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Grinding of Single-Crystal Silicon Along Crystallographic Directions

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ABSTRACT

This article studies the effect of grinding along crystallographic directions on the surface finish of single-crystal silicon. It also discusses new and/or improved processes for precision machining brittle materials, including silicon. Silicon samples were cut from (100) silicon wafers. These samples were then subjected to grinding along different crystallographic directions under the same experimental conditions. The surface roughness and the surface texture of these samples were then analyzed. The R_a and R_q values and the microphotographs of the ground silicon surfaces showed the dependency of surface finish on the grinding direction. Better surface finish was achieved when (100) silicon was ground along $\langle 110 \rangle$ directions. Samples ground along these directions also showed more ductile streaks on the silicon surfaces, compared with surfaces ground along the other directions.

Key Words: Grinding; Single crystal; Silicon; Crystallographic direction; Brittle material; Surface roughness; Wafer; Experiment; Surface texture; Slip direction; Ductile streak; Pitting damage; Crystal structure; Miller indices; Microphotograph.

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1.0. INTRODUCTION

Silicon is one of the most abundant materials on the earth's surface, representing approximately 25% of the earth's crust. Silicon is mainly used as an integrated circuit (IC) carrier in microelectronics. The silicon used in the fabrication of semiconductor devices is extremely pure. Before device manufacture is started, the silicon has a typical impurity concentration of less than one part per billion. ICs and discrete solid-state devices are manufactured on wafers made of single-crystal silicon. Single-crystal silicon is also the most widely used substrate material for microelectromechancial systems (MEMS) and microsystems. It is the prime candidate material for sensors and actuators, and is the common substrate for microfluidics.[1–3]

Semiconductors are commonly inorganic materials made from elements in the fourth column (group IV) of the periodic table. These materials are neither good conductors nor good insulators, hence the name, semiconductors. The two most common materials used in the production of semiconductor devices are crystalline germanium and silicon, although silicon dominates the market. Both these materials possess qualities that offer advantages for specific applications. Silicon can be modified in several ways to change its electrical, mechanical, and optical properties. The use of silicon in solid state and microelectronics has shown a spectacular growth since the early 1970s, and this growth pattern is still continuing.[4,5]

Silicon is also used for optical components in high-resolution thermal imaging systems. Si and Ge are the most widely used thermal imaging materials operating in the middle infrared to far infrared wavelength regions. Parabolic surfaces on Si prove to be a good choice for infrared applications.[6]

Two wafers with surfaces that are sufficiently smooth, flat, and clean can bond to each other without any adhesive or external forces at room temperature in ambient air. This technology is called wafer bonding and has been gaining interest for a number of microprocessing applications: high-performance microelectronics, photonics, optoelectronics, and MEMS. Modern wafer bonding is driven by the demand to enhance the IC performance.[7]

Apart from the increase in quantity of manufacturing of pure silicon, quality requirements have also increased. A steady increase in chip surface area produced annually is expected, and this will be accompanied by an increasing degree of component integration.[8]

In this article, past research work with new and/or improved processes for precision machining brittle materials, including silicon, is reviewed. Then the fundamental theories essential to this study are discussed. Finally, experiments carried out to study the effect of grinding along crystallographic directions on the surface finish of single-crystal silicon are reported with promising results.

2.0. LITERATURE REVIEW

Typical processes in the manufacturing of silicon-based devices are as follows. A seed crystal of silicon is placed on the end of a rod and dipped into a vat of molten silicon. The rod is slowly withdrawn from the vat, and during this withdrawal process, the silicon in contact with the seed crystal slowly cools and the crystal of

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silicon grows. The end result is an ingot of silicon that is usually not less than 50 cm long. This ingot is then sawed into slices called wafers, and both surfaces of the wafers are ground, lapped, and polished to form a smooth finish. The last step of wafer preparation is a chemical etching of one side to remove any final irregularities and possible damage that are left from the polishing process. The next step is to add the desired characteristics/devices to the material, then cut the wafer into many small pieces called dice or chips, and finally, assemble the chips into a protective package.[4]

There has been research in dealing with the traditional surface finishing processes such as cutting, grinding, and polishing of wafers, as well as more untraditional methods.[9] However, the industrial implementation of these new processes is still not possible due to reasons such as low throughput, high equipment cost, and so on.

Mechanical grinding gives high dimensional accuracy and good total thickness variation (TTV). Because it induces mechanical damage on surfaces, surface etching or polishing is necessary to remove the damaged area. During these etching and polishing processes, TTV is usually degraded. To improve TTV, etching and polishing should be reduced. In other words, reduction of surface damage depth during grinding is necessary.[7]

Precision machining of brittle material such as silicon and ceramics is based on a hypothesis, which states that all materials regardless of their hardness and brittleness will undergo a transition from a brittle to a ductile machining region below a critical depth of cut. Below this threshold, the energy required to propagate cracks is believed to be larger than that required for plastic deformation. Hence, plastic deformation is the predominant mechanism of material removal for ductile mode machining of brittle materials. Therefore, by cutting or grinding at an extremely small depth of cut, a brittle material is able to deform in a ductile manner, thus giving better surface finish.[10]

A cutting technique using a flying tool under negative pressure was proposed for cutting brittle materials without cracking.[11] A flying tool glided over a workpiece surface while maintaining a small height like a negative pressure slider of a magnetic disk drive. Using this tool system, ductile regime cutting of optical glass and single-crystal silicon was examined, and a mirror surface finish with no cracks was achieved on a lathe having a 0.1-μm order of error motion.

Diamond turning of single-crystal silicon was carried out along all the crystallographic directions on the (001) and (111) planes at depths of cut of 0.1 and 1 μm, and the mechanism involved in ductile regime turning was studied.[12] Pitting damage was observed along some crystallographic orientations. The crystallographic orientation dependence of the surface features was also observed to change with the depth of cut. By using transmission electron microscopy on the $\{111\}\langle 110\rangle$ slip systems, it was found that the orientation dependence of the surface features was closely linked to the ease with which slip deformation occurred.

Ultrasonic vibration was introduced into the grooving process of brittle materials by a vibration exciter exciting the cutting tool.[13] Roughness of the side surface was improved by low-frequency vibration, ultrasonic vibration, and combined vibration. When the amplitude of low-frequency vibration was increased, the surface roughness was further improved.

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The material removal mechanism in grinding of ceramics using diamond wheels was also studied.[10] Material pulverization was discovered on the surface layer of ground ceramics. The pulverized material was loosely connected in comparison to the bulk material, and could be recompacted by hydrostatic compressive stress in the contact region at the interface of the abrasive grain and the workpiece. Material flowed sideways in single-point grinding, forming pile-ups on both sides of a groove.

Grinding of toroidal and cylindrical surfaces made of Si and SiC was carried out by using diamond grinding wheels and an inexpensive computerized, numerically controlled (CNC) machining center.[14,15] Mirrors were successfully obtained by automatic grinding operations with good shape accuracy, mirror surface finish, and low roughness heights. Ductile-mode material removal was achieved by grinding with dressing. Scanning electron microscopy (SEM) microphotographs demonstrated the ductile mode in grinding of silicon. Ground silicon carbide had almost complete ductile mode surfaces, and the surface roughness was independent of the direction of measurement.

Nanogrinding was performed based on a lapping process.[16] The abrasive grains were completely embedded in a soft metallic plate that was the grinding tool. Pumice was embedded in the grinding plate and remained there throughout the process. Between pumice particles, the basic soft metallic-plate materials formed the plateaus. Diamond grains were then embedded by a conditioning ring with their summits aligned coplanar to the plate surface. This arrangement resulted in plastic material removal, minimal subsurface damage, and excellent surface finish.

A special grinding wheel was developed for machining silicon wafers.[17] The wheel acted like a grinding wheel when sufficient fluid was provided. It produced similar roughness and removal rate to a conventional lapping tool when the flow rate was below a certain value. Surfaces obtained by using this grinding wheel had better surface roughness than that obtained by conventional processes.

Electrophoretic deposition is a phenomenon whereby an electric field is applied to a solution of ionic particles. The particles will adhere to the anode. Making use of this theory, ultrafine abrasives can be deposited to the grinding wheel. It was reported that a mirror surface without chipping was achieved by using this method.[18]

By using a new device for dressing a resin-bonded diamond wheel and an improved coolant system, ductile-mode grinding of silicon and glass was achieved using an inexpensive, conventional surface grinding machine.[19] The low-cost dressing device also ensured minimum disruption to the grinding operation and a higher level of safety. A flooding supply of coolant at the grinding zone provided better cooling performance and lubrication.

An in-process dressing study was performed using a water jet.[20] It was found that the water jet removed the chips embedded in the space between the protrusion of the abrasive grains on the wheel. If the water pressure was too low, the in-process dressing was not effective. If the pressure was too high, the wheel became eroded.

Electrodischarge machine (EDM) dressing can be used for in-process dressing of the grinding wheel to obtain high truing efficiency.[21] The truing accuracy of EDM dressing not only depends on the electric parameters, but also on the precision of the equipment and balance of the wheel. For the grains of the grinding wheel not to be covered, removed, or emerged, the removal volume of a single EDM pulse must be less than the size of the diamond grain.

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3.0. SLIP DIRECTION AND SILICON LATTICE STRUCTURE

When dealing with crystalline materials, it often becomes necessary to specify some particular crystallographic plane of atoms or crystallographic directions. The most common way of doing this is using the Miller indices.[22,23]

Dislocations do not move with the same degree of ease on all crystallographic planes of atoms and in all crystallographic directions. There are preferred slip planes and specific slip directions along which dislocation motion tends to occur. In other words, plastic deformation occurs primarily by sliding over certain planes. Slip occurs predominantly on crystallographic planes of maximum atomic density. In addition, slip will occur in the closed-packed direction, which represents the shortest distance between two equilibrium atom positions and the lowest energy direction. Slip systems (combinations of slip planes and directions) are such that the atomic distortion that accompanies the motion of a dislocation is a minimum. The dominant slip systems vary with crystal structures of materials, because the relative atomic densities of planes and directions are different.[22,24]

Silicon is one of a very few materials that can be economically manufactured as a single-crystal substrate. It, like other group IV insulators and semiconductors including diamond, germanium, and gray tin, crystallizes in the diamond lattice structure that can be regarded as simple cube. In other words, the primitive unit, the smallest repeating block, of the crystal lattice resembles a cube.[3,25,26] It has an uneven lattice geometry for its atoms, but has basically a face-centered cubic (FCC) unit cell.[2] Indeed, the crystal structure of silicon is more complex than that of a regular FCC structure. The diamond structure consists of two interpenetrating FCC subcubes with the origin of one displaced $\frac{1}{4}\frac{1}{4}\frac{1}{4}$ from the other. That is, one atom of the second subcube occupies the site at one-fourth of the distance along a major diagonal of the first subcube.[26] Because of the asymmetrical and nonuniform lattice distance between atoms, single-crystal silicon exhibits anisotropic thermophysical and mechanical characteristics.[2]

The idea for the experiments reported in this article is that it should be possible to achieve better surface finish when grinding along certain specific directions where dislocation motions will most likely occur.

4.0. EXPERIMENTS

Silicon samples were cut from (100) wafers by using a method known as diamond scribing. The surface of the wafer was marked or scribed with a diamond cutter. Then, by bending the wafer along the scribed lines, the wafer would break along the lines.[1] However, the wafer would only break in specific directions. These preferred directions for breaking were perpendicular to each other.

As the wafer only broke in specific directions, it was not possible to cut out samples according to the crystallographic orientations that were of interest to the authors. Instead, 16 samples were cut with the same orientation and then placed with various orientations when they were subjected to grinding. The placement of the 16 silicon samples was according to the crystallographic directions as shown in Fig. 1.

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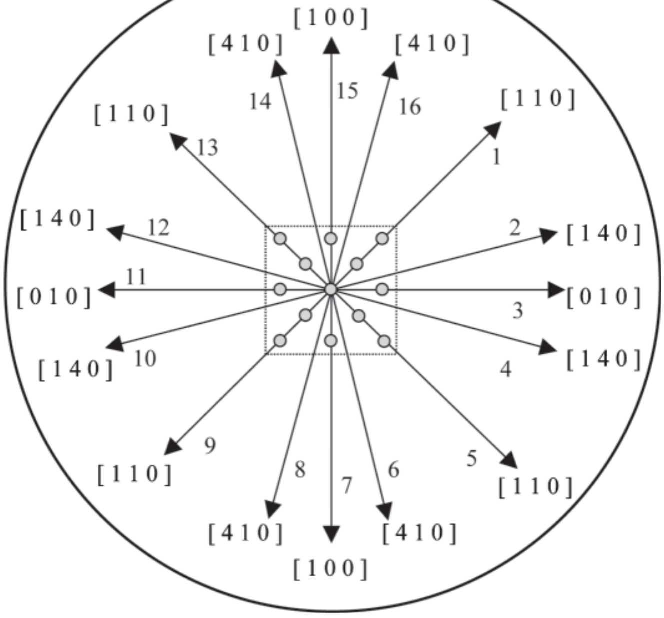

Figure 1. Grinding directions for silicon samples 1–16.

Grinding experiments were performed on an Okamoto Grind-X grinding machine (Singapore) with a fixed spindle speed of 1450 rpm using a resin-bond diamond wheel, grit mesh size 1500. The parameter settings for all the experiments were kept the same. The parameters included the worktable speed, worktable cross-feed rate, depth of infeed of the wheel, and total depth of infeed, as shown in Table 1. The parameters used might not be the optimum conditions for ductile-mode grinding of silicon. The objective of the experiments was to determine the effect of the grinding directions on the surface finish.

As the sample needed to be magnetized to the worktable of the grinding machine, it was first glued with wax to a sample holder that was made of mild steel. The sample holder, with the sample on top, was then placed onto the worktable of

Table 1. Grinding parameters for the experiments.

	Rough grinding	Fine grinding
Total depth of infeed, μm	20	5
Depth of infeed, μm	0.5	0.1
Total number of passes	40	50
Cross-feed rate, mm	1	1
Worktable speed, m min^{-1}	9	9

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the grinding machine such that the investigated crystallographic orientation of the sample was parallel to the grinding direction. The worktable was then magnetized to hold the sample holder in place. Because deep infeed could cause surface or subsurface damage to the silicon sample, the infeed depth of rough grinding was set at 0.5 μm. A dressing device developed[19] was used to dress the diamond wheel. This was to ensure that the condition of the grinding wheel was the same for fine grinding all the samples. The dressing sticks used were composed of WA400G aluminum oxide.

5.0. RESULTS AND DISCUSSION

The surfaces of the ground samples were measured perpendicular to the grinding direction for their roughness values using a Taylor-Hobson stylus profilometer. Then microscope pictures were taken to examine the surfaces.

Table 2 is the tabulated surface roughness R_a and R_q values of the ground silicon samples. Figures 2 and 3 are the graphical representations of these R_a and R_q values, respectively.

As shown in Figure 2 and Table 2, the best R_a values were obtained for sample 1 (0.047 μm) and sample 9 (0.043 μm), which were ground along the ⟨110⟩ crystallographic directions of the (100) wafer. The worst R_a values were obtained for sample 3 (0.083 μm) and sample 11 (0.084 μm), which were ground along the ⟨100⟩ crystallographic directions of the (100) wafer. Similar trends can be observed in Fig. 3, which shows R_q values.

The only two abnormalities are samples 4 and 5. Figures 2 and 3 seem to suggest that the surface finish (R_a, R_q) of sample 5 was poorer as compared with that of sample 4. However, as shown by the microphotographs of the two samples (Fig. 4), the surface texture in sample 4 was poorer than the surface texture of sample 5. The microphotograph of sample 4 shows more pitting damage compared with that of sample 5. Sample 5 had more ductile streaks than sample 4. To investigate the effect of grinding directions, the average roughness values and the microphotographs should also be analyzed.

Table 3 shows the average roughness R_a and R_q values of the 16 samples ground along different crystallographic directions. Figure 5 is the graphical representation of these average R_a and R_q values. They show clearly that the average roughness R_a and

Table 2. Surface roughness R_a and R_q values.

Sample	1	2	3	4	5	6	7	8
R_a, μm	0.047	0.065	0.083	0.060	0.066	0.076	0.080	0.078
R_q, μm	0.067	0.085	0.122	0.079	0.105	0.103	0.119	0.128
Sample	**9**	**10**	**11**	**12**	**13**	**14**	**15**	**16**
R_a, μm	0.043	0.073	0.084	0.081	0.062	0.078	0.073	0.067
R_q, μm	0.063	0.099	0.116	0.110	0.100	0.118	0.104	0.089

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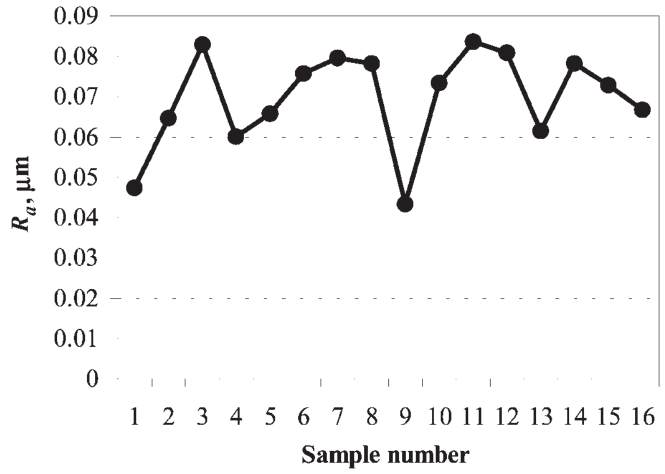

Figure 2. R_a values of the ground silicon samples.

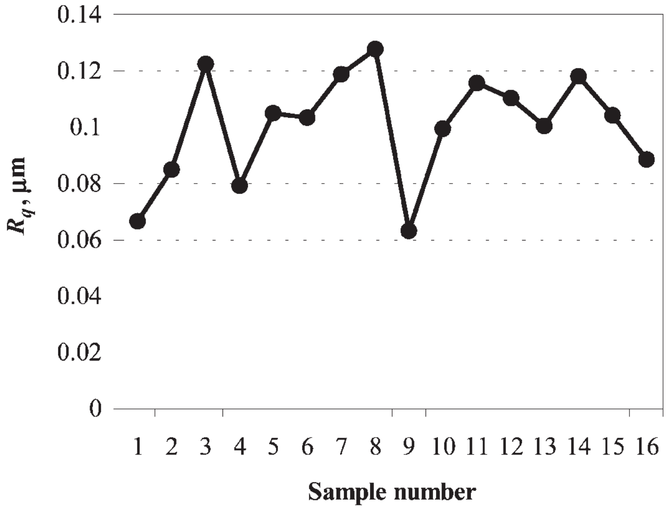

Figure 3. R_q values of the ground silicon samples.

R_q values of the surfaces ground along the ⟨110⟩ crystallographic directions of the (100) silicon are 68% and 73% of those values of the surfaces ground along the ⟨100⟩ crystallographic directions, respectively.

Figures 6, 7, and 8 show microphotographs of the surfaces ground along the ⟨110⟩, ⟨100⟩, and ⟨140⟩ directions of the (100) silicon, respectively. Although pitting damage can be observed on all of the surfaces, the pitting damage was more significant on the surfaces ground along the ⟨100⟩ and ⟨140⟩ directions.

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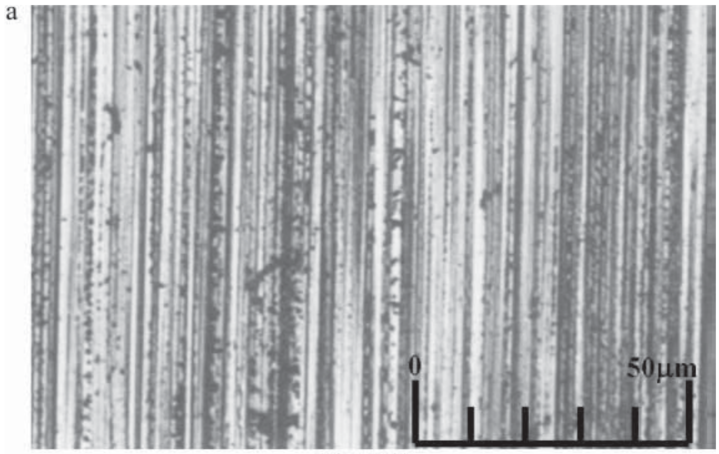
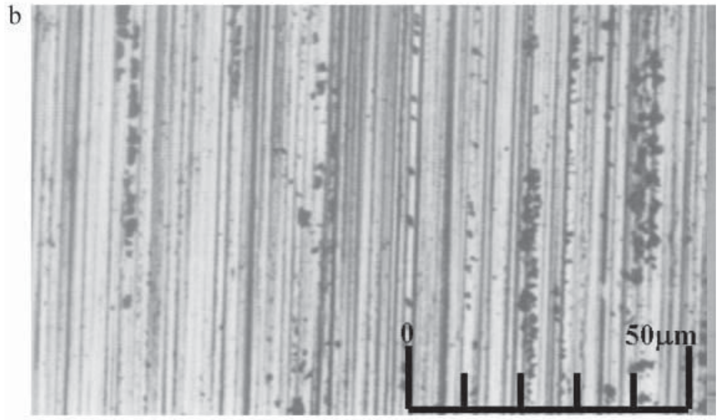


sample 4



sample 5

Figure 4. Microphotograph of ground silicon samples 4 and 5.

Table 3. Average roughness values of surfaces ground along different directions.

	R_a		R_q	
Grinding direction	µm	%	µm	%
$\langle 110 \rangle$	0.054	68	0.084	73
$\langle 100 \rangle$	0.080	100	0.115	100
$\langle 140 \rangle$	0.072	91	0.101	88

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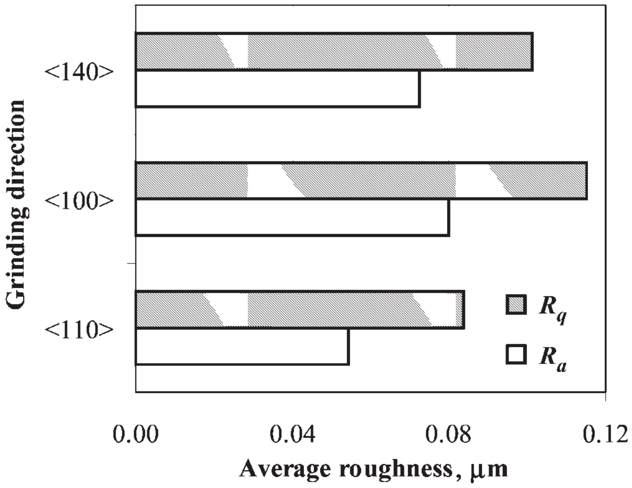

Figure 5. Graphical representation of the average R_a and R_q values of (100) silicon ground along ⟨110⟩, ⟨100⟩, and ⟨140⟩ directions.

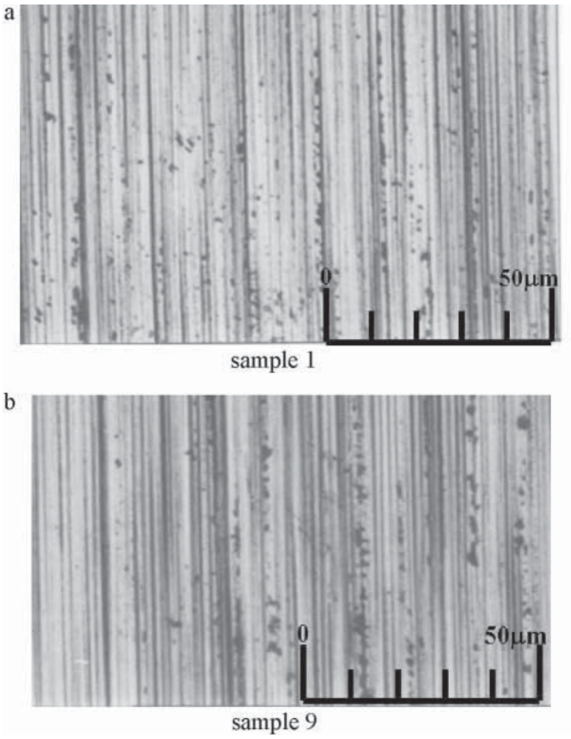

Figure 6. Microphotograph of (100) silicon samples 1 (a) and 9 (b) ground along ⟨110⟩ directions.

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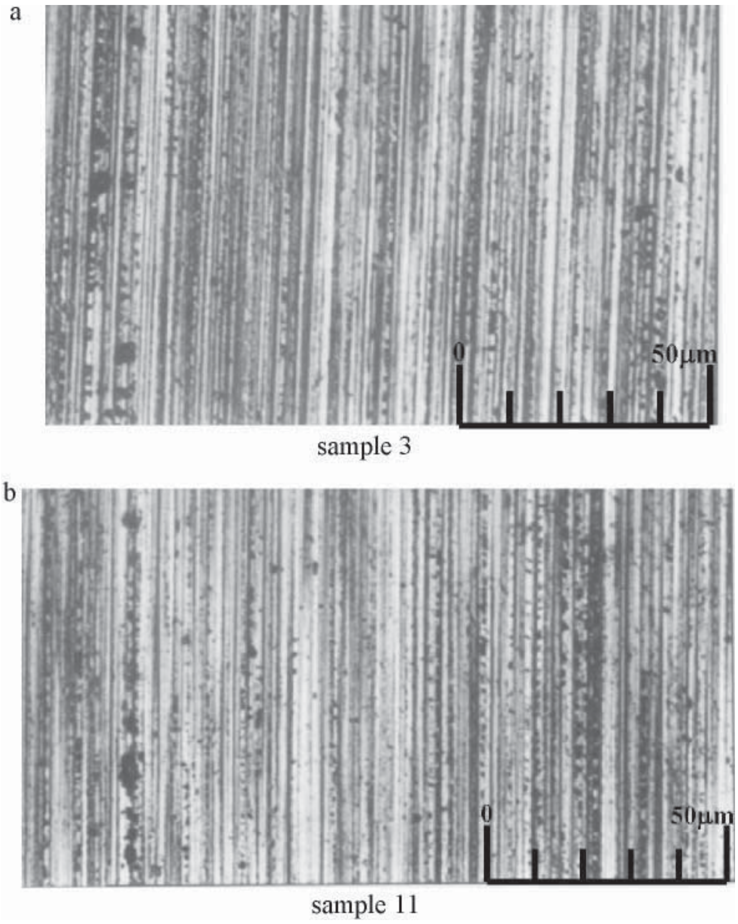

Figure 7. Microphotograph of (100) silicon samples 3 (a) and 11 (b) ground along ⟨100⟩ directions.

From the microphotographs of the ground silicon samples, we can also see that the surfaces ground along the ⟨110⟩ directions show more ductile streaks, as compared with those that are not ground in those directions. Ductile-mode machining is the very basis for precision machining of brittle materials such as silicon.

As stated in the previous section, the grinding parameters used might not be the optimum conditions for ductile-mode grinding of silicon. The objective of the experiments was to determine the effect of the grinding directions on the surface finish. We can conclude that grinding along the ⟨110⟩ directions of (100) silicon does show promising results.

The principle of grinding along a particular crystallographic direction may be applied to grinding of other single crystals if they are anisotropic (their material properties depend on crystallographic directions) like single-crystal silicon. If 100% ductile-mode surfaces can be obtained by grinding such materials along a

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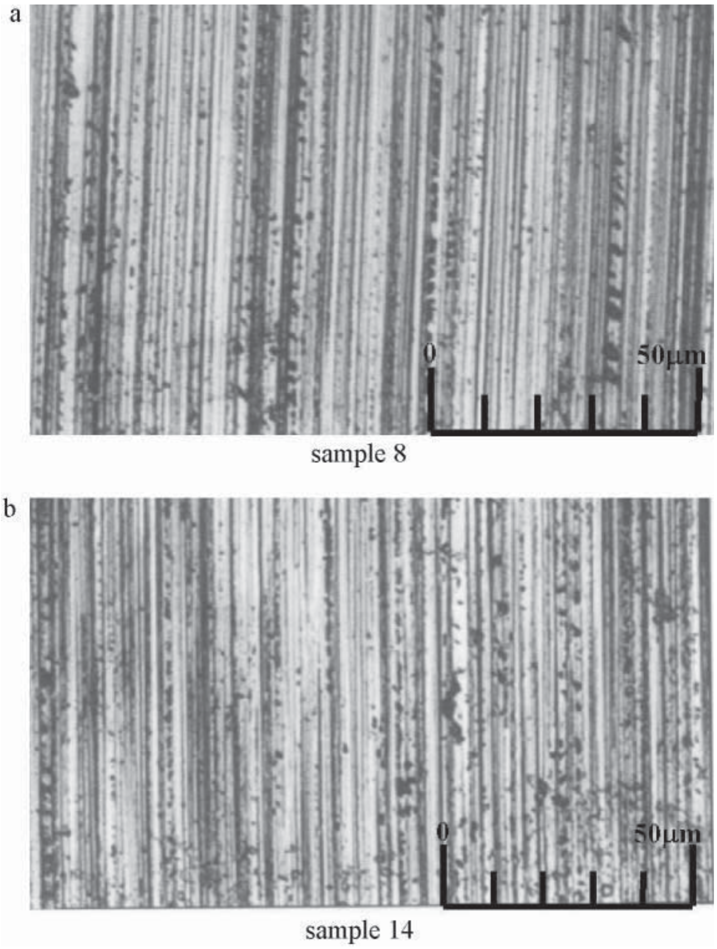

Figure 8. Microphotograph of (100) silicon samples 8 (a) and 14 (b) ground along ⟨140⟩ directions.

particular crystallographic direction, lapping and polishing are not required to produce mirror surfaces. Even if only partial ductile-mode surfaces can be obtained using this method, the polishing time required to produce mirror surfaces can be shortened, because grinding along a particular crystallographic direction can produce more ductile streaks than grinding along other directions and more ductile streaks help reduce the polishing time needed. Therefore, this method can be commercially useful. Further research can be carried out to verify this point of view.

CONCLUSION

Results from the experiments of grinding along crystallographic orientations of single-crystal (100) silicon suggested that better surface finish could indeed be

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achieved by grinding along ⟨110⟩ directions. The microphotographs also showed more ductile streaks on the silicon surfaces ground along these directions, compared with the surfaces ground along the other directions.

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