Slip on the surface of silicon wafers under laser irradiation: Scale effect*

Zhi-Chao Jia(贾志超)[1,2], Ze-Wen Li(李泽文)[1,2], Jie Zhou(周洁)[1,2], and Xiao-Wu Ni(倪晓武)[1,2,†]

[1] School of Science, Nanjing University of Science &Technology, Nanjing 210094, China
[2] Advanced Launching Co-innovation Center, Nanjing University of Science & Technology, Nanjing 210094, China

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The slip mechanism on the surface of silicon wafers under laser irradiation was studied by numerical simulations and experiments. Firstly, the slip was explained by an analysis of the generalized stacking fault energy and the associated restoring forces. Activation of unexpected {110} slip planes was predicted to be a surface phenomenon. Experimentally, {110} slip planes were activated by changing doping concentrations of wafers and laser parameters respectively. Slip planes were {110} when slipping started within several atomic layers under the surface and turned into {111} with deeper slip. The scale effect was shown to be an intrinsic property of silicon.

Keywords: slip, silicon, laser, scale effect

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1. Introduction

Silicon is the key material in the semiconductor industry. Lasers have many competitive applications in silicon machining, cleaning, and mechanical property enhancement.[1–5] Understanding laser-induced damage, including phenomena and underlying mechanisms, is critical for high efficient machining and long-term reliability of devices.

Laser-induced thermal effect is one of the damage mechanisms during the laser–silicon interaction process. In this case, laser irradiation increases the local temperature to melting or vaporization point. Investigations of thermal damages have focused primarily on the ablation effect, such as ablation threshold and ablation morphology.[6–8] The material is usually assumed to be homogeneous and isotropic. Thermal stress, induced by inhomogeneous heating, has seldom been taken into account.[9,10] Recent researches show that slip damage is the first state of permanent damage when silicon wafers are under millisecond and continuous-wave (CW) laser irradiation.[11,12] Since slip damage happens before ablation and can easily result in fracture, it is very important to ascertain the slip mechanism.

Silicon crystal has a diamond cubic crystalline structure in ambient conditions and the densest planes are {111} and {110}. However, mechanical experiments, including indentation experiments[13,14] and tensile tests,[15] have shown that slipping in bulk silicon only happens in the {111} planes. Slip planes remain {111} in the study of laser-induced slip damage.[14,16,17] Therefore, researches on slipping put particular emphasis on {111}⟨110⟩ slip systems.

In the present work, laser-induced slip on the surface of (001) silicon wafers was studied. The slip mechanism was discussed based on the concept of generalized stacking fault energy and the associated restoring forces. Activation of unexpected {110} slip planes was predicted to be a surface phenomenon. In the experiment, non-polarized Gaussian laser beams with low irradiances ($< 10^8$ W/cm^2) were used, so the effect of polarization and nonlinearity can be excluded.[18] The experimental results showed that slip planes were related to not only doping concentration but also laser parameters. These results offer a physical explanation for understanding the slip mechanisms at the atomic level.

2. Theoretical model and calculation

2.1. Usual slip model

In mechanical experiments such as tensile test, the generalized stacking fault (GSF) energy provides fundamental physics for understanding the slip mechanisms at the atomic level. It is obtained by moving one-half of the perfect bulk crystal with respect to the other along a slip direction on a slip plane (shown in Fig. 1 for the (011) slip plane).

An analysis based on the yield stress on different slip systems was performed. The yield stress is the resolved shear stress necessary to activate a slip in crystals. It can be likened to the maximum restoring force (RF), which is determined by the GSF energies. The RF corresponds to the derivative of the GSF energy respective to the slip displacement. The GSF energies for {011} and {111} slip planes along the $[01\bar{1}]$ directions were calculated with SIESTA.[19] First-principles calculations, using the density functional theory in its local density approximation for exchange and correlation potentials, were performed using norm-conserving pseudo-potentials.

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†Corresponding author. E-mail: nxw@njust.edu.cn
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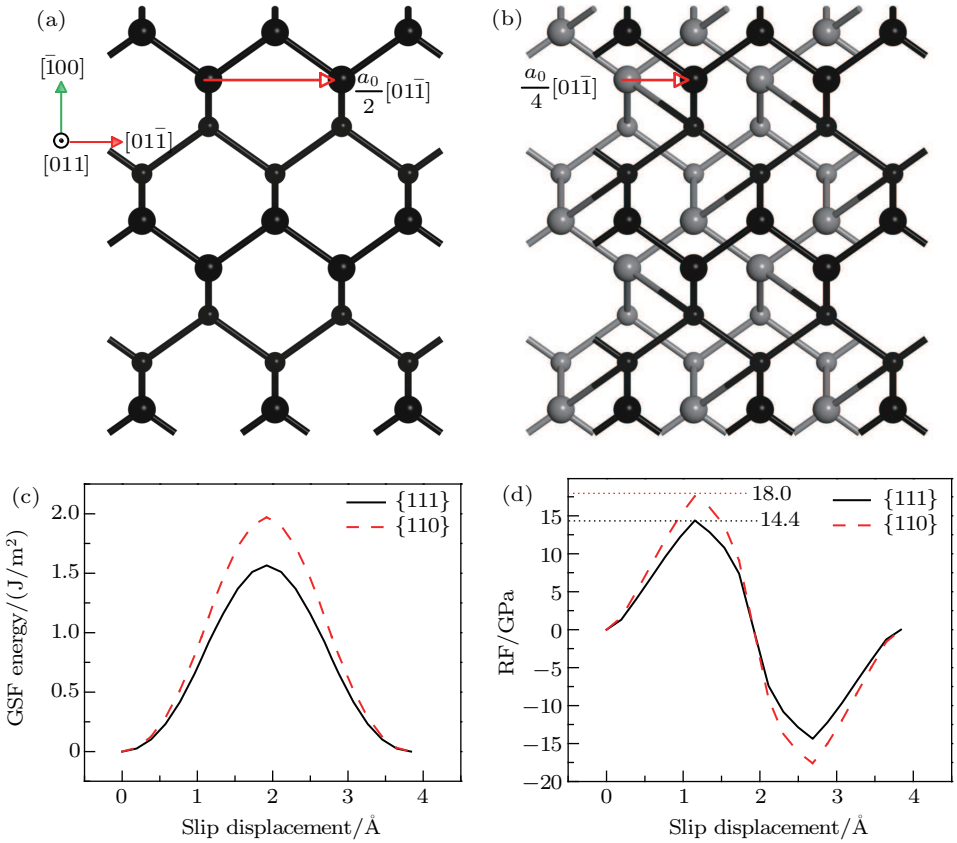


Fig. 1. (color online) (a), (b) The usual slip model to calculate GSF energy in the $\{110\}\langle 110\rangle$ slip system. Atoms in the (011) planes are represented by small-grey, grey, small-black, and black symbols from bottom to top. The slip plane is between the grey and the small-black atomic layers. (c) GSF energies and (d) RFs are presented for different slip systems.

The maximum of the GSF curve as shown in Fig. 1(c) is larger for $\{110\}$ than for $\{111\}$ planes. Consistently, the maximum restoring force, identified as $\mathrm{RF}_{\max}$, is larger for $\{110\}$ (18.0 GPa) than for $\{111\}$ (14.4 GPa) (shown in Fig. 1(d)). Slip would occur in $\{111\}$ if the two planes are submitted to the same shear stress τ. However, because of anisotropy in silicon, the resolved shear stresses $\tau = Sf$ are different in the $\{111\}$ and $\{110\}$ planes under the same stress f along $\langle 110\rangle$ directions. The Schmid factor S allows the direct calculation of the yield stress for slip systems: $S_{110} = 0.5$ and $S_{111} = 0.41$. The yield stress necessary to activate slip, identified as $\mathrm{RF}_{\max}/S$, is still lower in the $\{111\}$ planes (35.1 GPa) than in the $\{110\}$ planes (36.0 GPa). The results are close to those from classical calculations using semi-empirical potentials such as MEAM potential.[20] The usual slip model well explains the slip phenomenon in mechanical experiments.

2.2. Slip model under laser irradiation

In the case of laser irradiation, the slip mechanism is different, which leads to an interesting phenomenon as shown in Fig. 2. When silicon wafers are irradiated by lasers with low irradiances ($< 10^8$ W/cm^2), the laser energy will be absorbed and converted into heat.[6] The heating is not uniform and most of the heat is deposited in the layer below the front surface. Thermal expansion of the heated region is limited by the surrounding cool region. Therefore, thermal stresses keep increasing. Eventually, the spot center has the highest temperature and will slip first because the yield strength decreases with increasing temperature. From atomic scale, higher temperature corresponds to larger kinetic energy. Atoms in the spot center will be squeezed out by surrounding atoms while the atoms far away from the heated region keep equilibrium position, which will leave vacancies after slip.

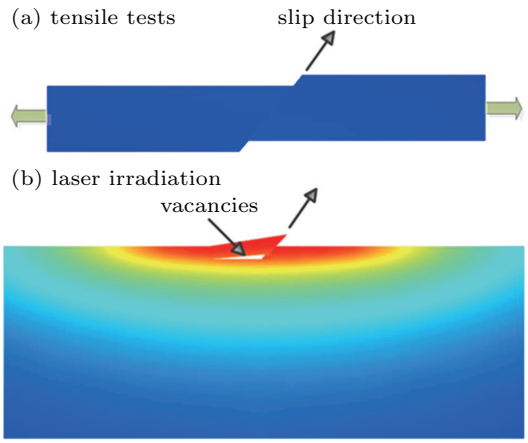


Fig. 2. (color online) Slip in tensile test (a) and under laser irradiation (b).

To ascertain the slip mechanism under laser irradiation, the GSF energies were calculated for {011} and {111} slip planes along the $[01\bar{1}]$ direction with the models shown in Figs. 3(a) and 3(b). The thicknesses for the two models were 7.68 Å and 5.43 Å, respectively. A vacuum layer (10 Å) was added on the (001) surface. The slip depth N is expressed by the number of slip atoms. Atoms in the dashed rectangle will slip together along the arrow.

When N is larger than 4, the GSF energy increment is stable and the total GSF energy can be expressed by $E_N = E_4 + (N-4)E_\Delta/2$ (Figs. 3(c) and 3(d)). Since the slip area $S_N = NS_1$, where $S_1^{111} = 12.8$ and $S_1^{011} = 20.8$ Å^2, then the restoring force RF can be expressed as

$$\mathrm{RF} = \mathrm{d}(E_N/S_N)/\mathrm{d}x. \tag{1}$$

Table 1 lists the calculated yield stresses. When $N = 4$, the corresponding yield stress σ_Y, identified as $\mathrm{RF}_{\max}/S$, is lower in the {011} planes (17.3 GPa) than in the {111} planes (19.0 GPa), so it is easier for the {011} planes to be activated. When N is larger than 4, the yield stress is less in {111} than in {110}, and therefore slip favors the traditional {111} planes. The results show the scale effect of slip under laser irradiation and that the activation of {110} planes is a surface phenomenon.

The slip mechanism has been discussed from the point of view of energy, however, why a slip occurs at a certain N is not clear. Since the unexpected slip takes place within several atomic layers under the surface, molecular dynamics (MD) simulations should be a useful tool to study the dynamic heating process. However, limited by computers, the simulation time of MD is about several picoseconds, which is too short to describe the process in milliseconds in the present paper. On the other hand, thermal stress arises from inhomogeneous heating of the silicon wafer, which contains too many atoms to deal with. So it is difficult to study the dynamic process and the analysis of (GSF) energy provides a realistic method to understand the slip mechanism.

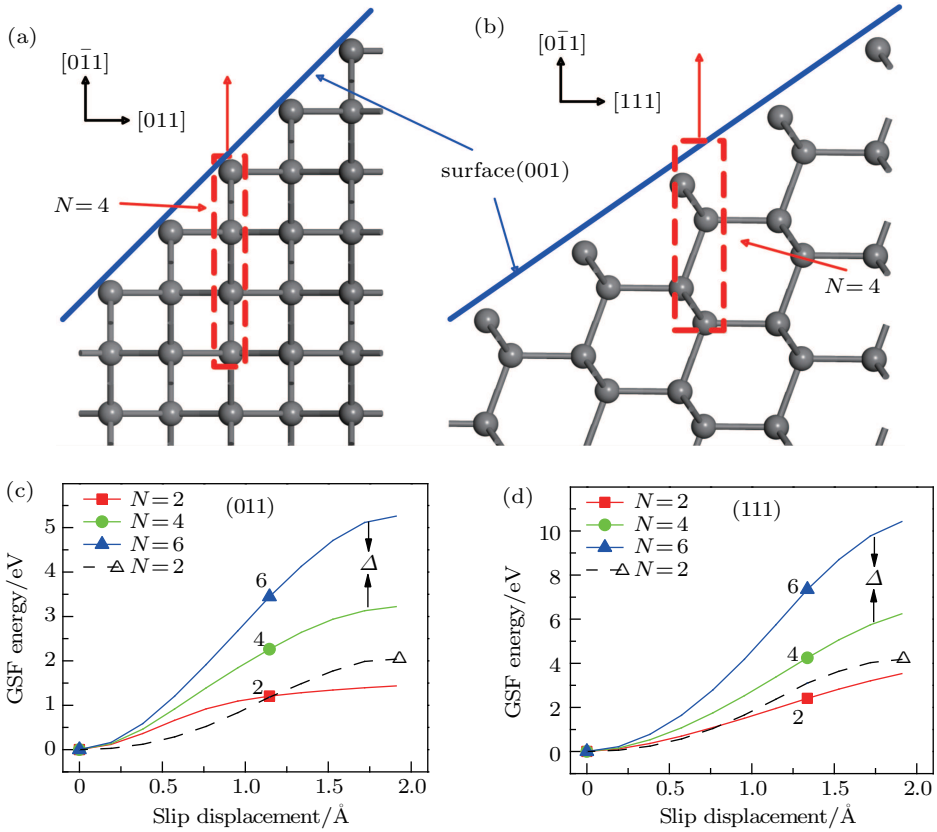


Fig. 3. (color online) Models of slip on {011} (a) and {111} (b) planes. There is a vacuum layer (10 Å) on the (001) surface. Atoms in the dashed rectangle will slip together along the arrow. (c), (d) GSF energies under the conditions in (a), (b) are presented.

Table 1. Yield stress σ_Y.

N		2	4	6	10	20	200	2000	20000
σ_Y/GPa	{111}	23.8	19.0	23.5	24.3	26.8	27.8	27.9	27.9
	{110}	18	17.3	24.5	25.3	27.3	29.1	29.3	29.3

3. Experiments

In Section 2, a slip model was built to describe the slip mechanism under laser irradiation. The results showed that it is possible to activate unexpected {110} slip planes. Since slip occurs in the heated layer, the heating depth L_H is a very important parameter. If the heating depth is small enough, slip will happen just below the front surface, which may activate the unexpected slip. When the laser irradiance is low, L_H can be expressed as $L_H = 1/\alpha + L_T$,[6] where the first item means the absorption depth and the second item $L_T = \sqrt{kt/\rho c}$ is the thermal diffusion length. The thermal properties of undoped silicon at 1000 K are taken as follows: mass density $\rho = 2.31$ g/cm^3, specific heat $c = 0.93$ J/(g·K), thermal conductivity $k = 0.31$ W/(cm·K), and absorption coefficient $\alpha = 1300$ cm^{-1}. We obtain the absorption depth 7.7 μm and $L_T = 72$ μm with pulse width $t = 50$ ms. It appears that there are two ways to reduce the heating depth. One is to reduce the absorption depth such as doping and the other is to reduce the thermal diffusion length such as shortening pulse width. Both methods make the energy deposited in a thinner layer under the surface, which may activate unexpected slip on {110} planes.

The Czochralski-grown, boron-doped silicon wafers with front surface mirror polished were commercially available. Dopant concentrations of samples 1–3 were 3.2×10^{18} atoms/cm^3, 1.0×10^{20} atoms/cm^3, and 1.1×10^{20} atoms/cm^3, respectively. The thicknesses of samples 1–3 were 270 μm, 400 μm, and 400 μm, respectively. The silicon wafers were irradiated by ∼ 1080 nm fiber lasers. The experiment was performed twice using different lasers. The CW laser emitted a laser beam continuously and the pulsed laser produced 120-ns (full pulse duration) pulses with a repetition rate of 80 kHz. The other parameters of the lasers were the same. The non-polarized Gaussian beam with average power 50 W was focused by a lens and the spot radius on the target surface was ∼ 530 μm ($1/e^2$ of the intensity). The surface morphologies after laser irradiation were observed by an optical microscope (OM). The experiment was performed at room temperature in air under normal atmospheric pressure.

4. Experimental results and discussion

4.1. Slip under CW laser irradiation

Firstly, the heating depth was reduced by changing the doping concentration of the samples. All samples were irradiated by CW laser beam. Doping greatly increases the absorption of lasers. For example, pure silicon wafer at 300 K has an absorption coefficient α of $\sim 10^3$ m^{-1}, while for doped silicon with boron (B) concentration of 10^{20} atoms/cm^3, the absorption coefficient is $\sim 10^5$ m^{-1}, which is two orders of magnitude higher than that of pure silicon wafer.[21] So laser energy is absorbed in a very thin layer. The absorption depth $L = 1/\alpha$ of sample 3 at 300 K is about 10 μm and reduces further with increasing temperature.

The evolution of slip patterns on the surface of sample 1 is shown in Figs. 4(a)–4(c). Rectangular slip loops are observed in the damaged region (Fig. 4(a)), and the rectangular edges tend to locate along ⟨110⟩, which are the intersections of {111} planes and the (001) surface. With further irradiation, the slip region enlarges a great deal (Fig. 4(b)). Eventually, ablation occurs and slip patterns disappear (Fig. 4(c)). These patterns are usually observed on the surface of silicon under CW laser irradiation.[22] It also shows that slip happens before ablation.

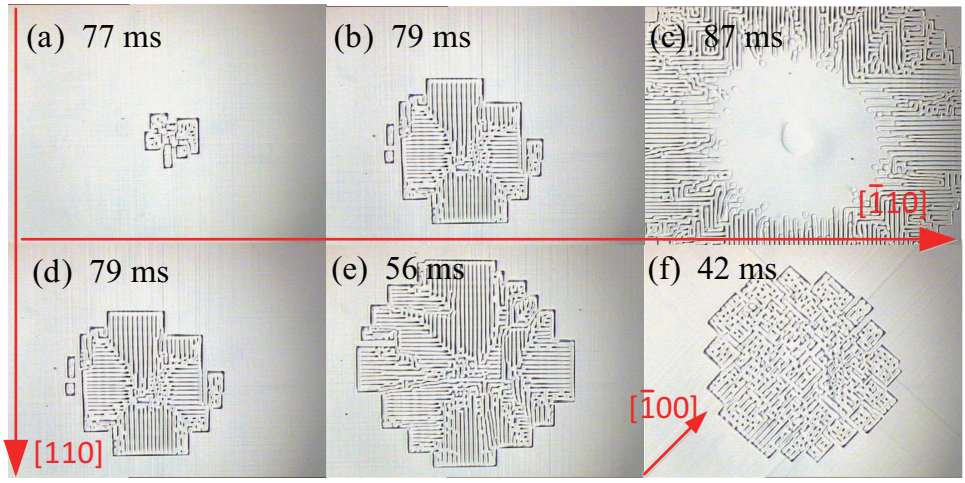


Fig. 4. (color online) (a)–(c) OM images of sample 1 with different irradiation time and (d)–(f) typical images for samples 1–3. Dopant concentrations increase from sample 1 to sample 3. The sizes are 80 μm×60 μm.

Typical images of samples 1–3 are shown in Figs. 4(d)–4(f). Unexpected patterns are observed in sample 3, where slip lines change to ⟨100⟩ directions, the intersections of {110} planes and (001) surface (Fig. 4(f)). These patterns are very repeatable and the directions of the slip patterns keep unchanged within the laser power range from 10 W to 500 W. The re-

sults show that slip is related to doping. Heavier doping corresponds to shorter absorption depth, so the heating depth of sample 3 is the smallest. Heat is deposited in the layer just below the front surface and unexpected slip is activated. In the following discussion, it is shown that the other effect of doping on slip is negligible.

4.2. Slip under pulsed laser irradiation

To reduce the heating depth by shortening the thermal diffusion length, the same experiment was carried out using a pulsed laser which produced 120-ns (full pulse duration) pulses with a repetition rate of 80 kHz. The other parameters are the same as the CW laser. Under pulsed laser irradiation, the thermal diffusion length has been reduced to 0.1 μm in one pulse.

As expected, the slip occurs on {110} planes in all samples. Figure 5 shows OM images of sample 1 under pulsed laser irradiation with different irradiation time. On the whole, slip lines tend to locate along ⟨100⟩ at the beginning (Fig. 5(a)), which means slip on {110} planes. However, the deviations of slip lines from ⟨100⟩ are obvious. Although slip takes place on {110} planes at the beginning, attempts to maintain slip on {110} end with propagation on {111} due to the deflection phenomenon, which is formed because {111} planes have less cleavage energy than {110} planes. As shown in Fig. 5(c), the slip planes have totally deflected into {111} at the rim of the damaged region. Thus slip on {110} planes is shown to be a surface phenomenon and deflects into a traditional {111} slip plane when slip extends.

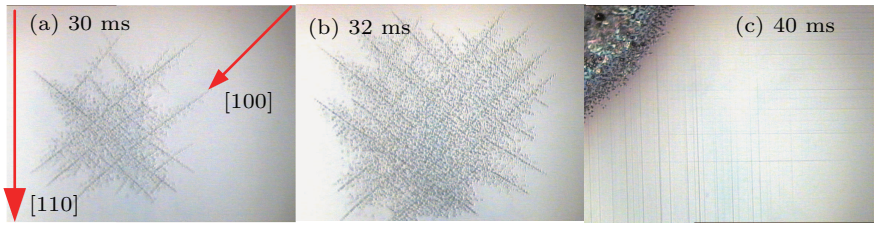


Fig. 5. (color online) (a)–(c) OM images of sample 1 under pulsed laser irradiation with different irradiation time. Panel (c) shows the image at the rim of the ablation region. The average laser power is 50 W. The sizes are 80 μm×60 μm.

4.3. Other factors affecting slip

In experiments, the heating depth was reduced by doping and changing laser parameters. Both methods made the energy deposited in a thinner layer under the surface, and successfully activated unexpected slip planes. The other factors affecting slip have not been discussed. Firstly, lattice deformation caused by doping should be ascertained. It has been shown experimentally that the doping of smaller boron atoms leads to a reduction of the lattice parameter. The concentration level of substitutional B (x) that can be reached is usually not higher than 1 at.%. In this case, a linear relation between the lattice parameter of B-doped Si and x is described by the well-known Vegard's rule: $a_{\mathrm{Si}_{1-x}\mathrm{B}_x} = (a_{\mathrm{B}} - a_{\mathrm{Si}})x + a_{\mathrm{Si}}$, where the lattice parameters a_{Si} and a_{B} are 5.43 Å and 3.78 Å, respectively.[23] Thus the relative variation of the lattice parameter is not higher than 0.3%.

Different from the mechanical experiment, where external stresses are applied, the laser irradiation process is non-contact. Therefore, the strain is limited by the mechanical properties of silicon and the maximum strain of the heated silicon can be expressed as

$$\varepsilon_{\max} = \int_{293}^{1685} \alpha_{\mathrm{T}} \mathrm{d}T \approx 5.7 \times 10^{-3}, \tag{2}$$

where α_{T} is linear expansibility along ⟨110⟩. The thermal strain is slightly larger than the lattice reduction caused by doping. Numerical results show that such small variances have little effect on GSF energies. Julien also pointed out that the relative change of $\mathrm{RF}_{\max}$ is less than 1% even at a strain of 20%.[20] Thus, we can exclude the effect of lattice deformation caused by either doping or heating.

In boron-doped P-type silicon, we activated {110} slip planes. The same experiment was done in phosphorus-doped N-type silicon with a doping concentration of 1×10^{19} atoms/cm^3. The slip patterns under two types of lasers were similar to those of sample 1, which showed that electronegativity of doped atoms was not a decisive factor. Attempts to activate unexpected slip planes in undoped silicon failed. Greater heating depth than the doped one is responsible. To the best of our knowledge, such a slip system has never been observed experimentally in bulk silicon. However, it has been noticed in nanostructures such as in epitaxial Ge layers on Si substrates.[24] In that case, the unexpected slip is activated due to high misfit, which exerts a force on the interface. Slip atoms are pulled out from the surface. In the present paper, laser irradiation leads to a similar surface phenomenon, but with a difference that slip atoms are squeezed out by surrounding atoms. At first glance, the doping and laser parameter greatly affect slip. Essentially, the scale effect is an intrinsic property of crystal silicon.

5. Conclusion

Two types of slips were observed on a silicon surface under laser irradiation: the usual {111} and unexpected {110}.

The generalized stacking fault energy and the associated restoring forces offer a physical explanation for understanding the slip mechanisms. In experiment, the change of the two slip planes is caused by heating depth, which is related to doping and laser parameters. Essentially, the scale effect is an intrinsic property of crystal silicon. The results presented in this paper deepen our understanding of silicon and offer both a theoretical and experimental basis for further investigation of the laser–silicon interaction.

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