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FACTORS INFLUENCING THE YIELD STRESS OF SILICON

Factors influencing the yield stress of silicon are investigated with advanced research methods. It is shown that elastic stresses which are concentrated at the structural defects (dislocation, crystalline grain boundary, dendrite and lamella) will influence on the yield stress of silicon.

1. INTRODUCTION

Further micro- and nano-miniturization of electronics elements produces enhanceable requirements to the semiconductor quality and to the technology. As it is known, sources of structural defects in semiconductors are stresses. Plastic deformation is always characterized by the yield stress. The stress level at which a material no longer behaves elastically, but instead experiences a small plastic deformation is known as the yield stress (point) or a plasticity threshold — τ_k . The great number of research papers is devoted to the problem of defect formation and, in particular, the yield point of monocrystallin silicon and systematize in monographs (see, e.g. [1, 2]). However, not all factors influencing the yield stress of silicon are sufficiently detailed investigated. This fact has conditioned the problem statement of the given work devoted to the investigation of the structural defects in silicon wafers and their influence on the yield point.

2. EXPERIMENTAL DETAILS

We studied Cz-Si wafers of different orientation, N-, P- type with $\rho = 4 — 10$ (Ohm·cm).

The following methods and equipment were used for researching the silicon wafers:

– method of selective chemical etching by Sirtle or Secco; Sirtle chemical selective etchant (50 g CrO3 + 100 ml H_2O + 100 ml HF (46 %)) is used to etch close-packed silicon planes (111) with the etching speed of about (2–3) µm/min. Knowledge of the etching speed enabled us to control the depth of analysis from the surface into the bulk of the silicon wafer.

– scanning electron microscopy (SEM), by means of scanning electron microscope analyzer "Cam Scan-4D" with a system of the energetic dispersive analyzer "Link-860" (with the usage of "Zaf" program, mass sensitivity of the device is 0.01 %, beam diameter ranges from $5\cdot10^{-9}$ to $1\cdot10^{-6}$;

– optical methods of researches with the usage of metallographic microscope "MMP-2P";

– Auger spectrometer LAS-3000 (beam diameter — 5 microns).

The technique of experiments consisted of the following: the selective chemical etching method allows one to carry out the level-by-level analysis of silicon by etching layers and to reveal defects simultaneously. After selective chemical etching application, the surface of wafers was investigated on deficiency with the usage of metallographic optical microscope "MMP-2P". To improve the defects image quality and to obtain the possibility of making the quantitative analysis of impurity, we applied such methods of analysis as scanning electron microscopy with energetic dispersive analyzers and Auger spectrometer.

3. RESULTS AND DISCUSSION

It is known, that stresses and deformations exceeding a plasticity threshold are the source of structural defects in solids. In case of a defectless material the yield stress depends on electrophysical and elastic parameters and other conditions (temperature, pressure, etc.). Alternative, the magnitude of a plasticity threshold can essentially vary. The relationship between the stress and strain that the material displays is known as a stress-strain curve (Fig. 1).

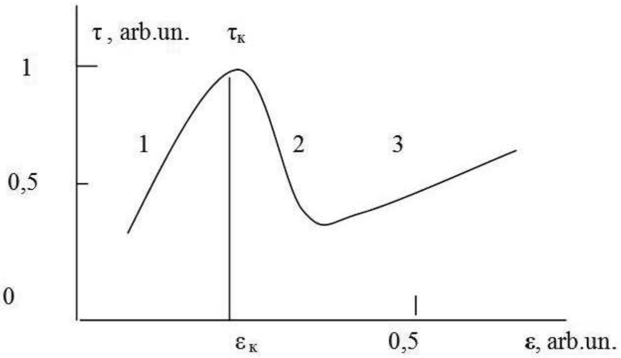


Fig.1. The quality stress-strain curve.

It is unique for each material and is found by recording the amount of deformation (strain) at distinct intervals of tensile or compressive loading. Up to this amount of stress, stress is proportional to strain (Hooke's law), so the stress-strain graph is a straight line, and the gradient will be equal to the elastic modulus of the material (region 1, Fig.1). Second region of stress-strain curve describe the increasing of dislocation density due to the formation of new dislocations and dislocation multiplication (region 2, Fig.1). At sufficiently large strains, the stress in materials increases with strain in a nonlinear manner, this is called hardening. On further straining, the material breaks (region 3, Fig.1) [2].

According to the Frank-Read source mechanism, presence of point defects of various type changes elastic parameters of crystals that at external actions leads to formation of structural defects. Thus, in this theory key parameter influencing the yield stress is the density of point defects [3].

Figure 2 illustrates the dislocation multiplication due to scribing of silicon wafers at a room temperature. Mechanical stresses are passed round approximately in the radial direction from a scribe channel because this direction is possible to relate with dislocations and areas with the changed mechanical potential and which can be related to Frank — Read sources. In the context of Alexander — Haasen model the dislocation multiplication happens by their recrawlings to the subsequent reproduction [4]. However, the problem related to the impurity atmosphere effecting on the yield stress will stand aside. According to models of static and dynamic dislocation “ageing”, impurity atmospheres interacting with dislocations, create starting stresses, which are necessary for overcoming to shift dislocation from a place [5]. Such interaction, also, creates the additional retardation rationing an impellent at dislocations moving. The dynamic “ageing” leads to astable dislocation jump moving and dislocation multiplication owing to their brakes-off from the impurities. The offered models well present some experimental data, according to which, increasing of initial dislocation density can lower the yield stress, however the presence of the impurity atmospheres increases the yield stress [6, 7].

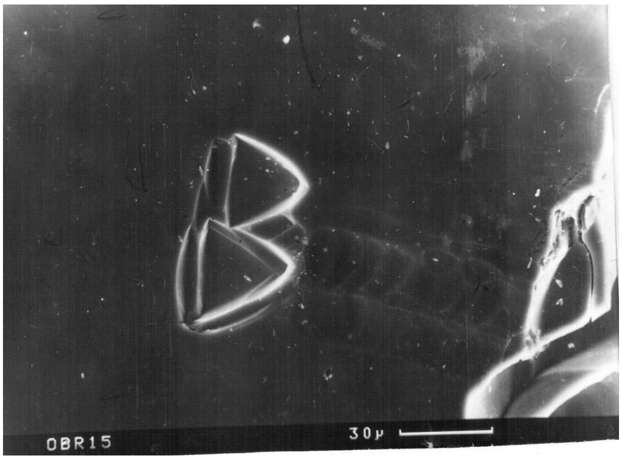


Fig.2. The SEM image of dislocation multiplication.

Elastic stresses are accumulated around the dislocation core during dislocation formation (Fig. 1, a region 2). For single crystalline silicon the yield stress ($\tau_к$), depending on orientation and other parameters, being over the range $\tau_k = (5 \cdot 10^8 - 2 \cdot 10^9)\, N/cm^2$ at magnitudes of the relative strains $\varepsilon_k = (10^{-5} - 2 \cdot 10^{-4})$ [8]. If the average distance between the 60° dislocations is 10^{-5} m, the relative strains counted by formula $\varepsilon = (b/D)k$, where D — average distance between dislocations, b-magnitude of a vector Burgers projection, $k \approx 0.5$, is equal $2.7 \cdot 10^{-5}$, i.e. is in the second region (fig. 1). Such relative strains are starting on further mechanical and thermal affecting. Dangling bonds are shaped around the dislocation core due to presence of compression and extension zone. These cause atomic bonds weakening and change the local threshold of plasticity.

The yield stress depends on temperature [5]. The yield stress decrease is caused by the temperature increasing. At temperatures $1000{-}1200^0$ C (the high-temperature oxidation) the yield stress falls down in 50—60 times. Thus, presence of strains around dislocations and temperature increase can lower the yield stress of single crystalline silicon.

The impurity atmosphere around dislocations can result not only “ageing”, but also generates compensation stresses and strains. Impurity atoms accumulate around dislocations in an extension zone if impurity atom radius more than radius of silicon atom. Thus there is a decrease of stresses and strains localized around dislocations. Impurity atoms accumulate in a compression zone if the radius of impurity atom is less, than radius of silicon atom. In this case there is a decrease of strains and stresses. Figure 3 shows the electronic image of 60° dislocation received on a surface p-Si (10 (100)) which come out after 2 minutes etching (Sacco etchant). The picture is received in a conductance mode.

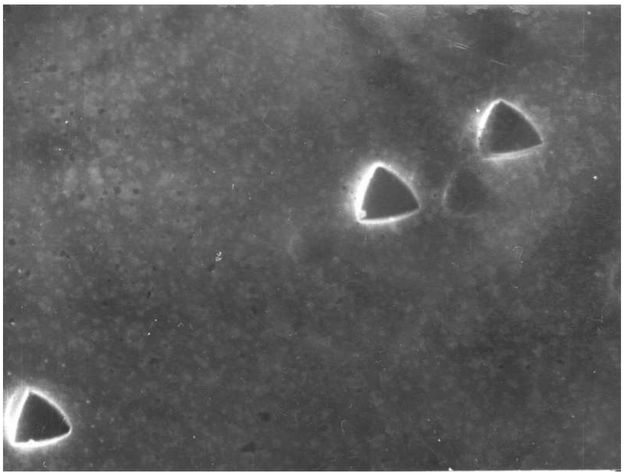
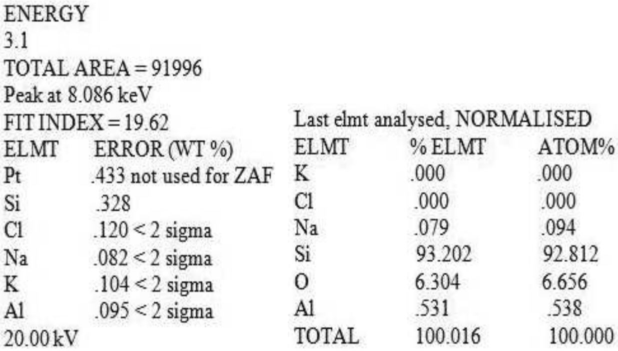


Fig.3. The SEM image of dislocations 1x3000 (conductance mode).

The X-Ray analysis of light areas of dislocation has shown presence of oxygen atoms (oxygen concentration is 6 atomic percents) (fig. 4). Oxygen atoms are located in interstitial position of a silicon crystal lattice, and being in an inactive electrical state. Oxygen atoms decrease stresses and strains localized around dislocation due to radius of oxygen atom more than radius of silicon atom occupying a position in an extension zone of dislocation. This causes that silicon crystal lattice begin more hardening and increase the yield stress.

If oxygen atoms create in dislocation-free silicon uncontrollable impurities in the form of interstitial position atoms accumulations or an accumulation of oxygen precipitates, it occurs the relative strains which it is possible to count approximately (taking into account known restrictions on sp^3-hybridizations), according to expression $\varepsilon = \omega C$ (Vegard’s law), where ω — Vegard’s coefficient, depending on a type of impurity atoms and their lattice position, C — impurity concentration. The calculations for the oxygen atoms have shown that the strain is approximately equated

10^{-5}. Such strain is starting to decrease the yield stress and cause the subsequent defect formation at the further affecting. If concentration of impurities considerably exceeds 6 atomic percents there are stresses and strains leading to generation not of one dislocation but their accumulations (fig. 5). Thus, impurity atoms are proportioned between dislocations, and process of dislocation generation stop, when stresses relax to level of elastic values.



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ENERGY
3.1
TOTAL AREA = 91996
Peak at 8.086 keV
FIT INDEX = 19.62                             Last elmt analysed, NORMALISED
ELMT     ERROR (WT %)                ELMT       % ELMT       ATOM%
Pt       .433 not used for ZAF       K          .000         .000
Si       .328                        Cl         .000         .000
Cl       .120 < 2 sigma              Na         .079         .094
Na       .082 < 2 sigma              Si         93.202       92.812
K        .104 < 2 sigma              O          6.304        6.656
Al       .095 < 2 sigma              Al         .531         .538
20.00 kV                             TOTAL      100.016      100.000
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Fig.4. The X-Ray analysis of dislocation core.

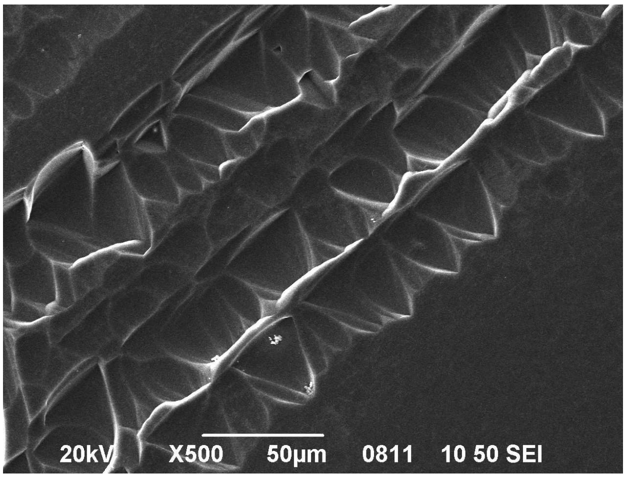

Fig.5. The SEM image of dislocation accumulation.

In very rare cases, when concentration of impurity atoms in silicon is more than solid solubility limit, it can organize macroimperfections known as dendrites (fig. 6). Dendrites consist of a mixture of solid solutions of iron or chromium (fig.7).

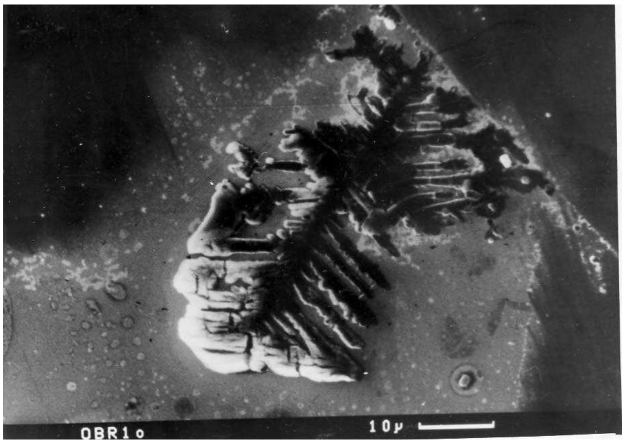

Fig. 6. The SEM image of dendrite on a silicon surface.

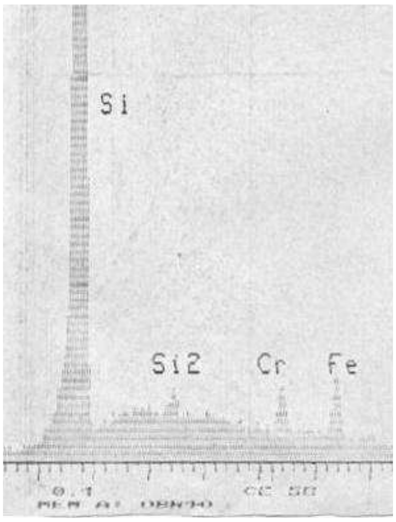

Fig. 7. The X-Ray analysis of dendrites in silicon.

When silicon atoms are clustering it can form twinning lamellas (fig.8). On the interface line dendrite — silicon are stresses often exceeding the yield stress of silicon. Thus, it is disordered silicon under a dendrite area and the area containing dislocation networks, consisting of 60^0 dislocations (fig. 9).

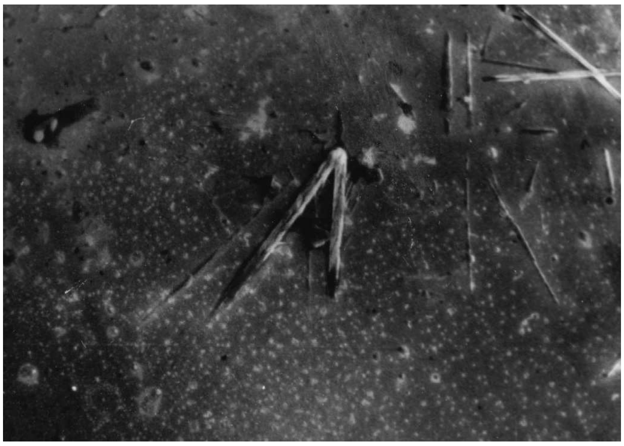

Fig. 8. The pattern of twinning lamellas, 1 × 5000.

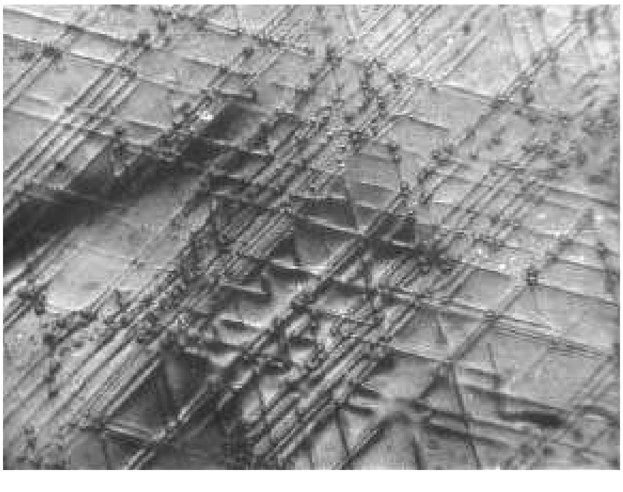

Fig. 9. The SEM image of dislocation networks, 1x2300.

In some cases, silicon wafers have layered structure that was revealed as a result of selective chemical etching (fig. 10) [9]. Boundary lines of layers are disoriented under different angles from each other and the strains are localized around boundary lines. These stresses exceed the yield point and can cause the generation of new defects and decrease a silicon plasticity threshold.

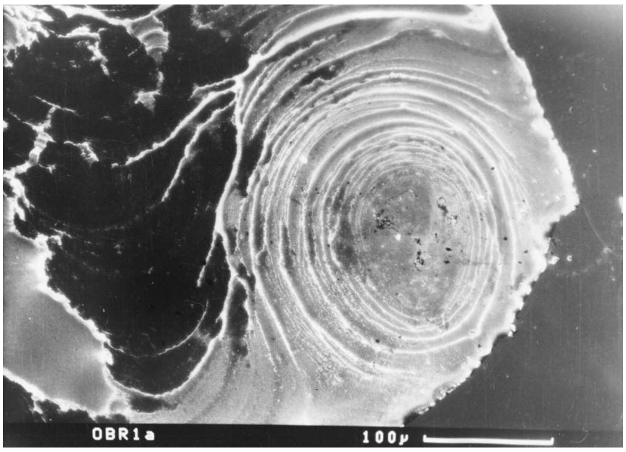

Fig.10. The SEM image of silicon layer structure defects.

4. CONCLUSIONS

On the basis of our researches, the following conclusions can be drawn:

– the yield stress of monocrystallin silicon decrease with increasing of a dislocation density and can vary in the presence of impurities atoms which localized around dislocations;

– in one case, impurity atmospheres participate in processes of “ageing” of dislocations that increases a plasticity threshold of silicon, in another one — presence of oxygen atoms near dislocations creates compensation stresses which can cause to the hardening of the crystal lattice of silicon and increase the magnitude of the yield stress;

– stresses and strains which decrease the yield point and are starting for formation of new defects are a consequence of the background uncontrollable impurity of oxygen atoms in dislocation-free silicon crystals;

– presence of dendrites, lamellas and layered structure of silicon decrease a local magnitude of yield stress due to strains accumulated around a boundary line of defects and monocrystallin silicon.

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Abstract
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Key words: silicon, structural defects, the yield stress.

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ФАКТОРЫ, ВЛИЯЮЩИЕ НА ВЕЛИЧИНУ ПОРОГА ПЛАСТИЧНОСТИ В КРЕМНИИ

Резюме
Используя современные методы исследования, определенны факторы, влияющие на величину порога пластичности монокристаллического кремния. Наряду с известными факторами, величина порога пластичности будет зависеть от упругих напряжений, локализованных в области нахождения структурных дефектов.

Ключевые слова: кремний, структурные дефекты, порог пластичности.

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ФАКТОРИ, ЩО ВПЛИВАЮТЬ НА ВЕЛИЧИНУ ПОРОГА ПЛАСТИЧНОСТІ В КРЕМНІЇ

Резюме

За допомогою сучасних методів дослідження, визначенні фактори, що впливають на величину порога пластичності в напівпровідниковому кремнію. Поряд з відомими факторами, на величину порога пластичності впливають пружні напруження, що локалізовані в області знаходження структурних дефектів.

Ключові слова: кремній, структурні дефекти, поріг пластичності.