Journal of Theoretical and Applied Physics, **4**-3, 37-41 (2010)

On the local homogenization of metallic sculptured thin films

F. Babaei[1], H. Savaloni[2,*]

[1]*Department of Physics, University of Qom, Qom, Iran.*
[2]*Department of Physics, University of Tehran, North-Kargar Street, Tehran, Iran.*

Received: 12 May 2010/Accepted: 8 November 2010/ Published: 20 December 2010

Abstract

The concept of local homogenization is employed for estimation of the relative permittivity scalars in copper Sculptured Thin Film (STFs). Three absorption transitions of dielectric to metal occur in the copper STFs. These transitions reduce to two in columns with circular cross section, when the volumetric fraction of metallic particles increases from zero to unity. The first transition occurs at low volumetric fraction of metallic inclusions and the other two transitions appear at high volumetric fraction of metallic inclusions. The influence of the column shape factors on the absorption transitions of dielectric to metal is also reported.

***PACs*:** 73.61.At; 78.66.Bz; 72.15.Rn; 78.40.Kc
Keywords*: Sculptured thin films; Homogenization; Absorption transitions of dielectric to metal*

1. Introduction

The Sculptured thin films (STFs) are columnar thin films that their columnar growth direction can change suddenly during their growth [1]. When the columnar thin films with a diameter of 10 to 300 nm are deposited at oblique incident and the two principal axes of rotation can change separately or together, then many kinds of morphologies in nano-scales can be produced [2-4]. The optional rotation of these two principal axes results in two groups of sculptured thin films, namely sculptured nematic thin films (SNTFs) [5] and thin film helicoidal bianistropic media (TFHBM) [6]. The SNTFs are two dimensional nano-structures with simple shapes such as oblique columns, chevrons, zigzags, and complex morphologies including shapes such as C, S and many other shapes. The TFHBMs are three dimensional nano-structures including morphologies from simple helicoidals to super helicoidals [7].
STFs are porous with anisotropic structures, and their structure can be designed in different useful shapes. Therefore their structure can be filled with gases, liquids, liquid crystals, organic monomers and other materials. This will change their optical activity considerably so that they can be used as optical sensors for detection and quantification of chemical, biological and nuclear media [8].

A STF is defined as a composite material consisting of two phases (i.e., material and vacuum). The mathematical processes that describe the transition from a nano-structure to continuum length scales is so called homogenization [9,10]. The homogenization has a principal role in the estimation of the relative permittivity scalars in STFs [11,12]. Three absorption transitions of dielectric to metal occur in composite material, out of which only two are sensitive to plane waves at normal incidence [13]. The Bragg peak results in higher reflectivity spectra when the absorption transition of dielectric to metal occurs at high volumetric fraction of metallic inclusions [11-13].
In this work the absorption transition of dielectric to metal in a composite STF made of copper is reported. In addition the influence of different columnar shape factors on these transitions are also investigated.

2. Theory

Each column in the STF structure is considered as a string of identical long ellipsoids. The surface of each ellipsoid in relation to its centroid may be considered in Cartesian coordinates by [14]:

$$x^2 + \left(\frac{y}{\gamma_2}\right)^2 + \left(\frac{z}{\gamma_3}\right)^2 = \delta^2, \qquad (1)$$

where δ is a linear measure of absolute size of an ellipsoid, while the factors γ_2 and γ_3 are the transverse aspect ratio and the slenderness ratio of the ellipsoid, respectively (Fig. 1) [15].
In order to obtain the relative permittivity scalars, the Bruggeman formalism was used [16]:

$$f_s \underline{\underline{A}}_s + (1 - f_s)\, \underline{\underline{A}}_\upsilon = \underline{\underline{0}}, \qquad (2)$$

Where $(0 \le f_s \le 1)$ is the volume fraction of the ellipsoidal inclusions. The polarizability dyadic of an ellipsoidal inclusion $\underline{\underline{A}}_s$, embedded in the homogenized composite medium is denoted, on a per unit volume basis, by [11]:

*Corresponding author: Hadi Savaloni;
E-mail: savaloni@khayam.ut.ac.ir
Tel: (+98) 21 88635776
Fax: (+98) 21 88004781

$$\underline{\underline{A}}_{s,\upsilon} = \varepsilon_0 \left(\varepsilon_{s,\upsilon}\, \underline{\underline{I}} - \underline{\underline{\varepsilon}}_{ref}\right) \cdot \left[\underline{\underline{I}} + \mathrm{i}\omega\varepsilon_0\, \underline{\underline{D}}_{s,\upsilon} \cdot \left(\varepsilon_{s,\upsilon}\, \underline{\underline{I}} - \underline{\underline{\varepsilon}}_{ref}\right)\right]^{-1} \tag{3}$$

where $\underline{\underline{0}}$ and $\underline{\underline{I}}$ are null and unit dyadics, respectively and ε_0, ε_s and ε_υ are the free space, bulk metal and vacuum permittivities, respectively. $\underline{\underline{\varepsilon}}_{ref}$ is given as [13]:

$$\underline{\underline{\varepsilon}}_{ref} = \varepsilon_a \underline{u}_z \underline{u}_z + \varepsilon_b \underline{u}_x \underline{u}_x + \varepsilon_c \underline{u}_y \underline{u}_y \tag{4}$$

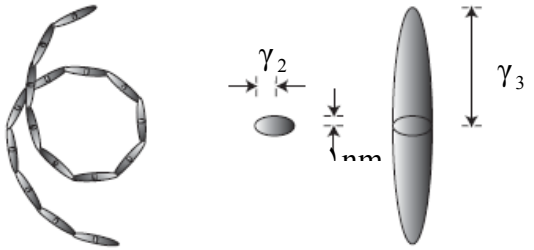

Fig. 1. A STF column which is considered as a string of identical long electrical ellipsoids with shape factors of γ_2 and γ_3.

The relative permittivity scalars $\varepsilon_{a,b,c}$ are implicit functions of frequency. $\underline{u}_x$, $\underline{u}_y$, and $\underline{u}_z$ are unit vectors in the Cartesian coordinate system. The permittivity of free space (vacuum) is, $\varepsilon_0 = 8.854 \times 10^{-12}\ F/m$.

The depolarization dyadic of an ellipsoidal region in the homogenized composite medium (HCM) is given by [12]:

$$\underline{\underline{A}}_{s,\upsilon} = \frac{2}{i\pi\omega\varepsilon_0} \int_{\phi=0}^{\pi/2} \int_{\theta=0}^{\pi/2} \sin\theta \times \frac{(\sin\theta\cos\phi)^2 u_z u_z + \left(\frac{\cos\theta}{\gamma_\tau^{s,\upsilon}}\right)^2 u_x u_x + \left(\frac{\sin\theta\sin\phi}{\gamma_b^{s,\upsilon}}\right)^2 u_y u_y}{(\sin\theta\cos\phi)^2 \varepsilon_a + \left(\frac{\cos\theta}{\gamma_\tau^{s,\upsilon}}\right)^2 \varepsilon_b + \left(\frac{\sin\theta\sin\phi}{\gamma_b^{s,\upsilon}}\right)^2 \varepsilon_c} d\theta d\phi \tag{5}$$

In order to concentrate on the absorption transitions from dielectric to metal due to metallic ellipsoidal shape, it is assumed that the vacuum topology is the same as metallic topology in all calculations (i.e., $\gamma_2^s = \gamma_2^v$, $\gamma_2^v = \gamma_2^s$) [14].

In order to obtain the relative permittivity scalars $\varepsilon_{a,b,c}$, equation (2) should be solved numerically. The solution can be readily obtained, using the iterative methods such as Jacobian technique [14].

4. Numerical results and discussion

It is assumed that the STF is produced from isotropic copper with bulk permittivity of $\varepsilon_s = -7.67 + 2.63i$ at wavelength of 590.38 nm [17], and let the ellipsoidal copper particles to be embedded in the dielectric medium (i.e., vacuum). The ellipsoids are considered to be electrically small (i.e., small in a sense that their electrical interaction can be ignored). In addition the film is considered to be porous and for vacuum $\varepsilon_v = 1$.

In order to obtain the real and the imaginary parts of the relative permittivity scalars $\varepsilon_{a,b,c}$, Eq. (2) was solved iteratively for columns with circular cross section, $\varepsilon_a = \varepsilon_b (\gamma_2 = 1\ nm)$, and for columns with non-circular cross section $\varepsilon_a \neq \varepsilon_b (\gamma_2 = 10\ nm)$ for different values of γ_3. The results are plotted as a function of volumetric fraction of metal inclusion f_s in Figs. 2 and 3, respectively.

In Figs. 2 and 3 it is obvious that when $f_s \to 0$ (the medium consists of only vacuum) and $\varepsilon_a = \varepsilon_b = \varepsilon_c = \varepsilon_v = 1$, and when $f_s \to 1$ (the medium consists of only metal) and $\varepsilon_a = \varepsilon_b = \varepsilon_c = \varepsilon_s = -7.67 + 2.63$ i. When $\gamma_2 = 1$ nm, the ellipsoids can have shapes similar to prolate spheroids ($\gamma_3 \succ 1\ nm$), spheres ($\gamma_3 = 1\ nm$), or oblate spheroids ($\gamma_3 \prec 1\ nm$).

From Fig. 2 it can be obviously deduced that when $\gamma_2 = 1\ nm$, the cross section of columns in xy plane is circular and ε_a's behaviour is similar to that of ε_c (different values of γ_3), and if $\gamma_2 = \gamma_3 = 1\ nm$, then each column of STF is composed of spheres ($\varepsilon_a = \varepsilon_b = \varepsilon_c$), and an isotropic composite material (copper-vacuum) is formed ($\gamma_3 = 1\ nm$).

In Fig. 3 it can be seen that when $\gamma_3 = 1\ nm$, the columns' cross section in xz plane is circular ($\varepsilon_a = \varepsilon_b$) and the behaviour of ε_a is the same as ε_b ($\gamma_3 = 1\ nm$). If $\gamma_2 = \gamma_3 \neq 1\ nm$, then the cross section of each column of STF in xy plane is circular ($\varepsilon_b = \varepsilon_c$), and ε_b and ε_c behave similarly ($\gamma_3 = 10\ nm$).

Generally, there are three absorption transitions from dielectric to metal (when $Re\left[\varepsilon_{a,b,c}\right] \prec 0$) in these films. There are only two transitions for columns with circular cross section (Fig. 2). When $\gamma_3 \prec \gamma_2$ the first transition happens in $\varepsilon_a = \varepsilon_c$ and the second transition occurs in ε_b. When $\gamma_3 \succ \gamma_2$ the first transition occurs in ε_b and second transition occurs for $\varepsilon_a = \varepsilon_c$.

For columns with noncircular cross section, all three transitions exist. When $\gamma_3 \prec \gamma_2$ the first transi-

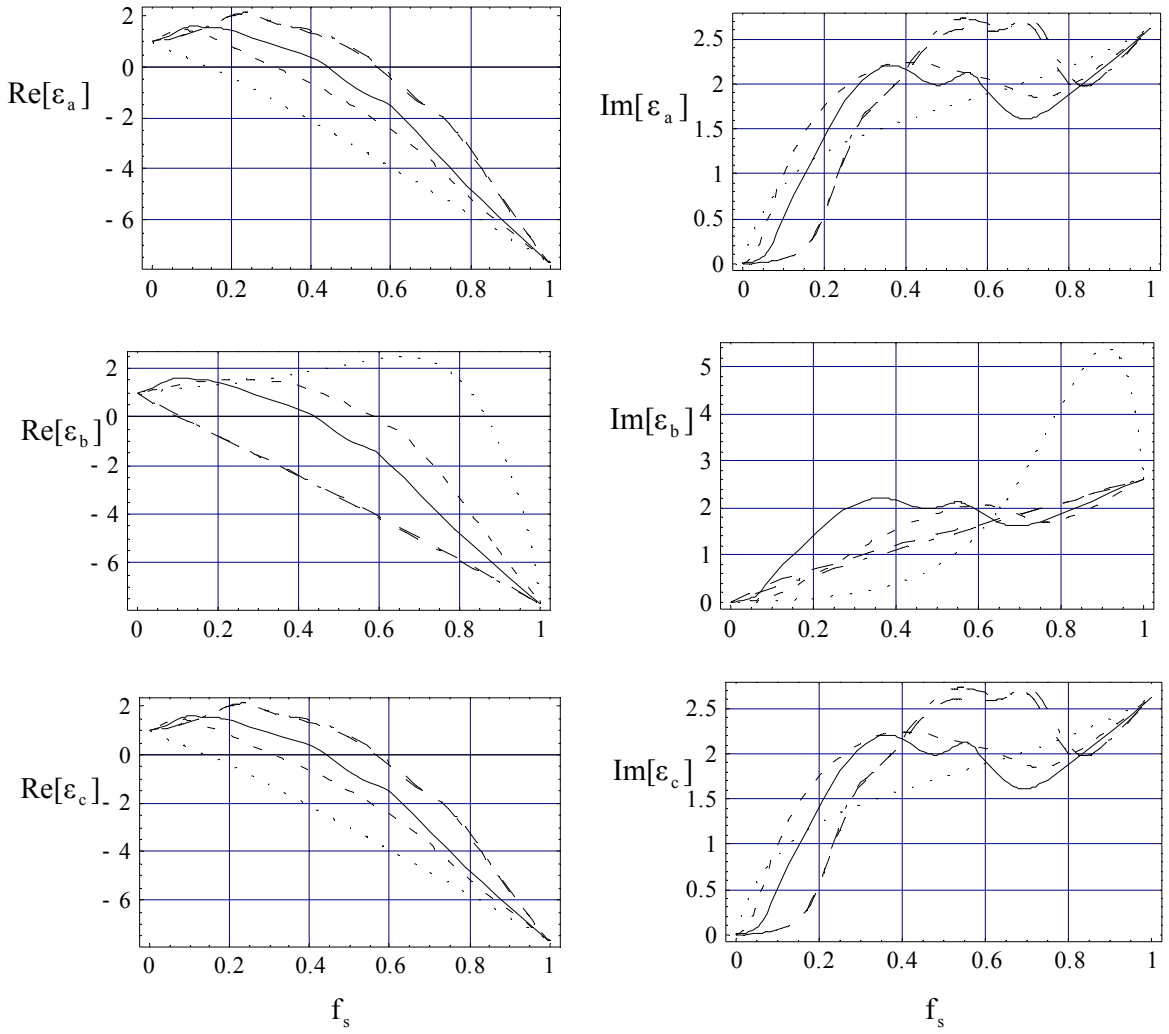

Fig. 2. Computed values of ε_a, ε_b and ε_c as a function of f_c in copper STF for different values of $\gamma_3 \cdot \gamma_3 = 1\ nm$, (..... $\gamma_3 = 0.1\ nm$, – – – $\gamma_3 = 0.5\ nm$, ——— $\gamma_3 = 1\ nm$, — — $\gamma_3 = 10\ nm$, — . — $\gamma_3 = 20\ nm$)

Table 1. The volumetric fraction of metallic inclusions f, when the real part of the relative permittivity scalars, $\varepsilon_{a,b,c}$ becomes negative.

	$\gamma_3 = 0.1$ nm			$\gamma_3 = 0.5$ nm			$\gamma_3 = 1$ nm			$\gamma_3 = 10$ nm			$\gamma_3 = 20$ nm		
	$*\varepsilon_a$	$*\varepsilon_b$	$*\varepsilon_c$	$*\varepsilon_a$	$*\varepsilon_b$	$*\varepsilon_c$	$*\varepsilon_a$	$*\varepsilon_b$	$*\varepsilon_c$	$*\varepsilon_a$	$*\varepsilon_b$	$*\varepsilon_c$	$*\varepsilon_a$	$*\varepsilon_b$	$*\varepsilon_c$
$\gamma_2 = 1$ nm	0.143	0.867	0.143	0.312	0.587	0.312	0.443	0.443	0.443	0.568	0.105	0.568	0.578	0.112	0.578
$\gamma_2 = 10$ nm	0.156	0.895	0.115	0.393	0.699	0.110	0.568	0.568	0.105	0.867	0.143	0.143	0.887	0.116	0.155

*) For the f_s values given in this table the corresponding real part of the relative permittivity scalar on that column (row 2) becomes negative

tion occurs in ε_c, and the second transition occurs in ε_a and the third transition occurs in ε_b. When $\gamma_3 \succ \gamma_2$ the first transition occurs in ε_b, and the second transition occurs in ε_c and the third transition occurs in ε_a.
In Table 1 the values obtained for the volumetric fraction of metallic inclusions f_s, when the real part of the relative permittivity scalars, $\varepsilon_{a,b,c}$ becomes negative are given. These values are obtained for both columns with circular and noncircular cross sections.

5. Conclusions

The relative permittivity scalars ε_a, ε_b and the composite relative permittivity ε_b for copper STFs consisting of columns of circular cross section and columns of noncircular cross section after hemogenization are computed, using Bruggeman formalism. For columns with noncircular cross section all three absorption transitions from dielectric to metal exist, while in case of columns with circular cross section the number of transitions reduces to two.

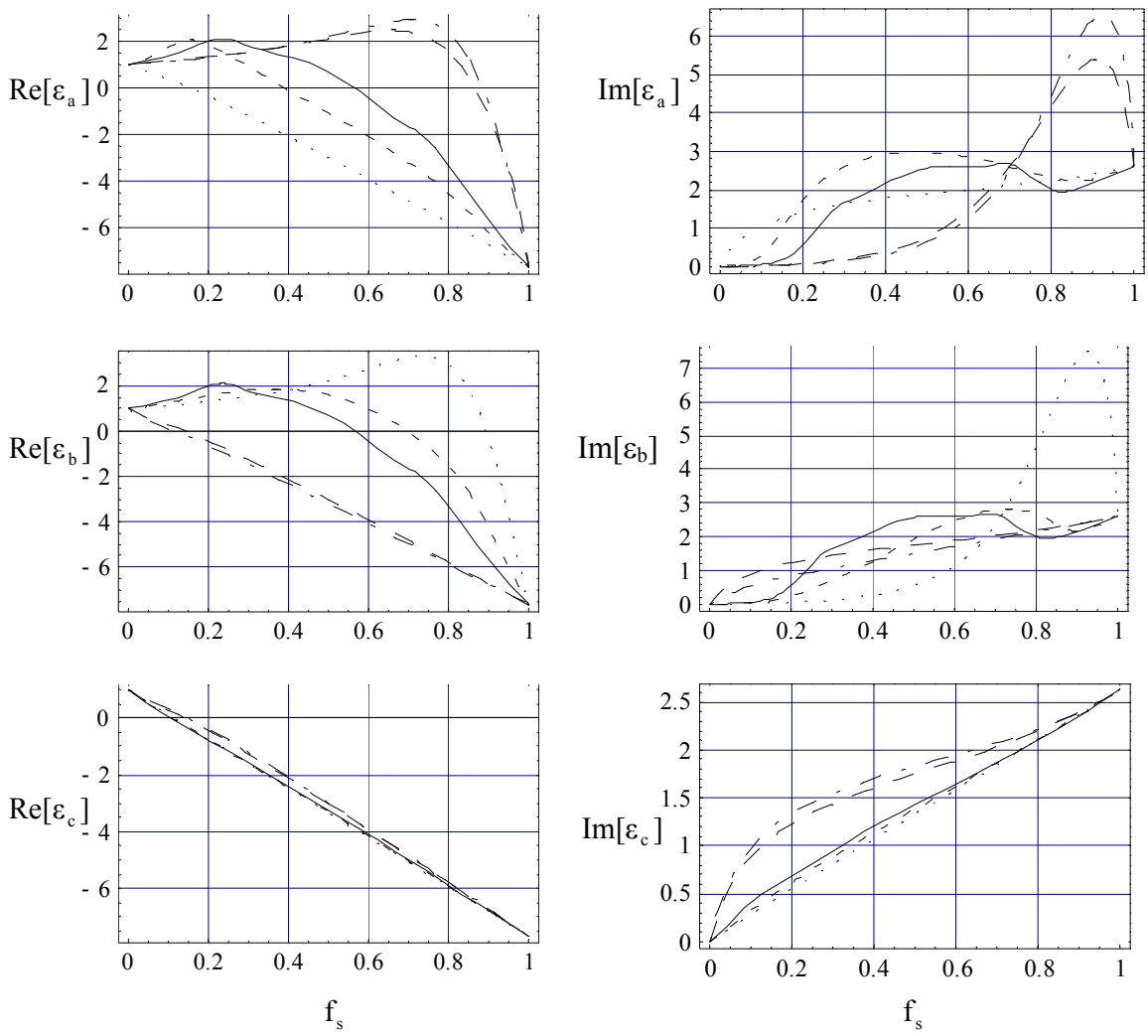

Fig. 3. Computed values of ε_a, ε_b and ε_c as a functions of f_s in copper STF for different values of γ_3. $\gamma_2 = 10\ nm$, (.....$\gamma_3 = 0.1\ nm$, - - - $\gamma_3 = 0.5\ nm$, —— $\gamma_3 = 1\ nm$, — — $\gamma_3 = 10\ nm$, — · - $\gamma_3 = 20\ nm$)

For columns with circular cross section consisting of oblate spheroids, the first transition occurs in $\varepsilon_a = \varepsilon_c$ and for low volumetric fraction of metal inclusion f_s (because of increased continuity of metallic ellipsoids) the second transition happens in ε_b. In case of prolate spheroids the results are opposite to those obtained for oblate spheroids.

For columns with noncircular cross section consisting of oblate spheroids the first transition occurs in ε_c, and the other two transitions occur at higher volumetric fraction of metal inclusion f_s, while for columns composed of prolate spheroids the first transition occurs in ε_b, and the other two transitions occur at higher volumetric fraction of metal inclusion. It is also observed that the absorption transitions from dielectric to metal (copper) in copper STF composite of (metal (copper)-vacuum) are strongly dependent on the columns shape factors, γ_2 and γ_3.

Acknowledgements

This work was carried out with the support of the University of Tehran and the University of Qom.

References

[1] A. Lakhtakia, R. Messier, M. J. Brett, K. Robbie, Mater. Res. Innovat. **1**, 165 (1996).
[2] K. Robbie, M. J. Brett, A. Lakhtakia, J. Vac. Sci. Technol., A **13,** 2991 (1995).
[3] K. Robbie, M. J. Brett, A. Lakhtakia, Nature **384**, 616 (1996).
[4] D. Vick, J. Friedrich, S. K .Dew, M. J. Brett, K. Robbie, M. Seto, T. Smy, Thin Solid Films **339,** 88 (1999).
[5] R. Messier, T. Gehrke, C. Frankel, V. C. Venugopal, W. Otano, A. Lakhtakia, J. Vac. Sci. Technol. A **15**, 2148 (1997).
[6] A. Lakhtakia, W. Weiglhofer, Proc. R. Soc. Lond. A **448**, 419 (1995).
[7] R. Messier, P. D. Sunal, V. C. Venugopal, Proc. SPIE **3790**, 133 (1999).
[8] R. Messier, V. C. Venugopal, P. D. Sunal, J. Vac. Sci. Technol. A **18**, 1538 (2000).
[9] A. Lakhtakia, Modelling Simul. Mater. Sci. Eng. **8**, 677 (2000).
[10] A. Lakhtakia, Mater. Sci. Eng. C **19**, 427 (2002)
[11] F. Babaei, H. Savaloni, Opt. Commun. **281**, 3120 (2008).

[12] F. Babaei, H. Savaloni, Opt. Commun. **278**, 321 (2007)
[13] A. Lakhtakia, Microw. Optical. Technol. Lett. **20**, 239 (2000).
[14] J. A. Sherwin, A. Lakhtakia, B. Michel, Opt. Commun. **178,** 267 (2000).
[15] A. Lakhtakia, Optik **114**, 556 (2003).
[16] A. Lakhtakia, R. Messier, Sculptured Thin Films: Nanoengineered Morphology and Optics (SPIE, USA, 2005) chap. 6.
[17] E. D. Palik, Handbook of Optical Constants of Solids (Acadamic press, Newyork, 1985).