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Free carrier density effects on DyN optical spectra

Abstract

The optical energy gap is a parameter of fundamental importance in semiconductors. However, concentration of free carriers may conceal the true absorption edge. In this paper, we show that the density of the free carriers can affect the onset of the direct absorption. The optical reflectance and transmittance spectra were obtained in the photon energy range of 0.5–5.0 eV thin films of the nitride compound of Dy metal. The films with the greater number of carriers exhibit a greater blue shift in the absorption edge.

Keywords: semiconductors, spintronics, thin films, optical absorption

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Introduction

The optical transmittance and reflectance measurements are popular techniques to experimentally determine the optical energy gap. Recently, the onset of absorption has been determined with great degree of certainty in various rare earth nitride thin films by using this technique.[1–3] Further, this technique has also been used successfully to resolve the spin split bands at point X which has an excellent agreement with the band structure calculations.[4] However, quite often the true absorption edge is masked by the interference fringes formed by the multiply reflected and transmitted rays from the sample as well as due to the artefacts in the spectra due to surface roughness. The most prominent parameter affecting the absorption, however, is the number of free carriers in a sample. Particularly for the case of thin films of monochalcogenides and monopnictides with rare earth or transition metals, the density of carriers can adversely affect the position of absorption edge on the photon energy axis.

It is not possible to determine the exact number of the free carriers in a particular thin film sample. However, certain estimates can be made by applying the Drude model on the optical spectra. Such an analysis can provide us information that how the density of free carriers may affect the properties of a material. In this report, we have collated reflectance and transmittance optical spectra on the DyN thin films fabricated at variable conditions. The films prepared at different dysprosium and nitrogen ion flux rates have different values of the free carrier density which clearly also affects the optical energy gap. Information about the crystal structure and lattice constant was obtained using X–ray diffraction (XRD).

Experimental details

The DyN thin films were prepared by thermally evaporating the Dy metal in the presence of ionized nitrogen gas as described in details.[1–3] The samples with the different values of N_2/Dy flux ratio were prepared. Films were deposited on the sapphire substrates. Since the compounds of rare earth metals oxidize in the atmosphere, samples were protected with an additional capping layer of MgF_2, which is transparent to the photon energy range of our interest.

Fourier transform infrared spectrometer was used to obtain transmission and reflection spectra from the multilayer samples. The DA8 model of BOMEM was used to make measurement in infrared region whereas in the visible regions, a conventional visible–UV spectrometer was used. A reference film was required to make the reflection measurements. A gold film was used in the infra–red region whereas a quartz wedge was in the visible region as the comparison standard for reflectance measurements. Reflectance measurements were made for the light incident on both the film and the substrate surfaces, but since the transmittance is unaffected by the direction that light traverses through the sample it was taken from one side alone. The light is partially reflected and transmitted at the every interface of the multilayer sample due to discontinuous refractive indices. These multiply transmitted and reflected rays then interfere to form a complex interference pattern. This results in the loss light which otherwise would signal the absorption edge. A commercial software, TFCalc,[5] was used to analyze the optical spectra obtained from the multilayer and to extract the optical constants of the DyN. The software makes use of the characteristic matrix method and the data were analyzed as three layers: two films (cap and DyN) and substrate.

Results and discussion

Figure 1 shows the XRD scan of a DyN film. The strongest peak is from the sapphire whereas the peak labelled as (111) and a rather weak (222) peak are contributed by the cubic structure of DyN, therefore the film is strongly textured in the <111> direction. The lattice constant of the films is approximately 4.970±0.003Å, slightly larger than the previously reported value[6,7] of 4.895Å. The average crystallite size is about 10 nm.

In this work, the reflection/transmission spectra and their sum, R+T, of the two films are being reported, one is the near stoichiometric while the other is affected by nitrogen vacancies. Figure 2 shows the R–T spectra from a nearly 300nm DyN thin film, prepared at the highest N_2/Dy flux ratio. In the region below 1.0eV, the absorptance is almost zero showing a very low free carrier density as expected of a semiconductor and also signaling that no interband transitions are present here. The interference fringes in both the reflection and transmission spectra are apparent in this region. Above 1.2eV the transmitted light falls gradually due to interband transitions and continues to fall till 5.0eV where it is less than 1%.

Figure 3 show the optical spectra from second DyN thin film, prepared at a considerably lower N_2/Dy & flux ratio as compared to the film 1. Significant differences can be seen immediately at low energy. The transmittance is as low as 70% in the subgap region due to high carrier density introduced due to the nitrogen vacancies. Following equation was used to calculate the free carrier density where $m^*=0.2m_0$, obtained from the band structure,[4]

$$\alpha = \frac{4\pi}{\lambda}\left(\frac{\sigma_{DC}}{2n\varepsilon_0\omega^3\tau^2}\right)$$

Here α is the absorption coefficient, σ_{DC} is the DC conductivity, τ is the relaxation time, ε_0 is the permittivity of the free space, ω is the angular frequency and n is the refractive index.

The effects of the free carrier are more prominent in Figure 4 where the DyN thin film with larger nitrogen vacancy concentration shows a more clear shift in the absorption edge. Note that this sample was prepared at a lower nitrogen partial pressure (6.8×10^{-5} mbar) while the deposition rate for the dysprosium metal was 2.0Å/s. DyN grown at a relatively larger nitrogen pressure of 1.7×10^{-4} mbar and a deposition rate 1.5Å/s had a nitrogen to dysprosium ratio closer to the stoichiometric value showed a relatively smaller shift of the absorption coefficient. Table 1 summarizes the effects of growth conditions on the fundamental absorption edges of various DyN thin films.

Table 1 Effect of nitrogen vacancies on the fundamental absorption edge

Sample number	N2/Dy flux ratio	Absorption coefficient at 0.5 eV (10^3 cm^{-1})	Absorption onset (eV)	Energy Shift	Film thickness (nm)
Sample 1	250	0	1.2		287
Sample 2	75	6.5	1.5	0.3	304
Sample 3	25	9.7	1.7	0.5	320

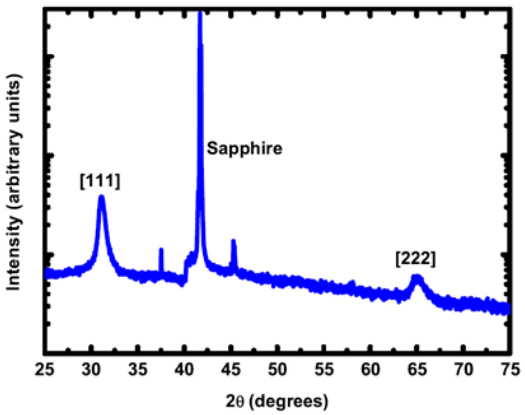

Figure 1 XRD pattern for a representative DyN thin film.

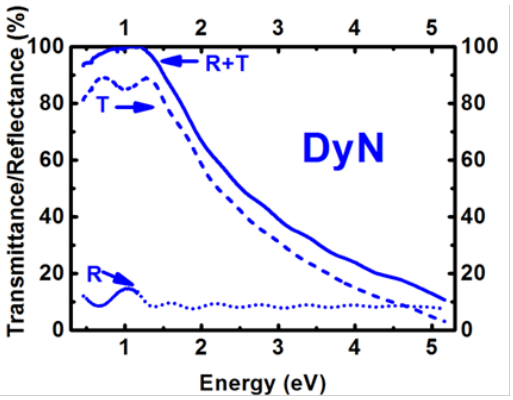

Figure 2 R,T and R+T from the substrate side of DyN thin film.

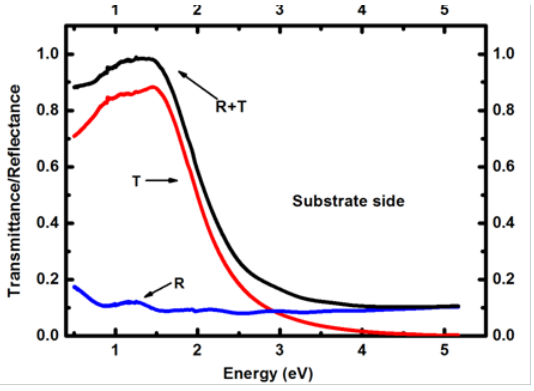

Figure 3 R,T and R+T spectra for a DyN film with greater nitrogen vacancies.

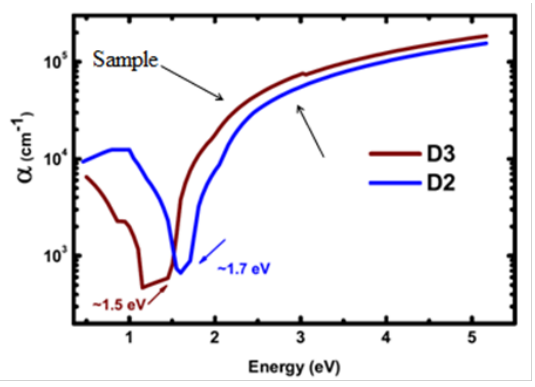

Figure 4 Absorption coefficients for DyN with higher nitrogen vacancies.

Conclusion

It is clear that the various growth conditions affect the carrier densities which in turn have some adverse effects on the position of the optical energy gap. As a matter of fact the number of charge carriers can change the nature of a material from semimetal to semiconductor. Therefore in order to observe optical energy gap with a reasonable certainty, the growth parameters need to be optimized first. The present work shows that the close to stoichiometric films have smaller number of nitrogen vacancies. However as the nitrogen vacancies increase, the onset of absorption is blue shifted.

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None.

Conflict of interest

Author declares there is no conflict of interest.

References

1. Azeem M, Ruck BJ, Do Le B, et al. Optical response of DyN. *Journal of Applied Physics*. 2013;113(20).
2. Trodahl HJ, Preston ARH, Zhong J, et al. Ferromagnetic redshift of the optical gap in GdN. *Physical Review B*. 2007;76(8).
3. Larson P, Lambrecht WRL, Chantis A, et al. Electronic structure of rare–earth nitrides using the LSDA+*U* approach: Importance of allowing 4*f* orbitals to break the cubic crystal symmetry. *Physical Review B*. 2007;75(4).
4. Azeem M. Spin split joint density of states in GdN. *Chinese Physics Letters*. 2016;33(2).
5. Noe TD. TFCalc, 3.5 ed. (Software Spectra Inc., 2011).
6. Preston ARH, Granville S, Housden DH, et al. Comparison between experiment and calculated band structures for DyN and SmN. *Physical Review B*. 2007;76(24).
7. Richter JH, Ruck BJ, Simpson M, et al. Electronic structure of EuN: Growth, spectroscopy, and theory. *Physical Review B*. 2011;84(23):1–10.