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Structural and optical properties of sputtered gadolinium nitride films

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Abstract

Rare-earth (RE) materials have high magnetic moments and form a wide range of magnetic structures. There has been speculation in the literature that rare-earth nitrides may form half-metallic ferromagnetics. This is surprising because, based on a simple ionic model, trivalent rare-earth nitrides would be expected to be insulators with a similar electronic structure to the divalent rare-earth chalcogenides. However if it is the case that they are half-metallic or narrow gap insulators, then they have potential applications in spin-filtering devices. In the present investigation, We have deposited *GdN* films on glass substrate at room temperature by Ar/N_2 mixed gas plasma-radio frequency (rf) sputtering method. The structure and the complex optical properties as well as the energy gap of *GdN* thin films as a function of N_2 partial pressure are determined.

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Keywords: Optical properties; Optical constants; Deposition by sputtering; Nitride

1. Introduction

Electron spin is becoming increasingly popular in electronics, where active control and manipulation of electron spin in semiconductors and metals provide the basis of a novel quantum technology. New devices now generally referred to as spintronics, exploit the ability of conduction electrons in metals and semiconductors to carry spin-polarized current [1]. Possible applications of spintronics include high-speed magnetic filters, sensors, quantum transistors, and spin qbits for quantum computers [2–4]. More fundamental research will however be needed before practical spintronics devices can be demonstrated.

Today's spintronics research involves virtually all-material families. However, particularly interesting appear to be ferromagnetic semiconductors, which combine complementary functionalities of ferromagnetic and semiconductor material systems.

Rare-earth (RE) materials have high magnetic moments and form a wide range of magnetic structures. An interesting aspect of these materials is the occurrence of localized strongly correlated 4f electrons that determines the magnetic properties while the other electronic properties are determined principally by the itinerant s–d electrons [5].

There has been speculation in the literature that rare-earth nitrides may form half-metallic ferromagnetics [5–7]. For example, *GdN* is found to be a semiconductor in the paramagnetic phase and a semimetal in the ferromagnetic phase [5]. Whereas, in [8] *GdN* is a narrow gap (0.7–0.85 eV) indirect gap semiconductor. This is surprising because, based on a simple ionic model, trivalent rare-earth nitrides would be expected to be insulators with an electronic structure similar to the divalent rare-earth chalcogenides. However if it is the case that they are half-metallic or narrow gap insulators, then they have potential applications in spin-filtering devices [9].

Some properties of rare-earth oxide and fluoride films has been reported by several workers [10–13]. In the pres-

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ent study, the structure of gadolinium nitride thin films has been analyzed by X-ray diffractometer and the complex optical properties as well as the energy gap of *GdN* thin films as a function of film thickness are determined. The fact that there is a lack of literature data concerning optical characteristics and the energy gap of *GdN* thin films highlights the significance of the present study.

2. Theory

Existing methods for the determination of the optical constants of thin films, are usually based on sophisticated computer iteration techniques [14–17], using both optical transmission and reflection spectra or only the transmission spectrum. A relatively simple method for computation of the optical constants, using only the optical transmission spectrum at normal incidence is employed here. The method is applicable to any transmission spectrum showing appreciable interference fringes and based on the idea to use the upper and lower envelopes of the spectrum. It was pioneered by Manificer et al. [18] and extended by Swanepoel [19,20]. Swanepoel's methods are advantageous because they are non-destructive and yield the dispersion relation over a large range of wavelengths without any prior knowledge of the film's thickness. From the transmission spectrum, envelops around the transmission maxima and transmission minima are constructed. Then, the envelopes around the maxima and minima are considered as continuous spectra in wavelength, $T_M(\lambda)$ and $T_m(\lambda)$, respectively. The optical constants n and k can now be calculated from T_M and T_m at each wavelength.

Consider now the following model in which the film and the transparent substrate are surrounded by air of refractive index $n_o \approx 1$, and the incident light from the spectrophotometer is normal to the substrate. The film has a complex refractive index $\mathbf{n} = n - ik$, where k is the extinction coefficient, and the absorption coefficient is given by $\alpha = 4\pi k/\lambda$. The substrate has a refractive index s and must be thick enough to eliminate any resonant modes except within the film. Finally the transmission spectrum will contain interference fringes that obey the basic formula:

$$m\lambda = 2nd, \tag{1}$$

where $m = 1, 2, 3, \ldots$ at maximum points in the transmission spectrum, $m = 1/2, 3/2, 5/2, \ldots$ at minimum points in the transmission spectrum, and d is the film thickness.

As already mentioned, Swanepoel's method requires an envelope construction through the peaks and troughs of the transmission spectra. These envelopes, $T_M(\lambda)$ and $T_m(\lambda)$, are very carefully drawn using the computer program created by McClain et al. [21]. Their work gives an accurate method for the calculation of the two envelopes of a given set of oscillatory data, based on the determination of the corresponding tangent points between the set of data and the envelopes. The main steps for calculation of envelopes are: (i) smoothing of the data; (ii) estimation of the locations of the upper and lower tangent points; (iii) interpolation of a cubic spline through the estimated upper tangent points and another through the estimated lower tangent points. Once the tangent points λ_i between the two envelopes and the transmission spectrum are known, the values of corresponding T_M and T_m can be obtained. By using all these values together with the refractive index of the substrate, the thickness and the optical constants can be calculated. Therefore, it is necessary to analyze them as follows:

2.1. Weak and medium absorption region (interference zone)

In the transparent region, (far below the band gap energy), the n value is given by the following relation [19,20]:

$$n = \left[N + (N^2 - s^2)^{1/2}\right], \tag{2}$$

where

$$N = \frac{s^2 + 1}{2} + 2s\frac{T_M - T_m}{T_M T_m}. \tag{3}$$

The refractive index for a pair of adjacent maxima or minima described by (n_1,λ_1) and (n_2,λ_2) can be obtained by solving Eq. (2). These values are subsequently used to determined the film thickness through the following relation:

$$d = \frac{\lambda_1\lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)}. \tag{4}$$

Having calculated the film thickness and the refractive index, the accuracy of the results can be greatly improved by using Eq. (1) to evaluate the fringe order. By rounding down and up m to its integer or half integer value, the film thickness can be recalculated, averaged and used to recalculate n via Eq. (1). Finally, the absorption coefficient α in the low absorption region of the interference zone can be calculated using the relation:

$$\alpha = -\frac{1}{d}\ln\left[\frac{E_M - [E_M^2 - (n^2-1)^3(n^2 - s^4)]^{1/2}}{(n-1)^3(n-s^2)}\right], \tag{5}$$

where

$$E_M = \frac{8n^2 s}{T_M} + (n^2 - 1)(n^2 - s^2). \tag{6}$$

2.2. Strong absorption region (interference free zone)

In this region, the refractive index is determined by extrapolating the curve of n vs. λ obtained previously at λ values within the interference zone. For that, a Cauchy relation can be used to fit $n(\lambda)$:

$$n(\lambda) = A + \frac{B}{\lambda^2}. \tag{7}$$

By extrapolating Eq. (7) to wavelengths in the region of strong absorption, the absorption coefficient can be