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Depth-resolved correlation between physical and electrical properties of stressed SiN_x gate insulator films

Jin-Seong Park · Chang Woo Lee · Jae Jin Yoon · Kwun-Bum Chung

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Abstract The physical and electrical properties of SiN_x gate insulator films with compressive and tensile internal stress have been investigated using various characterization techniques. The mechanical hardness measured by nano-indenter system showed the different distribution in the film depth direction according to the type of film stress. The uniformity of optical property inside films had a correspondence to the mechanical properties of stressed SiN_x films, as well. The contents and bonding states of hydrogen influenced the mechanical and optical properties of stressed SiN_x films. The leakage characteristics of tensile SiN_x films with uniform physical properties exhibited the lower current density than the compressive films with ~10^{-7} A/cm^2 until 8 MV/cm. The correlation between physical and electrical properties depending on the internal stress will suggest the appropriate optimization of SiN_x gate insulator films to enhance the device performance and reliability.

J.-S. Park
Department of Materials Science and Engineering, Dankook University, Dongnamgu Anseodong 29, Cheonan 330-714, South Korea

C. W. Lee
Department of Nano & Electronic Physics, Kookmin University, Seoul 136-702, South Korea

J. J. Yoon
Nano-Optical Property Laboratory and Department of Physics, Kyung Hee University, Seoul 130-701, South Korea

K.-B. Chung (✉)
Department of Physics, Dankook University, Dongnamgu Anseodong 29, Cheonan 330-714, South Korea
e-mail: kbchung@dankook.ac.kr

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1 Introduction

Silicon nitride (SiN_x) films are widely applicable as passivation films of semiconductor devices and a gate insulator of thin-film transistors (TFTs) for various device architectures including liquid crystal display (LCD) and light emitting diodes (LED) due to good dielectric property and thermally stability [1–5]. Several reports have studied the physical characteristics of SiN_x films deposited by plasma enhanced chemical vapor deposition (PECVD) depending on the deposition conditions [6–8]. These papers have focused on the variation of stress in SiN_x films, such as tensile and compressive stress, by the changes in the plasma conditions and the introduced amount ratio of process gases like SiH_4 and NH_3. In the fabrication of thin-film device, the internal stress of SiN_x films is very important factor because the type of stress and excessive stress may cause cracking and peeling in device structure, which are detrimental to the device operation [6]. Moreover, the device performance and reliability of TFT using SiN_x gate insulator films are strongly governed by the quality of film, such as stress and composition.

In this letter, we report the correlation between physical and electrical characteristics of SiN_x gate insulator films with different internal stress. In particular, the mechanical hardness, optical property, and hydrogen distribution investigated as a function of film depth. In addition, the bonding characteristics of hydrogen were examined according to film internal stress. The physical uniformity in the depth direction and different hydrogen bonding states of SiN_x films with tensile and compressive internal stress

Table 1 Deposition conditions and resulting properties of SiN_x films with compressive and tensile stress

	Deposition conditions						Film properties		
	Power (W)	SiH_4 (SCCM)	NH_3 (SCCM)	N_2 (SCCM)	Temperature (°C)	Pressure (Torr)	Stress (MPa)	Si (%)	N (%)
C1-SiN_x	650	25	125	1000	350	2	−890	48.5	51.5
C2-SiN_x	650	25	125	1000	350	3.5	−1419	47.2	52.8
T1-SiN_x	150	25	125	400	350	2.1	333	51.4	48.6

induces the electrically different properties as a gate insulator.

2 Experiments

P-type Si(100) wafers were chemically cleaned using the standard reduced calcium aluminate (RCA) method, which removes organic and metallic residues, resulting in the formation of a 1~2 nm thick SiO_2 layer. After the RCA cleaning, Si wafers were then dipped in a dilute HF solution to remove the SiO_2 layer. The stressed SiN_x gate insulator films with the thickness of 100 nm were grown on Si substrate by plasma enhanced chemical vapor deposition (PECVD) at the substrate temperature of 350°C. In order to systematically analyze the correlation between physical and electrical properties depending on film stress, the compressive SiN_x films with low (−890 MPa; C1) and high (−1419 MPa; C2) stress, and the tensile SiN_x film (333 MPa; T1) were prepared. The detailed deposition condition and corresponding properties of SiN_x films are summarized in Table 1. The film stress is mainly modulated by plasma power and amount of introduced N_2 gas during CVD process [9]. The given stress of SiN_x films after deposition was determined by measuring the curvature change of pre- and post-deposition of the films. The compositions of Si and N except hydrogen were examined using x-ray photoemission spectroscopy (XPS). The mechanical hardness of SiN_x films in the depth direction was performed by the nano-indentation measurement with vertical load resolution of 1 nN and vertical displacement resolution of 0.04 nm [10, 11]. The optical properties of grown film were measured by vacuum ultraviolet spectroscopic ellipsometry (VUV-SE) in the energy range from 0.75 to 8.5 eV with incident angles of 50˚, 60˚, and 70˚. The system uses a rotating analyzer with an auto retarder. To cover wide spectral range, Xenon arc and Deuterium lamp was used as a light source. The hydrogen contents and bonding states were examined by time-of-flight secondary ion mass spectroscopy (TOF-SIMS) and Fourier transform-infrared (FT-IR) analysis, respectively. To evaluate the difference of leakage current for SiN_x gate insulator films, the current-voltage (I–V) characteristics were investigated with metal-SiN_x films-semiconductor structure.

3 Results and discussion

Figure 1 shows the mechanical hardness of stressed SiN_x films as a function of indent penetration depth, measured by using a nano-indenter system. Penetration depth was controlled by the vertically loaded force and mechanical hardness was determined by the ratio of the maximum load to the projected contact area. The contact area was estimated from indenter probe calibration and the loaded force were calculated by fitting the following power law relation; $P = A\,(h-h_f)^m$ where A and m are arbitrary fitting parameters, h and h_f are the penetration depth and final penetration depth, respectively [11]. The hardness of compressive SiN_x film with low stress (C1) monotonically decreases in the depth direction. The changes in hardness of compressive SiN_x film with high stress (C2) according to depth direction appear the larger fluctuation with the

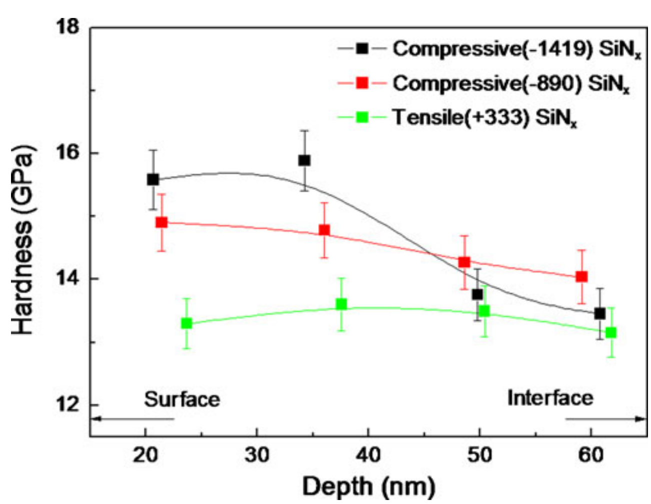

Fig. 1 Mechanical hardness changes of compressive SiN_x films with low (−890 MPa; C1) and high (−1419 MPa; C2) stress, and tensile (333 MPa; T1) stress in the depth direction, measured by a nano-indentor system. Arrows indicate the film surface and interface direction

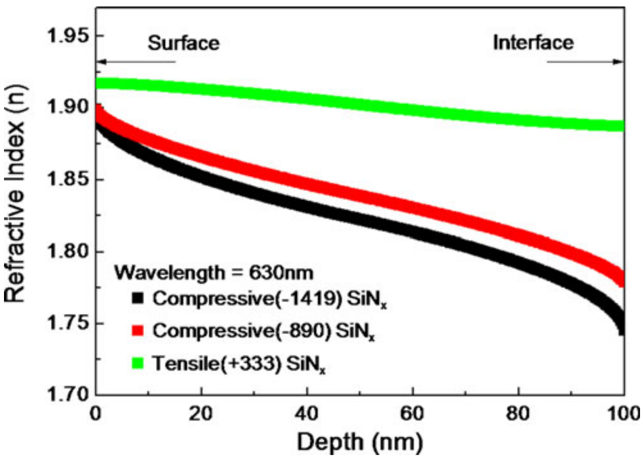

Fig. 2 Changes in refractive index (n) values of SiN_x films with compressive and tensile stress as a function of film depth. Arrows indicate the film surface and interface direction

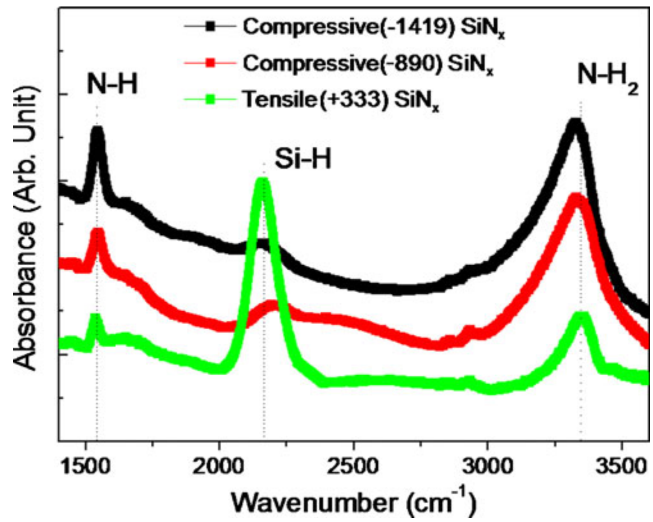

Fig. 4 FT-IR absorption spectra of SiN_x films with compressive and tensile stress

deviation of approximately 2 GPa through. On the other hands, the tensile SiN_x film has the similar hardness values through the whole film, regardless of film depth. These results indicate that the mechanical hardness in the depth direction depends on the given stress of SiN_x films by the different deposition conditions. Also, the tensile SiN_x film has more uniform distribution of hardness inside films, rather than the compressive films.

To obtain the optical properties, such as the complex refractive index (n, k) and dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$), Tauc Lorentz model dielectric function was applied for VUV-SE measurement data with multilayer structure comprised of graded layers [12]. Figure 2 shows the changes of refractive index (n) in the depth direction of SiN_x films, which was extracted from the physical values of each layer in the graded model structure. The obtained optical thicknesses from modeling are approximately 95 nm, 104 nm, and 102 nm for C1, C2, and T1-SiN_x films, which are well-matched with the results measured by ion scattering. The refractive index of tensile SiN_x film has slightly high value through the whole film, as compared to that of compressive films. This could be caused by the difference of Si/N composition ratio as shown in Table 1, which shows the slightly larger Si/N ratio in tensile SiN_x film with high refractive index [9]. In addition, similar to the results of mechanical hardness, the SiN_x film with tensile stress have more uniform depth profile of refractive index, than the films with compressive stress. The complex refractive index (n, k) is closely related to the density of films and the dielectric function ($\varepsilon = \varepsilon_1 + i\varepsilon_2$), which can affect the changes in electronic, ionic, and space charge polarization [13]. Therefore, the tensile SiN_x

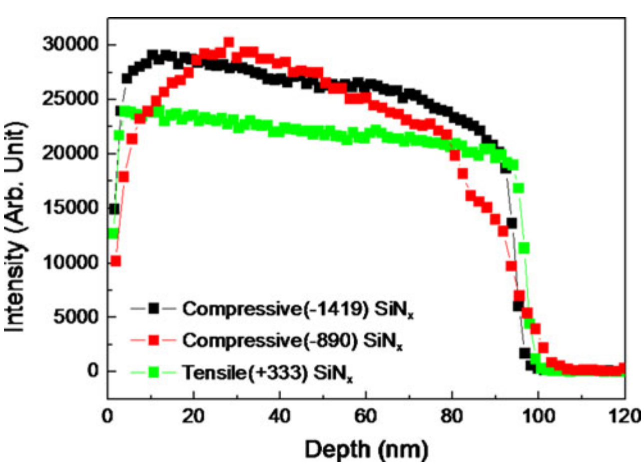

Fig. 3 TOF-SIMS depth profiles of SiN_x films with compressive and tensile stress

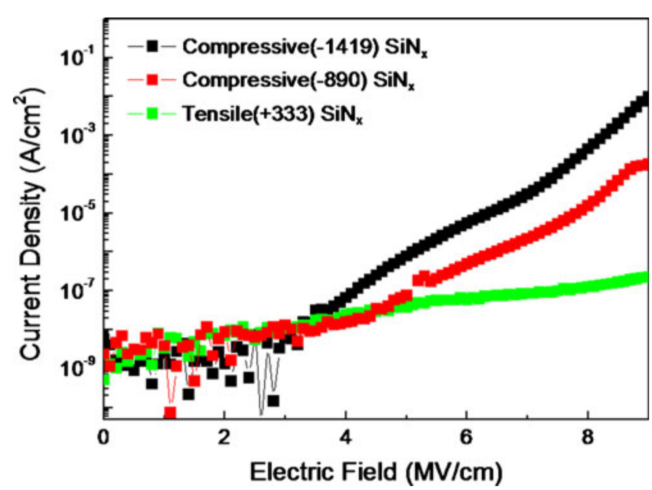

Fig. 5 Current density-Electric field (J-E) characteristics of SiN_x films with compressive and tensile stress

film with smaller fluctuation of refractive index might represent the better physical properties with the uniform film density and distribution of dielectric properties as a function of film depth, which can affect the performance of a gate insulator.

Figure 3 shows the results of TOF-SIMS depth profile for the measurement of hydrogen contents. The compressive SiN_x film has the larger contents of hydrogen through the entire films. Moreover, the hydrogen distribution of tensile SiN_x film in the depth direction is more uniform, rather than the compressive film. More contents of hydrogen in the compressive SiN_x films exhibit non-uniform distribution of hydrogen in the depth direction, even if the uniformity of hydrogen between films with low and high compressive stress shows a little inconsistency. In addition to the film composition, the contents of hydrogen are related to refractive index and stress of SiN_x films [1, 9]. The control of hydrogen in SiN_x films is key processing in device characteristics because hydrogen can be associated with detrimental effects such as negative-bias-temperature instability (NBTI), radiation induced interface traps, and oxide charges [14]. As considered the physical properties of SiN_x films with the depth profile of hydrogen, the distribution and contents of hydrogen in the film depth reveals the correspondence to the physical uniformity of films with different internal stress.

In order to analyze the bonding characteristics of hydrogen with hydrogen contents, FT-IR measurement was performed as shown in Fig. 4. The compressive SiN_x films (C1 and C2) represent the smaller Si-H absorption peaks and higher N-H and N-H_2 absorption intensities than the tensile film. The interesting finding is that the overall N-H absorption intensities are increased, as the SiN_x films become more compressive. The amount ratio of Si-H and N-H bonding states could causes the physical change in film density [15]. As compared to the result of hydrogen contents in Fig. 3, this implies that the contents and bonding states of hydrogen could be the origin which induces the changes in mechanical and optical properties of stressed SiN_x films in the film depth direction.

The electrical characteristics in relation to the different physical properties of SiN_x films were investigated by current-voltage (I–V) measurement as a function of film stress. Figure 5 shows the current density-electric field (J-E) characteristics of compressive and tensile SiN_x films, respectively. The compressive SiN_x film have higher leakage current density at the electric field above 4 MV/cm. As the SiN_x films become more compressive, the leakage characteristic shows the higher current level. As compared to changes in mechanical hardness and optical property as a function of film depth, in addition to the contents and bonding states of hydrogen, the tensile SiN_x film with uniform depth profile through the entire film lead to the better leakage characteristics. This correlation between physical and electrical properties means that the physical uniformity of film depending on the film stress can affect the electrical properties of its film and device. Therefore, the modulation of film stress could be important to control of physical and electrical properties of the SiN_x gate insulator film and to enhance the device performance and reliability.

4 Conclusion

The physical and electrical properties of SiN_x gate insulator films with compressive and tensile internal stress have been investigated. As SiN_x films become more compressive, the mechanical hardness of film has the larger fluctuation with the deviation of approximately 2 GPa between film surface and interface. However, the tensile film in the depth direction represent the uniform distribution of hardness. The refractive index of tensile SiN_x film has higher and more uniform in the depth direction, rather than the compressive film. The contents and distribution of hydrogen are smaller and uniform in tensile SiN_x film. The Si-H bonding is dominant bonding states of hydrogen in the tensile film. These characteristics of hydrogen could have an effect on the changes in physical properties of stressed SiN_x films. In addition, the electrical characteristics, evaluated by the result of current density-electric field (J-E) are strongly related to the mechanical and optical properties of SiN_x films with different stress. The uniform distribution of physical film properties has a key role of obtaining the better electrical performance. The correlated results between physical and electrical properties depending on the stress could be anticipated the appropriate optimization of Si-based gate insulator films to enhance the device performance and reliability in field effect thin film transistor (FE-TFT).

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