Available online at www.sciencedirect.com

SCIENCE DIRECT®

Thin Solid Films 478 (2005) 256–260

thin solid films

www.elsevier.com/locate/tsf

Characterization of bias magnetron-sputtered silicon nitride films

S. Guruvenket[a], Jay Ghatak[b], P.V. Satyam[b], G. Mohan Rao[a,*]

[a]Department of Instrumentation, Indian Institute of Science, Malleswaram, Bangalore 560 012, India
[b]Institute of Physics, Bhubaneswar 751 005, India

Received 14 February 2004; received in revised form 7 October 2004; accepted 25 October 2004
Available online 26 November 2004

Abstract

Influence of the deposition parameters and the substrate bias voltage on the optical, compositional and the surface properties of DC magnetron-sputtered silicon nitride thin films are studied. Silicon nitride thin films are deposited on silicon (100) and quartz substrates at different partial pressures of nitrogen and discharge currents. The variation in the refractive index and the optical band gap of these films is studied. Compositional variation has been studied using Rutherford backscattering spectroscopy (RBS). Silicon nitride thin films deposited at 3×10^{-2} Pa partial pressure of nitrogen with 2.5 mA/cm^2 cathode current density showed an optical band gap of 4.3 eV and refractive index of 2.04 (at 650 nm). Nitrogen to silicon ratio in the film is 1.31, and the roughness of the films is 2.3 nm. Substrate bias during deposition helped in changing the optical properties of the films. Substrate bias of −60 V resulted in films having near stoichiometry with N/Si ratio 1.32, and the optical band gap, refractive index, and the roughness are 4.8 eV, 1.92 and 0.78 nm, respectively.

Keywords: Magnetron sputtering; Silicon nitride; Ion-assisted deposition; Substrate bias; Rutheford backscattering

1. Introduction

Silicon nitride is an important material in the fabrication of the microelectronic devices [1]. Its properties, like high thermal stability, chemical inertness, hardness, and good dielectric behavior, make it more attractive and most commonly used material [2]. Transparency of silicon nitride over a wide spectral range from near-ultraviolet (UV) to infrared (IR) region along with the passivating property makes it suitable for many optical applications [3]. Conventionally, silicon nitride thin films are deposited at high substrate temperatures (700–900 °C) by chemical vapor deposition (CVD) [4]. In most of the abovementioned applications, a low-temperature deposition is preferred. However, films deposited with the low-temperature CVD technique show hydrogen entrapment, which deteriorates the properties of the silicon nitride thin films [5]. Several low-temperature techniques, like plasma-enhanced CVD and reactive sputtering, etc., have been adopted to deposit silicon nitride thin films.

Reactive sputtering at low temperature has been found to be the best alternative, which can result in films with minimum hydrogen content [6]. In sputter deposition, additional ion assistance during the film growth helps in improving the properties of the growing film. Ion assistance can be accomplished either by using a separate ion source (ion-beam-assisted deposition) or by biasing the substrate during deposition (bias sputtering).

In the present study, we investigated the effect of the substrate bias and the influence of the partial pressure of nitrogen gas, together with cathode current density on the optical, surface, and compositional properties of silicon nitride thin films prepared by DC-reactive magnetron sputtering. We correlate the composition and microstructure of the deposited films to the observed changes in the properties of the films, which are due to substrate bias effects.

* Corresponding author. Tel.: +91 80 2932349; fax: +91 80 3600135.
E-mail address: gmrao@isu.iisc.ernet.in (G.M. Rao).

0040-6090/$ - see front matter © 2004 Elsevier B.V. All rights reserved.
doi:10.1016/j.tsf.2004.10.031

2. Experiment section

We used a homemade magnetron-sputtering system for this study. A planar silicon disk (99.99% pure and 100 mm diameter) is mechanically clamped to the magnetron sputtering cathode assembly. The ultimate pressure obtained in the sputtering chamber is 10^{-3} Pa using a combination of diffusion and rotary pump. Sputtering was done in $Ar+N_2$ mixed gas, and the total pressure during the sputtering was maintained at 10^{-1} Pa. The partial pressures of the two gases are controlled individually. The distance between the substrate and the target is maintained at 100 mm. Polished Si (100) (p-type, 10 Ωcm resistivity) was used as the substrate, which was maintained at the ambient temperature without any deliberate heating. For the optical studies, films were deposited on quartz substrates. The deposition was carried out at different partial pressures (2×10^{-2}, 3×10^{-2}, and 4×10^{-2} Pa,) of nitrogen while maintaining the total pressure at 10^{-1} Pa and at different cathode current density of 1.9, 2.5, and 3.10 mA/cm^2. A bias potential was applied to the substrate and varied in steps of 20 V from 0 to −120 V for the films deposited at 3×10^{-2} Pa partial pressure of nitrogen and with the cathode current density of 2.5 mA/cm^2. Optical characterization of the silicon nitride films was carried out using Fourier transform infrared (FTIR) spectroscopy (Perkin-Elmer) with 2 cm^{-1} resolution and UV–VIS spectroscopy (Hitachi 330A). Compositional analysis of the films was carried out using Rutherford backscattering spectroscopy (RBS), using 2 MeV, He^+ ion beam. Spectra were analyzed using GISA simulation code [7]. Surface roughness of the films was measured using atomic force microscopy (AFM). Thickness of the silicon nitride films used in this studies varied from 270 to 300 nm (measured using the stylus profiler).

3. Results and discussion

3.1. Spectral studies

FTIR spectra have been used as the basic tool for identifying silicon nitride formation in the films deposited under different conditions. All the spectra recorded have been corrected for the absorption due to substrate. Fig. 1 shows the FTIR spectra of the silicon nitride films deposited at a cathode current density of 2.5 mA/cm^2 with nitrogen partial pressure of 2×10^{-2}, 3×10^{-2}, and 4×10^{-2} Pa. These spectra show a small absorption band around 3340 cm^{-1}, which corresponds to hydrogen bonding groups. As no hydrogen-based gas has been used in the process, this band could be due to the water vapor absorption in the silicon nitride films after the deposition [8]. Fig. 2 shows the FTIR spectra of silicon nitride thin film deposited at 3×10^{-2} Pa partial pressure of nitrogen and cathode current density of 2.5 mA/cm^2 at different

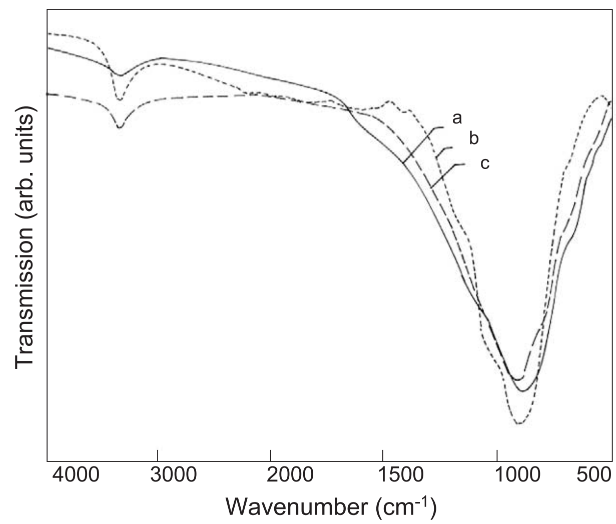

Fig. 1. FTIR spectra of the silicon nitride film deposited at different nitrogen partial pressures (a) 2×10^{-2}, (b) 3×10^{-2}, and (c) 4×10^{-2} Pa.

substrate bias voltages. In the case of ion-assisted deposition, it has been generally observed that the packing density will be high, and hence the water vapor absorption would be less. It can be observed from Fig. 2 that, with the increase in the bias voltage, there is no absorption band at 3340 cm^{-1}. It can also be observed that only the films deposited at higher negative bias voltage (above −40 V) show absorption band at 2190 cm^{-1}, which is due to Si–N_2 stretching band [9]. All the films showed an absorption band in the range 840–870 cm^{-1}, which corresponds to the stretching vibration mode of the Si–N bond. In Fig. 2, it can be noticed that, with increase in the substrate bias voltage, the absorption band of Si–N shifts towards the higher energy value. This shift could be due to the increased nitrogen incorporation in the film.

Optical band gap of the silicon nitride films has been calculated from the optical spectra using the Tauc's relation [10].

$$(\alpha h\nu)^{1/2} = A\left(h\nu - E_g\right),$$

where α is the absorption coefficient, A is a constant, hν is the photon energy, and E_g is the band gap. Optical band gap value for the films deposited at various conditions is shown in Table 1. It can be seen from Table 1 that, at lower cathode current density, lower optical band gap value of 2.5 eV is obtained. With increase in the partial pressure of nitrogen and cathode current density, optical band gap value increased up to 4.5 eV. Variation in the band gap as the function of the substrate bias voltage for the films deposited at the cathode current density of 2.5 mA/cm^2 and 3×10^{-2} Pa partial pressure of nitrogen is shown in Fig. 3. When the substrate bias voltage is increased, it is observed that the optical band gap value increases gradually from 4.3 eV and attains a constant value around 4.8 eV at the bias voltage of −60 V, which is much closer to the optical band gap of the