Optical Characterization of Radio-Frequency Magnetron-Sputtered Gallium-Arsenide Films under Non-Uniform Thickness Conditions

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Abstract

Measurements were carried out on radio-frequency magnetron-sputtered amorphous and microcrystalline gallium-arsenide (GaAs) films, which were fabricated under various sputtering conditions such as annealing temperature (up to 450˚C), substrate temperature (up to 200˚C), sputtering pressure (up to 20 mTorr), rf sputtering power (up to 800 W), and hydrogen partial pressure (25% H_2 in a mixture with 75% Ar). The experimental goals were to obtain GaAs films exhibiting a low optical absorption coefficient (< 100 cm^{-1}) and a high index of refraction (n > 3.5) for wavelengths greater than 1,000 nm. The key contribution of this work is the introduction of a novel, simple technique to calculate the absorption coefficient under conditions of non-uniform film thickness. The absorption coefficient calculated using the new technique generally decreases as a function of increases in annealing temperature (up to 450˚C), substrate temperature (up to 200˚C), sputtering pressure (up to 20 mTorr), rf sputtering power (up to 800 W), and hydrogen partial pressure (25% H_2 in a mixture with 75% Ar). Index of refraction, on the other hand, generally decreases as a function of the parameters above except for the case of rf sputtering power, where the index of refraction significantly increases. The absorption coefficients obtained in this research are the lowest values ever published using conventional spectrophotometry.

INTRODUCTION

GaAs thin films find many potential applications in the semiconductor industry. The most prominent is the multiple-layer bandpass thin-film filter for Dense Wavelength-Division Multiplexing (DWDM) used in fiber-optic communications where each signal is transmitted on a different wavelength using a combination of multiple optical signals into a single fiber. Therefore, the determination of the film's optical constants, i.e. the absorption coefficient, α and the index of refraction, n is very vital in realizing minimal loss optical filter design consisting of multiple layers of a quarter-wave film.

We have endeavored into the determination of the absorption coefficient using a simple, yet precise technique by finding the thickness of the film to within 2% precision. [1] Then, n can be calculated to define the theoretical transmittance. By varying α iteratively, we were able to match the experimental transmittance to the theoretical transmittance to within 0.1%. In this paper, first, we will describe how to obtain optical constants. Then, we will present some of our key findings of the optical constants under various sputtering parameters with some conclusions.

OPTICAL CONSTANTS

The transmittance was obtained using Perkin-Elmer Monochromator model 128A, which was detailed elsewhere.[3] Since the measurements were carried out in the mid infra-red region that corresponds to the band gap region, the measurement exhibits interference fringes. To determine α as low as 100 cm^{-1}, the thickness precision to within 2% is required. This α determination was achieved by averaging all transmittance lying between two adjacent extrema rather than finding α on each transmittance value that is very dependent on the thickness non-uniformity.

The transmittance was measured on a two-layer structure consisting of the film on a substrate layer. The reflected electric field at the air-film interface undergoes a phase shift of 180˚; on the other hand, no phase shift occurs at the film-substrate interface. However, this electric field travels a path length of $\lambda/2$ where λ is the wavelength in free space. Both electric fields will add constructively if the optical thickness is $\lambda/4$. This constructive interference yields a maximum reflectance. The index of refraction is described by

$$2nd = m\lambda \quad (1)$$

where m is the order of the fringes, and d is the thickness of the film.

Furthermore, the thickness measurement shows no noticeable phase shift at the boundary between the air and the film.[1] The transmittance maxima correspond to a multiple of an integer order (m = 1,2,3…) while the transmittance minima (reflectance maxima) corresponds to an odd multiple of a half-integer order (m = 1/2,3/2…).

Once the correct order is assigned to each extremum value, n of the film can be calculated. We can determine n using the order of the transmittance fringes and the thickness of the film. However, Swanepoel pointed out that this method is very sensitive to the thickness and the error is proportional to the accuracy of the film's thickness.[2] For the case of a 2 μm film, a precision of 2% requires the thickness measurement to be accurate to within 40 nm. Fortunately, this is an achievable requirement using the interferometry technique since the thickness can be resolved within 30 nm (1/10 of a fringe).[3] Since we have more than one extremal point (typically about 6 to 7 maximum points from the 950 to 1900 nm wavelength range), we propose a new means for determining n by choosing the appropriate order that corresponds to the correct dispersion for the wavelength range of interest.

Dispersion is the variation of n as a function of wavelength or photon energy. One way to determine n of a film is by comparing the dispersion between a-GaAs and c-GaAs. Once the order is correctly identified, the dispersion of a- GaAs is similar to that of c-GaAs within experimental precision. This argument is validated by comparing the dispersion of a-Si to that of c-Si, which exhibits the same dispersion relation within experimental precision.[5] If the fringe order is less by an integer number, the dispersion will increase and it will not be comparable to that of c-GaAs.

The index of refraction can be obtained by utilizing the coherent nature of the transmittance data over the measured wavelength range. Fig. 1 illustrates the same dispersion relation between a-GaAs:H and c-GaAs within experimental precision when the correct order m is used. When the order m is increased by one (m+1), it causes wrong dispersion in which n increases as a decreasing function of the photon energy. On the other hand, when order m is decreased by one (m-1), it results in "too much" dispersion relative to c-GaAs. This is a very useful method to calculate n providing that the thickness of our films is precise to within 2%.

Using Selmeir fit, we have the following expression for the index of refraction: [3]

$$n^2 = \varepsilon + \frac{A}{\lambda^2} + \frac{B\lambda_1^2}{\lambda^2 - \lambda_1^2} \quad (2)$$

where ε is the relative permittivity in the medium. A, B, λ_1 are the fitting parameters. This expression is utilized to fit n at other wavelengths besides the extrema.

The rule of thumb is to have the non-uniformity to be less than $\lambda/20n$, which corresponds to 14 nm at wavelength of 1 μm on the film that has a thickness of 2 μm. This condition ensures the calculation of the absorption coefficient to as low as 100 cm^{-1}. Fig. 2 illustrates the averaging of transmittance for both uniform film and non-uniform film when α is taken into consideration. In this plot, α is varied from 10^4 cm^{-1} at λ = 500 nm to 0.1 cm^{-1} at λ = 1500 nm as given by Swanepoel.[2]

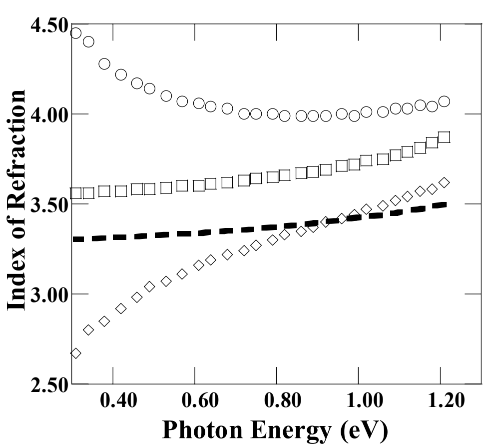

Fig. 1: Index of refraction shown for a-GaAs:H for 3 cases: the correct order m (square); the correct order plus one, m + 1 (circle); and the correct order minus one, m-1 (diamond). Index of refraction of a-GaAs:H is compared to c-GaAs given by Zollner (dotted-line).[4]

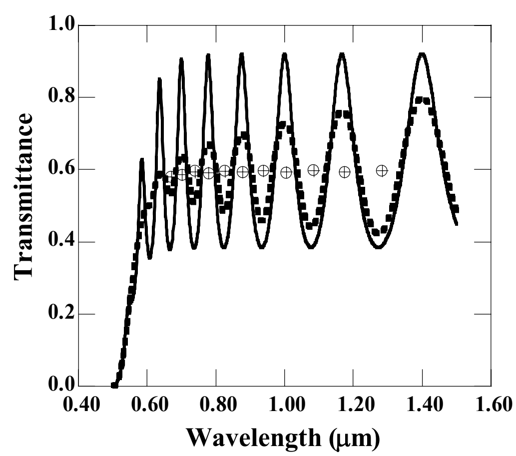

Fig. 2: Transmittance shown between uniform (solid line) and non-uniform film (dotted line) under lossy condition. The circle and the plus indicate the average of the uniform and the non-uniform film, respectively. In this plot, α is varied from 10^4 cm^{-1} at λ = 500 nm to 0.1 cm^{-1} at λ = 1500 nm. In this figure the thickness of the Si sample is 1 μm, with the thickness variation of Δd = 40 nm. (Adapted from Swanepoel's work).[2]

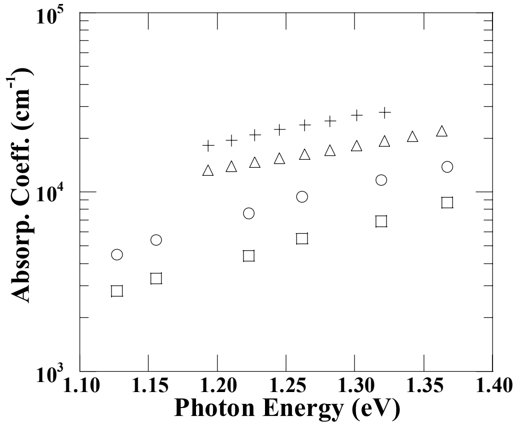

Fig. 3: Absorption coefficient for annealed a-GaAs films sputtered at rf-power of 500 W (triangle) versus unannealed one (plus). Similar condition was established at 800 W for annealed (square) and unannealed samples (circle).

We average the transmittance that yields an agreement between the uniform and the non-uniform film to within 0.5%. Therefore, we justified the use of averaging technique between two extrema for both cases, i.e. the lossless and the lossy case. We also vary Δd between 8 nm and 16 nm. The transmittance excursion decreases as the film becomes non-uniform. Therefore, shorter wavelength is the constraint to achieve 2% agreement between the uniform and the non-uniform film.

RESULTS

In this section, we present our results based on 4 experiments: the annealed *versus* unannealed conditions, substrate temperature samples, sputtering pressure samples, and rf power samples.

Fig. 3 shows α against photon energy for a-GaAs annealed at 450ºC *versus* unannealed one. The plot results in reduction of α value to 17,000 cm^{-1} at 1.28 eV (500 W rf-power film) and 6,000 cm^{-1} (800 W rf-power film) at the same photon energy. The detailed explanations into the mechanism of α change were discussed elsewhere. [3]

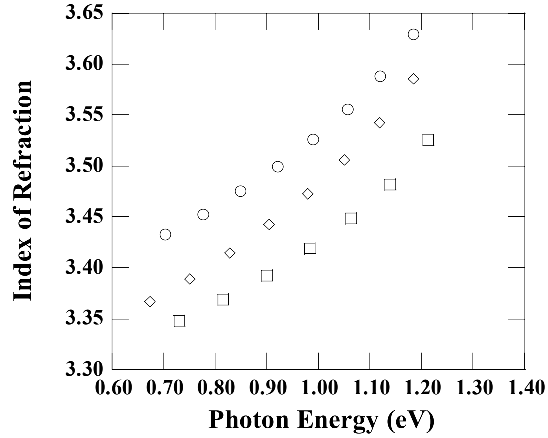

Fig. 5: Index of Refraction as a function of photon energy for various substrate temperatures; 149˚C (circle), 169˚C (square) and 200˚C (diamond).

Fig. 4 shows the absorption spectra as a function of photon energy for a-GaAs sputtered under 3 different substrate temperatures: 149ºC, 169ºC and 200ºC. We observed that α decreases by a factor of four at 1.00 eV. However, the index of refraction remains fixed within 2% precision as illustrated in Fig. 5.

Fig.6 illustrates an order of magnitude decrease in α as we vary the sputtering pressure from 2.25 to 20 mTorr. Despite this significant improvement in lowering α, n decreases significantly by 20% at 1.00 eV as shown in Fig. 7.

Fig. 8 shows the effects of increase in rf power from 400W to 800W, which exhibits more than an order of magnitude reduction in α as the rf power is decreased. Fig. 9 illustrates the increase in n by 10%, albeit the increase in power to 800W. This condition seems to be the best condition in realizing low α, high n.

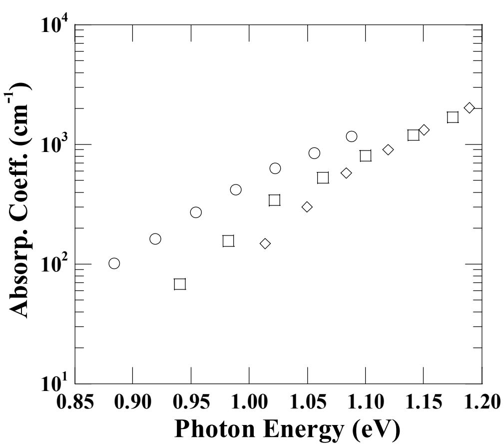

Fig. 4: Absorption coefficient as a function of photon energy for various substrate temperatures; 149˚C (circle), 169˚C (square) and 200˚C (diamond).

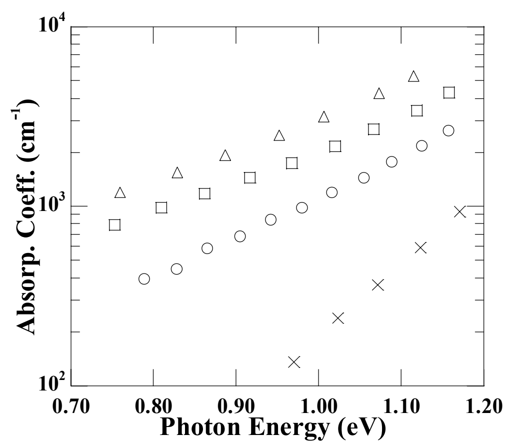

Fig. 6: The absorption coefficient as a function of photon energy for sputtering pressure variation: 2.25 mTorr (triangle), 5 mTorr (square), 10 mTorr (circle), and 20 mTorr (x).

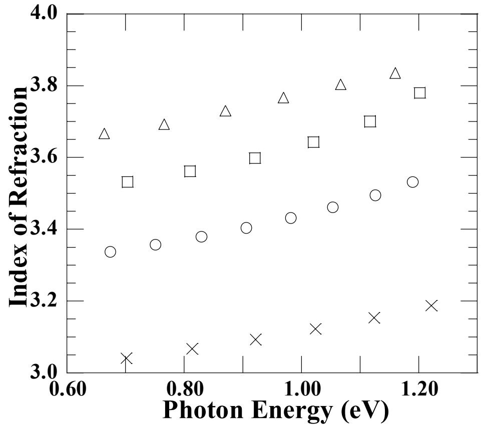

Fig. 7: The index of refraction as a function of photon energy for sputtering pressure variation: 2.25 mTorr (triangle), 5 mTorr (square), 10 mTorr (circle), and 20 mTorr (x).

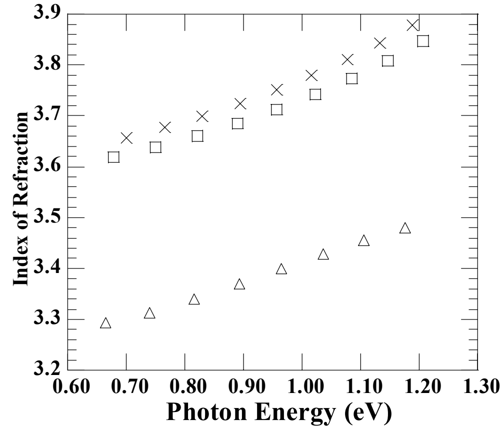

Fig. 9: The index of refraction as a function of photon energy for rf sputtering power variation: 400W (triangle), 650W (square), and 800W (x).

Conclusions

We have shown a simple, precise procedure to obtain both n and α. This procedure yields results that clearly points to the influences of all 3 parameters on α. The influence of rf sputtering power shows the most considerable decrease of α as a function of rf sputtering power. Surprisingly, this improvement in α is coupled with an increase in the refractive index. However, the use of high rf sputtering power must be carefully carried out due to the possibility of thermal shock to the sputtered target as the power is increased. Murri *et al.* replaced the target as a result of target cracking when they varied the power from 100-400W.[6] One way to avoid this occurrence is by making sure the target has a uniform thermal contact, using Galium-Indium eutectic.

The second most important parameter that can improve α is by increasing the hydrogen concentration in the GaAs film. Decreasing the number of dangling bonds is the cause of α reduction.[1] Another parameter is the decrease of wrong bonds, which can be achieved if the amorphous structure is maintained at a stoichiometric ratio of 1:1 between Gallium and Arsenic. However, the reduction of α is accompanied by a significant decrease in n. Index of refraction is very crucial in designing an interference filter where higher n will allow for the fabrication of fewer layers.

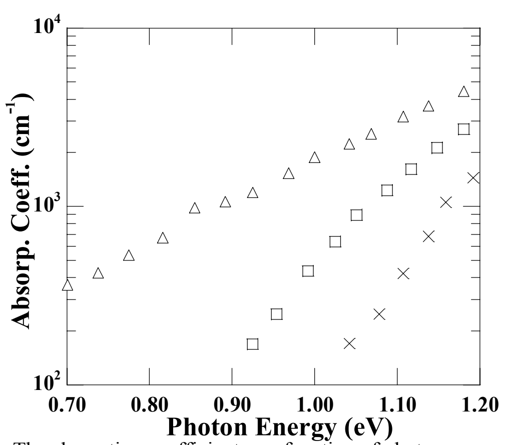

Fig. 8: The absorption coefficient as a function of photon energy for rf sputtering power variation: 400W (triangle), 650W (square), and 800W (x).

The last important parameter to achieve a lower α is by sputtering at a higher temperature. At higher temperatures the film evolves into a more microcrystalline phase that causes the film to comprise fewer dangling bonds, together with the improvement towards a stoichiometric film.

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References

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Acronyms

Absorp. Coeff.: Absorption Coefficient
a-GaAs:(H): (hydrogenated) amorphous/microcrystalline Gallium Arsenide
a-Si: amorphous Silicon
c-GaAs: single-crystal Gallium-Arsenide
c-Si: single-crystal Silicon
rf: Radio Frequency