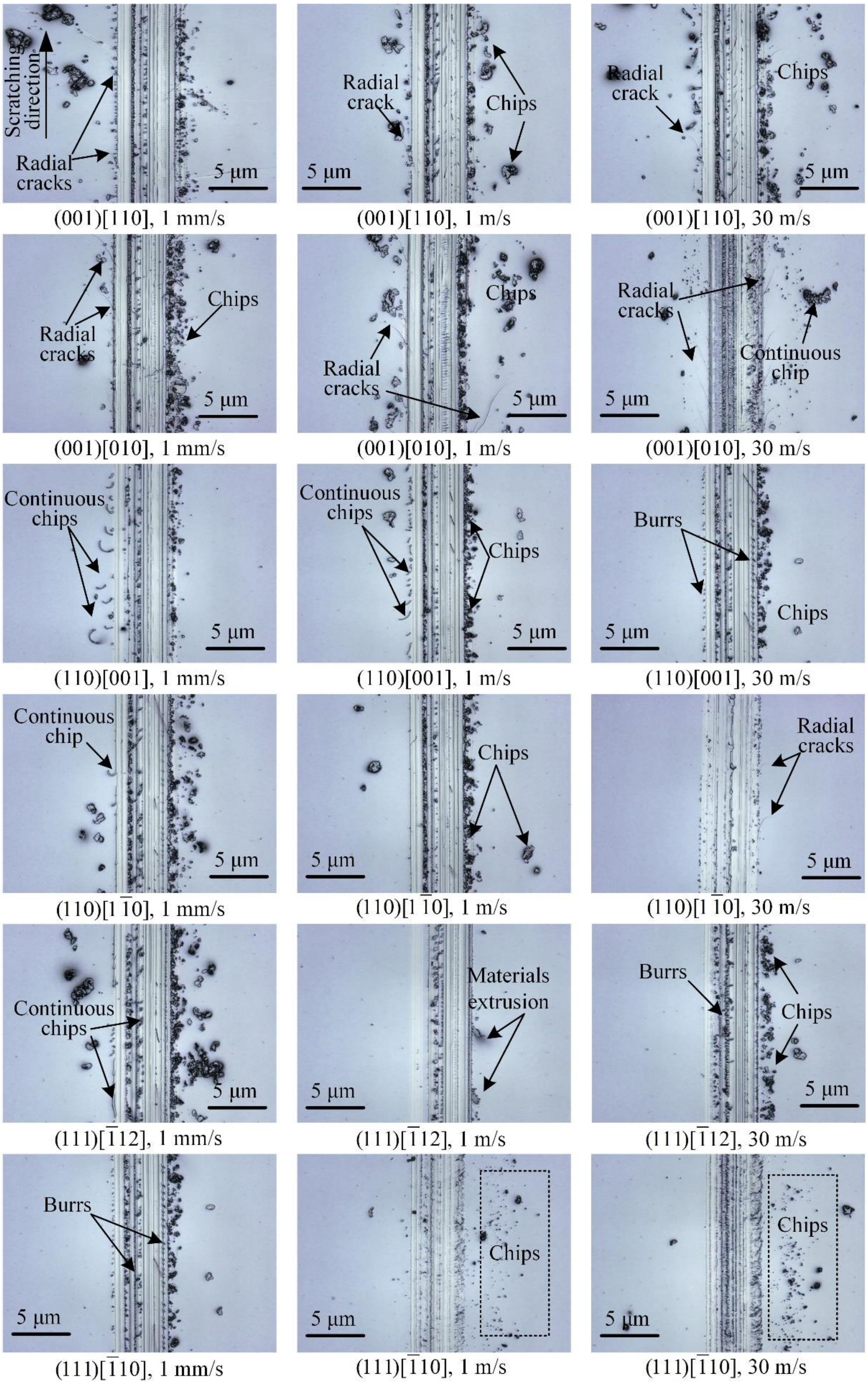

Fig. 2: Morphologies of the scratched grooves generated with constant scratching depth of 300 nm for tests at different crystallographic orientations.

dominates ductile deformation and removal of silicon during scratching process. It is noteworthy that no crystal phase Si-I was found on the (110) plane. It indicates that Si-I has fully transformed into Si-IV and amorphous phase a-Si.

Existing literatures demonstrate that the full width at half maximum (FWHM) of the Raman peak represents the degree of crystallinity, and the intensity ratio of crystalline phases to amorphous phase can characterize the amorphization degree of scratched surface [Yan 2008]. To clarify the amorphization degree of monocrystalline silicon during high speed scratching along different crystallographic orientations, the Lorentzian and Gaussian functions were employed to fit the intensity distribution of sharp crystalline peaks and broad amorphous peaks of the Raman spectra. Fig. 3(d) shows an example of the fitting result of different Raman spectra peaks for scratching test along crystallographic direction of [110] on (001) plane. Table 1 summarizes the FWHM values of crystalline and amorphous peaks of Raman spectra as well as their ratios at different crystalline orientations. Obviously, while phase transformation dominates the plastic deformation of monocrystalline silicon, it exhibits different characteristics during high speed scratching along different crystalline orientations. Smaller values of the ratio indicate a higher degree of material amorphization. It can be identified that scratching tests in [$\bar{1}$10] direction on (111) plane demonstrate the largest degree of material amorphization. This is attributed to the greater ductile machinability in this crystallographic orientation which leads to greater deformation of the chips during the removal process and further promotes the generation of phase transitions.

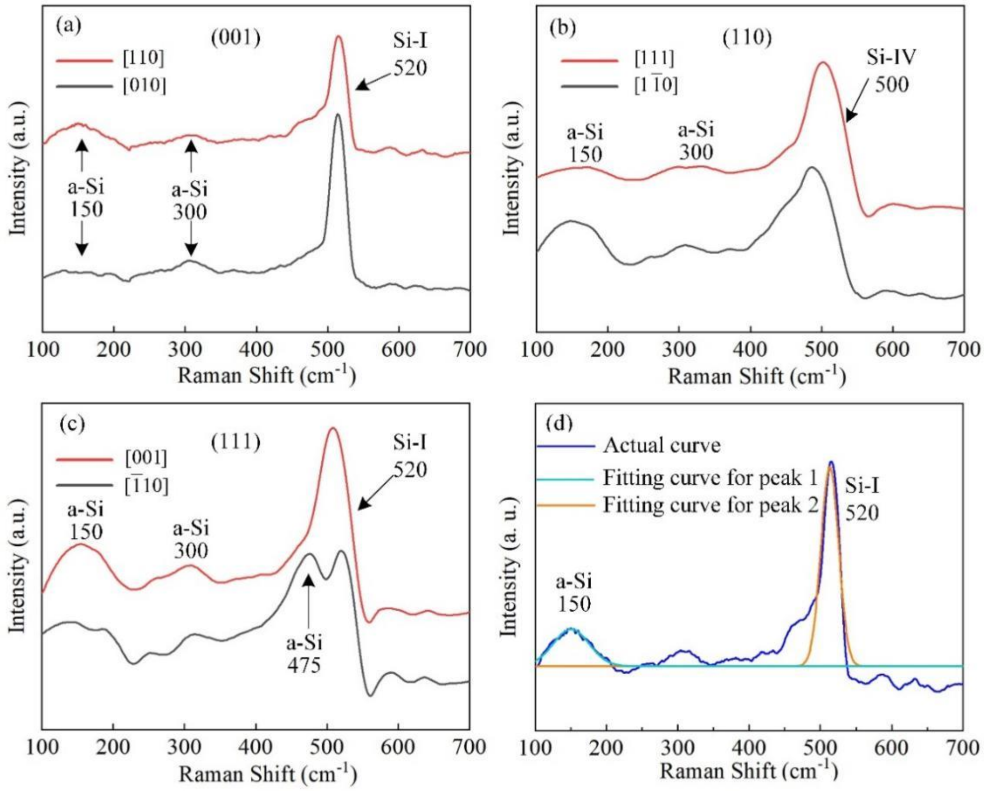

Fig. 3: Raman spectra of chips produced with high scratching speed of 30 m/s at different crystallographic orientations (a) [110] and [010] on (001) plane, (b) [111] and [1$\bar{1}$0] on (110) plane, (c) [001] and [$\bar{1}$10] on (111) plane, (d) an example of Raman peaks fitting with Lorentzian and Gaussian functions.

Tab. 1: Gaussian and Lorentzian fitting results of Raman spectra peaks for chips produced with high scratching speed of 30 m/s.

Plane	Scratching direction	Crystalline peak		Amorphous peak		Ratio
		Centre (cm^{-1})	FWHM (cm^{-1})	Centre (cm^{-1})	FWHM (cm^{-1})	
(001)	[110]	518	29.36	150	60.17	31.81%
				300	32.12	
	[010]	518	31.23	150	62.18	35.18%
				300	26.84	
(110)	[111]	500	48.32	150	76.56	30.82%
				300	80.21	
	[1$\bar{1}$0]	500	59.81	150	58.20	46.32%
				300	70.91	
(111)	[001]	519	47.10	150	70.16	28.67%
				300	94.15	

[$\bar{1}$10]	520	45.11	150	65.32	23.82%
			300	74.16	
			475	49.87	

3.2 Ductile-to-brittle transition during inclined scratching tests

In the inclined scratching tests, the material removal mode changes from ductile to brittle as the scratching depth increases. The critical residual depth d_c at the position of ductile-to-brittle transition was employed to quantify the effect of crystallographic orientation on material removal behavior. The critical depth was defined as the residual scratching depth at the first radial crack formed on the scratched surface along the scratching direction [Fig. 4(a)]. Fig. 4(b) shows the cross-sectional profile of the selected position of the scratched groove, while the distance between the profile bottom and undeformed surface is defined as the residual depth.

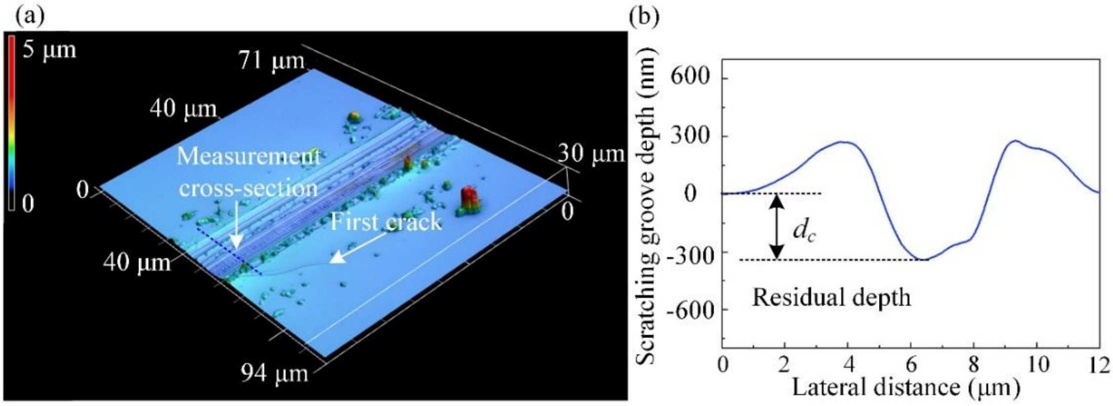

Fig. 4. Measurement of critical residual depth for ductile-to-brittle transition (a) measurement position, (b) cross-sectional profile of the selected position within scratched groove.

Fig. 5 shows the effect of crystallographic orientation on the critical residual depth of ductile-to-brittle transition during high speed scratching. The results indicate that the critical residual depth varies at different scratching speeds. In the same scratching direction, the scratching tests at speed of 30 m/s present a smaller critical residual depth than at speeds of both 1 mm/s and 1 m/s. This can be explained by the material embrittlement of monocrystalline silicon during high strain rate loading process [Wang 2020]. As shown in Fig. 5, the critical residual depths generated on (111) plane are significantly higher than other planes, which implies a greater ductile machinability of (111) plane. Scratching tests in [010] direction on (001) plane present the smallest critical residual depth, while and the largest critical depth occurs in [$\bar{1}$10] direction on (111) plane. Although the scratching directions of [110], [1$\bar{1}$0], and [$\bar{1}$10] belong to the <110> family, scratching tests in the direction of <110> on different planes demonstrate different critical depths as shown in Fig. 5. This is because the major loading directions during the scratching tests are the normal force perpendicular to the silicon wafer and the tangential force parallel to the scratching direction. The varied normal forces cause the same crystallographic orientation on different planes to exhibit anisotropic attributes during scratching process.

Fig. 6 shows the variance of critical residual depths at three scratching speeds and corresponding fracture toughness values at different crystallographic orientation. Fracture toughness is a parameter that characterizes the ability of a material to resist brittle fracture. The results indicate the magnitude of the effect of scratching speed on the critical residual depth in the same direction condition. As shown in Fig. 6, different crystallographic orientations exhibit different sensitivities to the variation of scratching speed. In the direction of (001) [010], fracture toughness presents the minimum value and variance of critical residual depth presents the maximum value at different scratching speeds. The variance of critical residual depth also presents a significant negative correlation with the fracture toughness also in other crystallographic orientations.

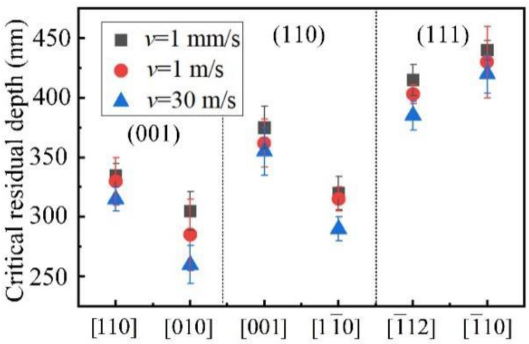

Fig. 5. Effect of crystallographic orientation on the critical residual depth of ductile-to-brittle transition at scratching speed of 1mm/s, 1 m/s, and 30 m/s (the error bars represent one standard deviation of four repeated tests performed at the same scratching condition).

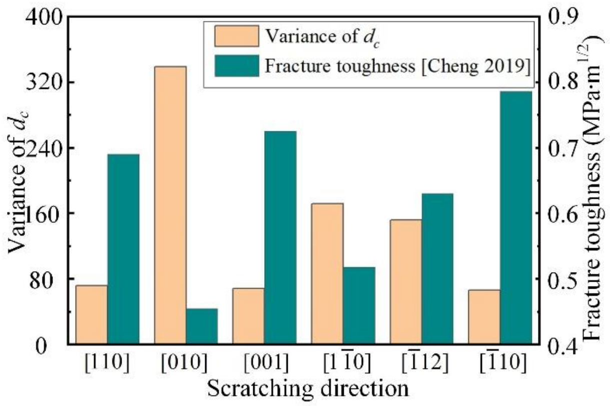

Fig. 6. Variance of critical residual depth generated at three scratching speeds and their relationship with fracture toughness at different crystallographic orientation.

4 SUMMARY

This paper investigates the effect of crystallographic orientation on material removal behavior during high speed scratching of monocrystalline silicon. Scratched grooves morphologies and ductile-to-brittle transition behavior of silicon during scratching process are analyzed under different conditions. The results show that (111) plane exhibits greater ductile machinability than (001) and (110) planes. Phase transformation from Si-I to the phases of Si-IV and a-Si dominates ductile deformation and removal of silicon during scratching process. Scratching tests in [$\bar{1}$10] on (111) plane direction present the largest degree of material amorphization. Scratching tests in [010] direction on (001) plane present the smallest critical residual depth, while the largest critical residual depth exists for [$\bar{1}$10] direction on (111) plane. Due to the anisotropy of monocrystalline silicon in the normal direction, the same crystallographic orientation on different planes exhibit different machining characteristics. The sensitivity of critical residual depth to scratching speed is correlated with the fracture toughness of different crystallographic orientation, i.e., the lower the fracture toughness, the higher sensitivity of critical residual depth to scratching speed.

5 ACKNOWLEDGMENTS

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