Optical properties of low pressure chemically vapor deposited silicon oxynitride films from $SiCl_2H_2$-NH_3-N_2O mixtures

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In this work results are reported on our investigation of the optical properties of low pressure chemically vapor deposited (LPCVD) silicon oxynitride films deposited from $SiCl_2H_2$-NH_3-N_2O gas mixtures. This investigation has been made with the aid of a physical model proposed by Forouhi and Bloome (FB) (1) to describe the optical dispersion in amorphous semiconductors and dielectrics. Theoretical reflection spectra of the system oxynitride film/silicon substrate were generated and fitted to those experimentally recorded. It was shown that the FB model describes satisfactorily the refractive index dispersion of these films and, moreover, it is able to provide an approximate picture of the energy distribution of the density of states near the absorption edge.

Oxynitride films were deposited on RCA cleaned (100) 4 in. Si wafers in a conventional LPCVD reactor at 812 ^oC and 230 mTorr from $SiCl_2H_2$-NH_3-N_2O gas mixtures with variable compositions. Depositions were carried out keeping the flows of $SiCl_2H_2$ and of NH_3 constants at 20 and 60 sccm respectively while that of N_2O was varied from 0 to 180 with increments of 60 sccm.

The physical model used to simulate the optical dispersion of the SnO_2 films (FB model) (1) considers the electronic structure of disordered insulators to be described by two parabolic bands (valence and conduction bands) separated by an energy gap, E_g. Within the FB model the dispersion of the real, n, and imaginary, k, part of the refractive index are given as functions of the energy gap, the distance between the gravity centers of the two parabolic bands, B, their magnitude and the lifetime of electronic transitions. Thus, once the above parameters determined from the fit of the theoretically calculated to the experimentally recorded reflection spectra, except of the dispersions of n and k, an approximate picture of the density of states (DOS) near the band gap is obtained.

The mathematical description of the reflection spectrum of a homogeneous and smooth film deposited on an absorbing substrate was taken from the literature. The fit of the calculated spectra to those recorded has been made using standard regression analysis techniques and yielded, except of the FB parameters, also the film thickness.

In Fig. 1 are shown the calculated spectra for a film deposited with an N_2O flow of 60 sccm together with the corresponding experimental one. It is observed that the two spectra are in satisfactory agreement indicating the suitability of the physical model to describe the optical dispersion of silicon oxynitride LPCVD films. In Fig. 2 are shown the energy dispersions of the real (upper) and imaginary (lower figure) parts of the refractive index of four films deposited with various N_2O flows.

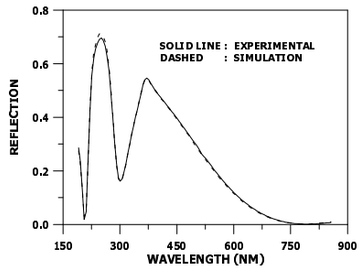

Fig. 1. Experimentally recorded and calculated reflection spectra of a silicon oxyntride film deposited with an N_2O flow of 60 sccm.

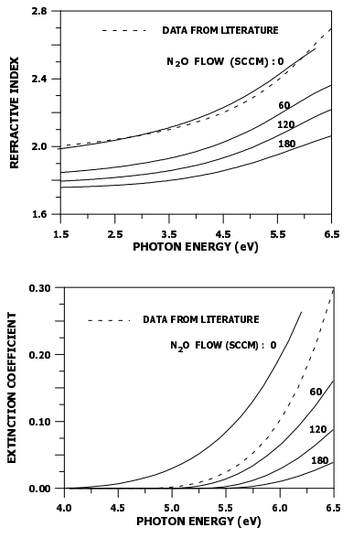

Fig. 2. Dispersion of the real (upper) and imaginary (lower) part of the refractive index of four samples deposited with various N_2O flows.

In Fig. 3 the energy distribution of the DOS, designed using the FB parameters, as obtained from fits like those in Fig. 1, for a silicon nitride LPCVD film is shown, together with the corresponding calculated for the crystalline material (2). It is observed that the overall features of the DOS are well reproduced by the FB model.

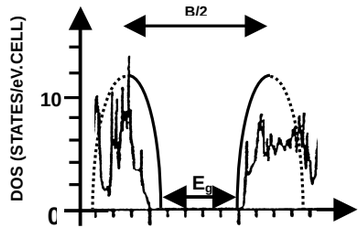

Fig. 3. Density of electronic states (DOS), as predicted by the FB model, for an LPCVD silicon nitride sample. The DOS for crystalline Si_3N_4 (2) is also shown.

In conclusion, it was shown that the FB model describes satisfactorily the refractive index dispersion of silicon oxynitride films and also provides an approximate picture of the energy variation of the DOS near the band gap coherent with theoretical calculations.

1. R. Forouhi and I. Bloomer, Phys. Rev B34 7018 (1986).
2. Y.-N. Xu and W. Y. Ching, Phys. Rev. B 51, 17379 (1995).