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MODELS OF EFFECTIVE REFRACTIVE INDEX FOR THIN FILMS

Literature review

ABSTRACT

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PREFACE

Tampere,

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LIST OF ABBREVIATIONS AND SYMBOLS

The abbreviations and symbols used in the thesis are collected into a list in alphabetical order. In addition, they must be explained upon first usage in the text.

1. INTRODUCTION

!!!TODO: introduction to the topic and about the relevance

In this paper a few effective medium approximations for the complex refractive index are introduced. The aim of this literature review is to compare the findings of studies related to the usage of these models with thin film structures and provide an overview of the types of materials these models could be used with.

2. EFFECTIVE MEDIUM APPROXIMATIONS

Effective medium approximations or EMAs are models made to predict the effective properties of heterogeneous materials. So, the purpose of these EMAs is to homogenize a physical property, e.g. dielectric constant, of a material composed of two or more constituent materials with different physical properties. In this chapter some of the most commonly used EMAs for the permittivity of heterogeneous thin films are introduced and the intended use cases for these EMAs are discussed briefly.

The first model introduced here is the Volume Averaging theory or VAT. VAT seems to be an EMA that effectively describes the optical properties of a few different types of heterogeneous materials [1, 2]. VAT was originally derived by del Rio and Whitaker for inclusions of arbitrary shape of one material embedded in a different background medium. The main assumption made in the VAT model is that the arbitrarily shaped inclusions form a relatively isotropic composite and that the volume fraction of the materials is effectively homogeneous throughout the composite. [3, 4]

The VAT model for the refractive index of a composite described above can be expressed with the equations [2]

$$n_{eff}^2 = \frac{1}{2}[A + \sqrt{A^2 + B^2}] \tag{2.1}$$

$$k_{eff}^2 = \frac{1}{2}[A + \sqrt{A^2 + B^2}] \tag{2.2}$$

$$A = f_v(n_i^2 - k_i^2) + (1 - f_v)(n_c^2 - k_c^2) \tag{2.3}$$

$$B = 2n_i k_i f_v + 2n_c k_c(1 - f_v). \tag{2.4}$$

In equations 2.1 to 2.4 n is the real part of the complex refractive index, k is the imaginary part of the refractive index, f_v is the volume fraction of the inclusion in the material, subscript eff signifies the effective values for the composite, subscript i signifies the inclusions and subscript c signifies the surrounding material. So, to model the effective refractive index of a composite described by the VAT model one only needs to know the bulk refractive index of the constituent materials and the average volume fraction of the inclusions.

The second model is the Maxwell Garnett model, which was originally derived by J.C. Maxwell Garnett to model the dielectric properties of a composite with spherical inclusions. So the assumptions made in this model are that the composite, again, consist of two different materials with the other one being the background in which the other material forms spherical inclusions.[5] This original Maxwell Garnett formula for 3-dimensional spherical inclusions is called the 3D Maxwell Garnett model (3D MGT) and according Hutchinson et al. the equation for the effective refractive index according to this model can be expressed as [1]

$$\tilde{n}_{eff}^2 = \tilde{n}_c^2 \left[1 - \frac{3f_v(\tilde{n}_c^2 - \tilde{n}_i^2)}{2\tilde{n}_c^2 + \tilde{n}_i^2 + f_v(\tilde{n}_c^2 - \tilde{n}_i^2)} \right], \tag{2.5}$$

where $\tilde{n}$ represents the complex refractive index $\tilde{n} = n - ik$.

Relating to this Maxwell Garnett model, Sihvola introduced a model for describing the optical properties of elliptical inclusions. From this model for elliptical inclusions Sihvola derived a model for the case of cylindrical inclusions. This model is called the 2-dimensional Maxwell Garnett model (2D MGT) and it is designed to model the optical properties of spherical inclusions embedded in a different material while the electric field of light traveling through it is perpendicular to the axis of rotation of the cylinders.[6] This model,,in terms of the refractive index, was presented by Sihvola [7] and according to Hutchinson et al. it is of the form [1]

$$\tilde{n}_{eff}^2 = \tilde{n}_c^2 \left[1 - \frac{2f_v(\tilde{n}_c^2 - \tilde{n}_i^2)}{\tilde{n}_c^2 + \tilde{n}_i^2 + f_v(\tilde{n}_c^2 - \tilde{n}_i^2)} \right]. \tag{2.6}$$

The third EMA introduced here is the symmetric Bruggeman model. It is similar to the Maxwell Garnett model but it doesn't assume that any of the materials in the composite is the host or the continuous phase [8]. Therefore, the Bruggeman model is assumed to be more suitable for composites where there clear background material exists and all the component are present in almost equal proportions [8]. For composites composed of two different materials the Bruggeman model takes the form [1]

$$(1 - f_v)\frac{\tilde{n}_c^2 - \tilde{n}_{eff}^2}{\tilde{n}_c^2 + 2\tilde{n}_{eff}^2} + f_v \frac{\tilde{n}_i^2 - \tilde{n}_{eff}^2}{\tilde{n}_i^2 + 2\tilde{n}_{eff}^2} = 0. \tag{2.7}$$

As can be seen from equations 2.1 to 2.7, the only information required to use these models is the refractive indexes of the constituent materials and the volume fraction of these materials in the composite. Therefore, these models are relatively simple to use, provided that the refractive indexes of the constituent materials are known and the volume fractions of the sample can be measured.

!!!TODO: add parallel and nonsymmetric Brugge and remove symmetric Brugge?

3. USAGE OF EMAS

In general, EMAs have some limitations as they try to approximate a heterogeneous medium as a homogeneous one. For example, according to Hutchinson et al. the scattering from the pores is assumed to be negligible in most EMAs. Because of this, there usually is a minimum wavelength after which scattering from the pores becomes too large for the model to accurately predict the optical properties of the medium. [1] According to Sihvola, as a rule of thumb, the minimum wavelength used should be 10 times greater than the size of the inclusion [6]. Hutchinson et al. also give a general rule for the minimum wavelength stating that $\frac{2\pi D}{\lambda} << 1$ for the EMAs to work [1]. The ratio of thin film length to the size of the inclusions has also been shown to affect the optical properties of porous thin films [1, 2]. Although, according to Garahan et al., this phenomenon is only related to the interference between different pores and is present only because of the numerical modeling methods used in the study. So, this limitation shouldn't be present when dealing with a real thin film with multiple pores and not a mathematical model of a simplified system. [2] This analysis by Garahan et al. seems to hold at least when looking at the data by Hulkkonen et al. where the ratio of film thickness to pore diameter is almost unity but the 2D maxwell Garnett model was able to predict the porosities of the used samples from their optical properties [9].

As stated before, the VAT model was originally designed to predict the optical properties of a composite with arbitrarily shaped inclusions in a continuous matrix. In thin film systems however, VAT seems to work the best when dealing with cylindrical inclusions [1, 2, 9]. In their study Garahan et al. mostly focused on the use of the VAT model with simulated nanowire and cylindrical pore films. In it they found that the VAT model can predict the optical properties of these films accurately with non-absorbing and slightly absorbing materials. This is supported by the findings of Hutchinson et al. but only when the light is polarized along the axis of rotation of the cylinders which is the polarization used in the study by Garahan et al. .[1, 2]

However, the optical properties of cylindrical pores seem to be modeled more accurately by the 2D Maxwell Garnett model when the incoming light is polarized perpendicular to the axis of rotation of the cylinders. These two polarizations are

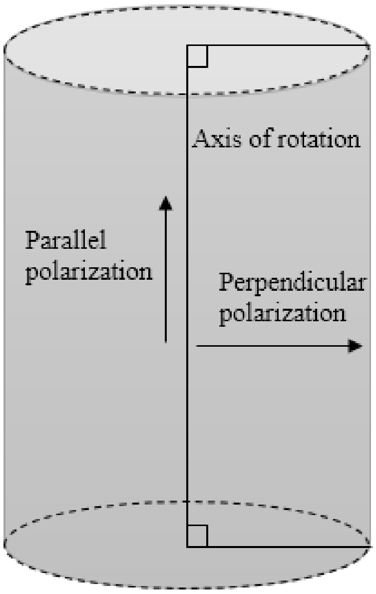

Figure 3.1 *Diagram of the different polarizations in terms of cylindrical inclusions.*

depicted in figure 3.1. Hutchinson et al. reported that the 2D Maxwell Garnett model accurately predicts the real part of the refractive index for cylindrical pores when the aforementioned polarization is used. However, they also found that the imaginary part is predicted more accurately by the parallel model but, when looking at their data, it seems that the 2D Maxwell Garnett model isn't much more off from the simulated values. [1] Hulkkonen et al. also found that the 2D Maxwell Garnett model predicts the porosity of real samples of thin films with cylindrical pores more accurately than the VAT model. Their data also shows that the 2D Maxwell Garnett model can be used to model the imaginary part of the refractive index in certain cases.[9]

For spherical inclusions, Hutchinson et al., found that the 3D Maxwell Garnett model did what it was intended to do, and accurately predicted the optical properties for these inclusions. However their numerical modeling also showed that, as with the 2D Maxwell Garnett model, the 3D Maxwell Garnett model wasn't the best at predicting the imaginary part of the refractive index. Although the imaginary part wasn't too far off from the values predicted by the 3D MGT, the nonsymmetric Bruggeman model described it more accurately. [1]

!!!TODO: add 1 more article on spherical inclusions, preferably experimental

4. CONCLUSIONS

!!!TODO: conclude the discussion in previous chapter and provide short guide according to the findings

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