Effects of PECVD temperature and RF power on surface structure and refractive index of amorphous and polycrystalline silicon films

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Abstract. The amorphous and polycrystalline silicon films were obtained by plasma enhanced chemical vapor deposition. The effect of power and temperature over a wide range on the surface morphology and structure, deposition rate films and refractive index have been investigated by atomic force microscopy, profilometry and ellipsometry. The deposition rate increased from 19.1 to 58.2 nm/min with RF power from 10 to 40 W. The refractive index of the films obtained at a temperature of 550 to 700 °C was in the range from 3.5 to 5.5.

1. Introduction
Silicon in all phase states is extremely demanded material in electronics, e.g. solar cells [1], thin films transistors (TFTs), micro- and nanoelectromechanical systems (MEMS/NEMS) [2,3], and others. Solar cells based on monocrystalline silicon are most effective maximum up to 21.3%, however their spread is limited by high cost [4]. To reduce the cost, the multi-layer structure of a thin film solar cell is formed on inexpensive glass and plastic substrates, which greatly limits the maximum process temperature. The elements based on amorphous hydrogenated silicon (a-Si:H, nc-Si:H) are actively used in mass solar cell production [1,4]. This is a consequence of a combination of low deposition temperature, high productivity, ease of manufacture, a sufficiently high optical absorption coefficient, and relatively low cost compared with the elements based on GaAs, InP, ZnP. It has been possible to increase the efficiency of solar cells based on a-Si:H to a maximum of 15% in experimental studies, by improving the properties of materials and developing new multilayer structures [5]. However, the main problem of thin-film silicon solar cells, which limits their effectiveness, is the light-induced degradation effect (Staebler-Wronski Effect) [6]. To reduce this effect, nano- and microcrystalline hydrogenated silicon films (nc-Si:H, μc-Si:H) with grain sizes from several units to tens of nanometers placed in an amorphous matrix were used [7]. They demonstrate greater stability in lighting, better electrophysical properties and lower defect density than a-Si:H. To increase the efficiency of thin-film solar cells, a combination of carbon nanotubes and silicon was used [8]. CNT are not only transport charge carriers, but also act as some photoactive thin films use in elements of solar cells, due of the large number of physical effects that occur in the bulk and at grain boundaries [9]. The high temperature and low deposition rate is limiting factor.

Amorphous, nano- and microcrystalline hydrogenated silicon and crystalline silicon films depending on the application can be prepared by various methods of chemical vapor deposition (CVD). This method allows deposition amorphous hydrogenated, nano- and polycrystalline silicon films in a wide temperature range from 100 to 1300°C [3]. However, the possibility of reducing temperature to 700°C
and less is interesting. To date, the most flexible method in terms of parameters process is plasma enhanced chemical vapor deposition (PECVD) [10]. Obtaining silicon films with reproducible properties requires the establishment of key parameters of process and fine adjustment in the deposition process.

The purpose of this study is to investigate the grain size and shape, deposition rate and refractive index of amorphous and polycrystalline silicon films depending on the temperature and RF power of plasma enhanced chemical vapor deposition.

2. Experiments
Polycrystalline silicon and silicon dioxide films were prepared by PECVD used Oxford Instruments PlasmaLab 100 [10, 11]. The substrate was n-type silicon wafer (100). Previously, the substrates were covered with a layer of silicon oxide in plasma of Ar:SiH\textsubscript{4}:N\textsubscript{2}O (161.5:8.5:710 sccm). Pressure, RF power and temperature were 1 Torr, 20 W and 350 °C, respectively. The film thickness of 0.45 μm, RMS roughness not more than 0.6 nm and compressive stresses of 380 MPa observed by profilometry. Further, plasma deposition of amorphous and polycrystalline silicon films was carried according to [11]. The surface morphology and grain size of the films were studied by atomic force microscopy (NTEGRA Probe Nanolaboratory) [12]. The thickness of the films was determined by profilometry (KLA Tencor D-100) of patterned steps formed by photolithography (MJB4). The refractive index was determined by ellipsometry (LEF-3M).

3. Results and discussion
Silicon films on the SiO\textsubscript{2}/Si (100) structure were obtained at temperature from 550 to 700°C (power was fixed to 40 W). The deposition rate was 150 nm/min. Investigations of the films by AFM and profilometry showed an increase in the grain size with increasing temperature and inflection of RMS curve (Fig. 1). The grain size of the films was in the range from 40 to 140 nm, and RMS roughness – 1.79-3.54 nm. Analysis of the AFM data (Figure 1,2) and previous RHEED findings of the same films [10] allowed to compare the flex point to the temperature of the phase transition from amorphous to polycrystalline at 550-600°C, which corresponds to the transition temperature of LPCVD films [9].

Figure 1. Grain size and RMS roughness vs deposition temperature curves.
Moreover, this process is characterized by a transition from tensile stresses, prevailing in the amorphous phase, to compressive stresses (~300 MPa). Further increasing in temperature above 600°C, contributes to the gradual decrease of internal stresses.

It is established that with increasing RF power from 10 to 40 W the deposition rate substantially increases almost linearly from 19.1 to 58.2 nm/min. Thus, the use the RF plasma allows to increase the deposition rate film by 6 times, compared to LPCVD. The shape of grains also changed (Figure 2). At a power of 40 W, the films have spherical and elliptical textures. With power decreasing below 20 W, it turns to columnar texture with a square cross-section. This behavior can be explained by the different kinetics of nuclear centers growth and deposition mechanism. The columnar structure is obtained under more equilibrium conditions (normal growth), and more dense. Whereas the elliptic structure is related to the inclusion of silicon particles formed in plasma. The density of such films is lower.

Values of the refractive index obtained at temperatures of 550-700°C ranged from 3.5 to 5.5 with the change from amorphous phase to polycrystalline.

Figure 2 (a-c). AFM images of silicon films: (a) amorphous and (b,c) textured polycrystalline.
4. Conclusion
In order to achieve efficiency enhancement of thin film-devices, it is desirable to increase structural and optical properties of the film by optimization deposition conditions. A study has been conducted on estimating effects of deposition parameters on surface morphology and optical parameter of silicon films by using plasma-enhanced chemical vapor deposition.

Films of amorphous and polycrystalline silicon on the PECVD-SiO$_2$/Si(100) structure were obtained. Deposition conditions providing grain size control have been identified in the range of 40-140 nm and ensure the control of the shape from nanoscale spherical crystallites to columnar elliptical and squared. The deposition rate of PECVD films was up to 60-90 nm/min, which is several times higher typical rates of low pressure chemical vapor deposition. Results of the investigations have shown that the fine adjustment of the deposition conditions allows to obtain a silicon films with the desired properties (grain size and shape, roughness and refractive index), and increase their stabilized performance and simultaneously increase their deposition rates. It can be used in the design and development of multilayer solar cells and microelectromechanical systems and devices fabrication.

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