Spectroscopic ellipsometry studies of nanocrystalline silicon in thin-film silicon dioxide.

G. E. Jellison, Jr., C. M. Rouleau, S. P. Withrow, C. W. White, Oak Ridge National Laboratory, Oak Ridge, TN, and C. O. Griffiths, Hinds Instruments, Inc., Hillsboro, OR.

It has been known for many years that nanocrystalline silicon (nc-Si) can be formed in silicon dioxide (SiO_2) by ion implantation followed by thermal annealing. The nc-Si/SiO_2 composite material has many interesting properties, including a broad luminescence spectrum between 700 and 900 nm when the sample is illuminated with UV light. Recent reports [i.e., L. Pavesi, et. al., Nature **408**, 440-444 (2000)] have shown that nc-Si/SiO_2 exhibits optical gain, which may make this material a candidate for the lasing medium in a Si-based laser. However, mainly due to its complexity, there has been little work on its linear optical properties.

In this paper, we examine samples of nc-Si/SiO_2 fabricated by ion implanting a uniform silicon concentration into a thin film of SiO_2 followed by an 1100 °C anneal for 1 hr in flowing Ar+4%H_2 to produce nc-Si in the SiO_2 matrix. The samples will be characterized using Rutherford backscattering and photoluminescence. However the main focus of the present work is spectroscopic ellipsometry measurements of the samples performed using the 2-modulator generalized ellipsometer (2-MGE). The complexity of the nc-Si/SiO_2 material requires that the optical model used in the analysis of the ellipsometric data include at least 4 layers: a surface roughness or transition layer, the primary layer, which can be modeled using a Maxwell-Garnett effective medium approximation of strained SiO_2 and amorphous-like inclusions, a transition layer, and the crystalline silicon substrate. The results of this analysis are spectroscopic optical functions of both the nc-Si/SiO_2, as well as an estimate of the optical functions of the nc-Si inclusions. For example, a preliminary determination of the refractive index of 10% nc-Si/ 90% SiO_2 material shows that it is only slightly higher than that of bulk SiO_2 (1.527 for nc-Si/SiO_2 compared to 1.458 for SiO_2 at 600 nm).