Optical investigation of $Si:SiO_2/SiO_2$ film

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The optical properties of 30-layer $[nc\text{-}Si:SiO_2/ SiO_2]_{30}$ periodic films have been studied. The films were prepared by alternately evaporating SiO and SiO_2 onto Si(100) substrates, followed by annealing at 1100 °C. Spectroscopic ellipsometry spectrum analysis was used to deter-mine the optical constants of the samples via the Forouhi–Bloomer model. The optical bandgap of a single periodic film is calculated. The photoluminescence (PL) spectra of three samples with different thicknesses clearly show that there are two physical origins of the PL process.

Keywords: Optical; Si; Oxide.

1. INTRODUCTION

Silicon is an indirect bandgap semiconductor with a forbid-den gap width of 1.12 eV. Its irradiance efficiency is so low that silicon is commonly regarded as an inefficient photo- electronic material in the visible range, and its application in this field is limited. In 1990, Canham found that porous sili-con produced strong visible radiation (1 %) under excitation at room temperature [1]. There has also been considerable research work on the irradiance efficiency of nanocrystalline silicon (nc-Si) in the visible and near-infrared ranges [2–4]. This work indicates that it is feasible to prepare nc-Si materials for photoelectronic device applications. This type of nanostructured silicon material has therefore become an active research area. Many preparation methods for nc-Si have been adopted, including Si ion injection into SiO_2, the use of a Si/SiO_2 superlattice structure [5], and Si and SiO_2 cosputtered films. The nc-Si/SiO_2 periodic multilayered film structure has been chosen as an ideal prototype to investigate the quantum confinement effect, because the sizes and contributions of the Si quantum dots can be controlled well in the superlattice structure. The fabrication process is compatible with standard ultra-large-scale integrated (ULSI) cir-cuit processes [6]. Xie reported the enhanced irradiance of Si/SiO_2 superlattice structure samples [7, 8]. In this article, spectroscopic ellipsometry (SE) analysis is adopted to study the optical properties of a single $[nc\text{-}Si:SiO_2/SiO_2]_n$ periodic multilayered film [9], including its optical bandgap and photoluminescence (PL) mechanism.

2. EXPERIMENTAL

The [SiO/SiO_2]n periodic multilayer film with 30 periods of 3 nm-thick SiO layers and 5 nm-thick SiO2 layers was prepared by electron-beam evaporation, alternating between the two target materials, SiO and SiO2, onto a Si(100) substrate in a high vacuum. The Si(100) substrate was cleaned by a normal ultrasound process with acetone, alcohol, and deionized water step by step in 45 min. The native oxide
3 nm-thick thin layer is still present covered upon the Si(100) substrate. In the experiments, the background pressure in the chamber was 2 10−4 Pa, the evaporation rate was controlled with a speed of 0.5 nm/s, and the film thickness was monitored using a quartz oscillator during evaporation. Thermal treatment was then performed in a quartz tube furnace in a nitrogen ambient at 1100 ◦C for 30 min.

3. RESULTS AND DISCUSSION

The Forouhi–Bloomer model (FB model), which is used to analyze the optical properties of various systems, was pro- posed by Forouhi and Bloomer [10, 11]. The expression of the extinction coefficient *k* is derived from the single electron model lifetime, which in the excited state is limited. Then the expression for the refractive index *n* can be obtained according to the Kramers–Kronig relation.
The abscissa position of the *k(E)* spectrum can be fixed by *B/*2, and the value of *C* is a little larger than the square of *B/*2; the peak value of the *k(E)* spectrum can thus be determined by both *B* and *C*. To obtain all of the optical properties of the [nc-Si:SiO_2/SiO_2]$_{30}$ sample film, experimental ellipsometric spectra are calculated from a regression analysis using a three-layered model, assuming an ambient/film/substrate (AFS) structure. Here, the [nc-Si:SiO_2/SiO_2]$_{30}$ film can be deemed to be a well-proportioned single-layer film system for the 280 nm to 820 nm wavelength range under study, although the actual film contains 30 periods of 3 nm-thick nc-Si:SiO_2 and 5 nm-thick SiO_2 alternating layers. This avoids the difficulty and complexity involved in performing the calculations layer by layer and by including the defects between the interfaces in the film. Also, the main aim is to obtain the optical proper- ties and optical bandgap for the whole film. The PL spectrum of the sample film excited at a wavelength of 300 nm at room temperature is shown in Fig. 1.
The peak energy located at 1.68 eV is higher than that of the previous work [12], but is less than the optical bandgap of 1.845 eV calculated from the SE data. This energy difference of 0.165 eV is close to the energy of 0.135 eV at the Si–O vibration peak of the nc-Si embedded in the SiO2 matrix in the sample film [13]. This indicates that the nc- Si/SiO2 interface plays an important role in the light emission. Consideration of the influence of the exciton effect induced by the quantum confinement effect indicates that this difference is reasonable [14].

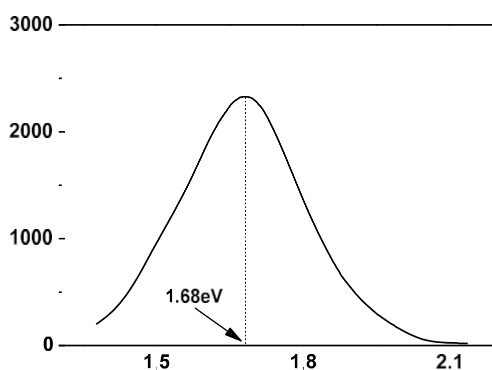

Figure 1 PL spectrum of the sample excited at a wavelength of 300 nm at room temperature

The curves of the 2 nm-thick nc-Si:SiO_2 layered sample and the 5 nm-thick nc-Si:SiO_2 layered sample can then be decomposed as shown in Fig. 2. The two peaks overlap for the curve of the 3 nm-thick nc-Si:SiO_2 layered sample and, therefore, there is no discernable shoulder.

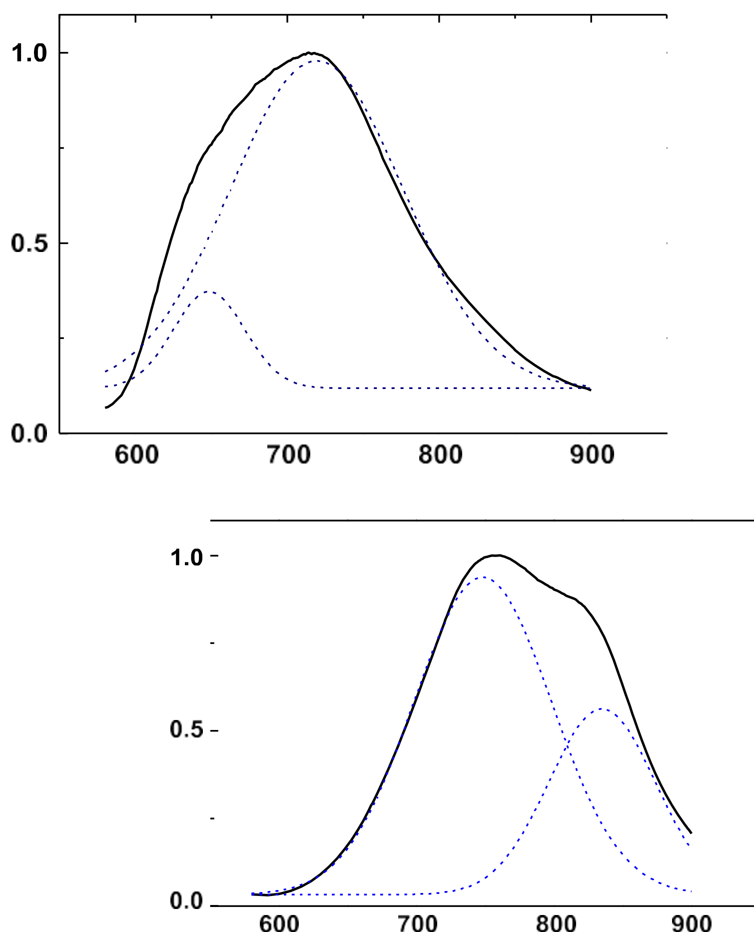

Figure 2 Decomposition of PL spectra of the samples with nc-Si:SiO_2 layer thickness of (**a**)2 nm, (**b**)5 nm

4. CONCLUSIONS

A [nc-Si:SiO_2/SiO2]30 periodic film was prepared by alternately evaporating 30 periods of 3 nm-thick SiO and 5 nm- thick SiO2 layers onto a Si(100) substrate, followed by annealing. An optical bandgap of 1.845 eV was calculated ac- cording to the relationship between $(ah\nu)^{1/2}$ and the pho- ton energy E of the [nc-Si:SiO_2/SiO_2]30 film. There is a 0.135 eV band-gap difference between the calculated and experimental values for the Si–O vibration of the nc-Si embedded in the SiO_2matrix. The interface between nc-Si and SiO_2 plays an important role in the PL process, and two competing processes, the QCLC process and the QC process, are observed. The former process dominates the PL characteristics.

References

[1] L.T. Canham, Appl. Phys. Lett. 57, 1046–1048 (1990)
[2] L. Pavesi, L. Dal Negro, C. Mazzoleni, G. Franzo, F. Priolo, Na-ture 408, 440–444 (2000)
[3] B. Zheng, J. Michel, F.Y.G. Ren, L.C. Kimerling, D.C. Jacobson, J.M. Poate, Appl. Phys. Lett. 64, 2842–2844 (1994)
[4] [D. Kovalev, H. Heckler, G. Polisski, F. Koch, Phys. Status Solidi B 215, 871–932 (1999)
[5] M. Zacharias, J. Heitmann, R. Scholz, U. Kahler, M. Schmidt, J. Blasing, Appl. Phys. Lett. 80, 661–663 (2002)
[5] L. Needs, K. Willams, Exp. Theo. NANOTECHNOLOGY 4 (2020) 93
[6] Z.Q. Xie, J. Zhu, M. Zhang, Y.Y. Zhao, M. Lu, Appl. Surf. Sci. 255, 3833–3836 (2009)
[7] Z.Q. Xie, D. Chen, Z.H. Li, Y.Y. Zhao, M. Lu, Nanotechnology 18, 115716 (2007)
[8] L.Y. Chen, X.W. Feng, Y. Su, H.Z. Ma, Y.H. Qian, Appl. Opt. 33, 1299–1305 (1994)
[9] A. M. Ahmed Alwaise, M. Ibrahim Alwiase, A. Y. Qasim, Exp. Theo. NANOTECHNOLOGY 4 (2020) 99
[10] A. Hassani, S.A. Hussain, N. Abdullah, S.Kmaruddin, M.K.Alomar, A. Rasedee, M. Al-Qubaisi, R. Rosli, Exp. Theo. NANOTECHNOLOGY 4 (2020) 109
[11] M.N. Kamalasamnan, S. Chandra, P.C. Joshi, A. Mansingh, Appl. Phys. Lett. 59, 3547–3549 (1991)
[12] Y. Liu, T.P. Chen, Y.Q. Fu, M.S. Tse, J.H. Hsieh, P.F. Ho, Y.C. Liu, J. Phys. D, Appl. Phys. 36, L97–L100 (2003)
[13] L. Ding, T.P. Chen, Y. Liu, C.Y. Ng, S. Fung, Phys. Rev. B 72, 125419 (2005)

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