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Analysis of ion energy impact on the refractive index of silicon nitride films by use of neural network model

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ABSTRACT

Physical ion bombardment plays a crucial role in determining refractory properties of silicon nitride films. The duty ratio is also a critical parameter that controls the amount of radio frequency power delivered to a plasma. In this study, impacts of duty ratio-induced ion energy on the refractive index are investigated. Silicon nitride films are deposited using a pulsed-plasma enhanced chemical vapor deposition. Ion energy variables and their relationship with the refractive index are studied. We report a decrease of the refractive index with decreasing duty ratio as well as a strong relationship of the refractive index with the ratio of high (or low) ion energy to high ion energy flux. A neural network model is developed to predict the effect of ion energy parameters.

1. Introduction

Due to good thermal stability, high electrical resistivity, and good chemical inertness, silicon nitride (SiN) films have been widely used as anti-reflective layer in manufacturing Si solar cells. Using plasma enhanced chemical vapor deposition (PECVD) or pulsed-PECVD, they have recently been deposited at low temperatures including room temperature [1–10]. The duty ratio in the P-PECVD plays an important role of controlling energy transfer to plasma, thereby changing film properties. Apart from the reduced particle sizes at lower duty ratios, the use of P-PECVD provides higher average charged particle density at the same average power and lower plasma damage during the off-time plasma. Low hydrogen content at room temperature has been reported [6]. Higher deposition rate [7] and smoother surface roughness [10] at lower duty ratio were observed. Among the film properties, the refractive index is an important film quality that determines cell efficiency. The effect of duty ratio on the refractive index has been investigated in a SiH_4–NH_3 plasma [9]. Its role in other plasmas still remains to be explored. The refractive index is considerably influenced by physical ion bombardment through the process of breaking chemical bonds such as [Si–H] or [N–H]. The impact by ion bombardment may differ with ion energy and flux. Therefore, the ion bombardment effect needs to be detailed in view of these variables. Strong dependency of the refractive index on the ion energy flux has been reported [9]. However, this has not been examined for the plasma employed in this study.

As reported from an earlier work [9], certain ion energy variables such as the ion energy flux are closely related to the refractive index of SiN films. Identifying influential ion energy variables may provide useful clues to understanding physical mechanisms and optimizing deposition processes. It is possible to determine nfluential ion energy variables as they are individually investigated given a plasma condition. However, it becomes an extremely difficult task to find out any tendency that can be applied to all plasma conditions of concern in an experiment. This becomes much worse as certain ratios between the variables are examined due to the division of different nonlinearities. This may be circumvented by constructing a prediction model using a neural network technique. The use of the neural network becomes more effective as the number of diagnostic or process variables to model is very large or as the complexity of non-linearity to capture increases. This is mainly attributed to neural network's inherent data processing method, i.e. an adaptive learning by distributive neurons acting as a processor of nonlinear information. This unique feature enables the neural network to process a huge number of input variables such as a data set comprising several thousands of intensities measured by an optical emission spectroscopy. In the context of PECVD of SiN at room

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temperature, the neural network has been applied to build a prediction model of the surface roughness in a SiH_4–NH_3–N_2 plasma [11], the refractive index in a SiH_4–NH_3 [8]or in a SiH_4–NH_3–N_2 plasma [9]. Constructing a neural network model plays a role of extracting additional knowledge about statistical tendencies over a wide range of diagnostic variables. This indicates that by coupling neural network model with experimental data more detailed and plentiful information are able to be acquired. Potential advantages of the combined approach stated are well represented by the recent works [8,9,11].

In this study, we investigate a refractive index from experimental and simulation point of view. SiN films have been deposited using a P-PECVD at room temperature from a SiN_4 and N_2 plasma. Ion energy diagnostics has been conducted and is related to the refractive index with the variation in the radio frequency (rf) source power and duty ratio. A neural network model constructed is utilized to assess the significance of diagnostic variables, composed of ion energy and ion energy flux. Rather than single variable, the model was built with several ratios between the diagnostic variables because both ion energy and flux are involved in deposition simultaneously.

2. Experimental details

SiN films were deposited on p-type, single side polished Si wafers of (100) orientation. The thickness and resistivity of wafers were about 525 ± 25 μm and 1 ~ 30 Ω cm, respectively. Using a P-PECVD operating at a radio frequency of 13.56 MHz, SiN films were deposited. The equipment was explained in greater detail in our recent work [5]. The deposition was conducted in the SiH_4 and N_2 gas as a function of source power in the range of 500–900 W. The bias power was set to zero. For a given source power, the duty ratio was varied from 50 to 90% by 10%. The flow rates of SiH_4 and N_2 gases were set to 8 and 100 sccm, respectively. The deposition time was 5 min. The refractive index measured with ellisometry is examined. Ion energy distribution functions were collected in-situ using an ion energy analyzer (PLASMART^{TM}). One ion energy distribution is shown in Fig. 1. This was collected at 30% and 500 W. Fundamental ion energy variables are indicated in Fig. 1, and they are E_h (high ion energy), E_l (low ion energy), N_h (high ion energy flux) and N_l (low ion energy flux). As shown in Fig. 1, both E_h and E_l represent the location of high and low energy peaks, respectively. The other N_h and N_l correspond to the height of high and low energy peaks, respectively. From them, various ratios were calculated and they are E_h/E_l, E_h/N_h, E_h/N_l, E_l/N_h and E_l/N_l. The relationship between the calculated variables and the refractive index is then modeled.

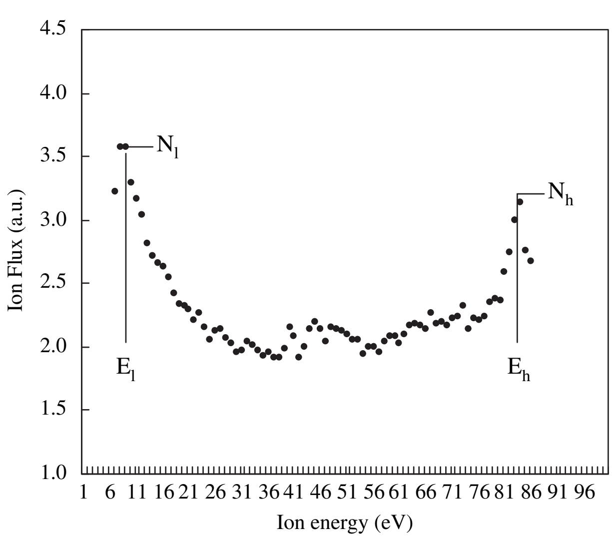

Fig. 1. Ion energy distribution function collected at 500 W source power and 30% duty ratio.

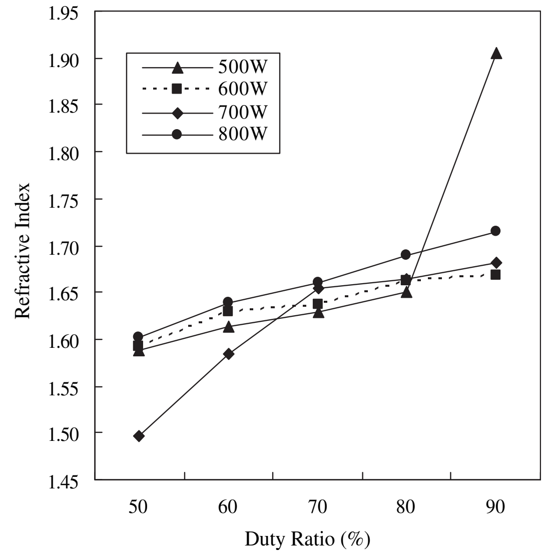

Fig. 2. Impact of duty ratio on the refractive index at fixed source powers.

3. Results and discussion

3.1. Experimental investigation

Fig. 2 shows the effect of source power and duty ratio on the refractive index. The bias power, SiH_4 and N_2 were set to 0 W, 8 and 100 sccm, respectively. As shown in Fig. 2, decreasing duty ratio at 500 W decreases the refractive index and the decrease is the most significant for the decrease from 90 to 80%. A similar phenomenon is observed at other source powers. Meanwhile, close relationships between the refractive index and the atomic Si/N or [Si–H]/[N–H] have been reported [12,13]. The decrease of the refractive index at lower duty ratio indicates the formation of N-rich film with higher [N–H] than [Si–H]. It is noted that less energy is required to break [Si–H] due to its lower bonding strength. Under given ion bombardment, more Hs are released from the [Si–H] than the [N–H]. The excess Hs are subsequently bonded to the dangling N, resulting in a larger [N–H] and hence a smaller refractive index.

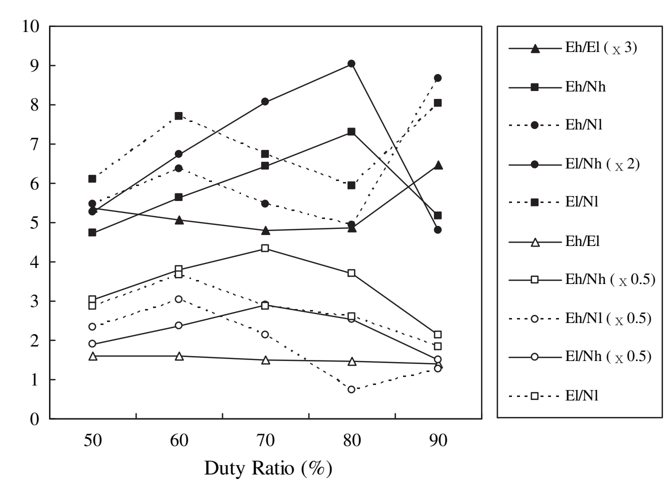

Fig. 3. Ion energy variables as a function of the duty ratio (closed symbols: 500 W, opened symbols: 600 W).