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The Albedo of Metallic Nanoparticles Computed from FDTD

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Abstract*— *This manuscript presents the albedo, a measure of a nanoparticles light retention capability, for silver, aluminum, gold, chromium, copper, nickel and titanium throughout the visible spectrum. Lumerical's finite-difference time-domain Maxwell's equation solver was employed to analyze how light of various angles and polarizations interacts with such materials in three dimensions. All of the particles in this study are 50 nm in radius.

Keywords*— *albedo, finite-difference time-domain (FDTD), organic light emitting diodes (OLEDs), scattering.

I. INTRODUCTION

Recently, several researchers have been focusing on enhancing the internal quantum efficiency and out-coupling efficiency of light emitting diode materials[1-5]. Baldo et al. have reported internal quantum efficiencies near 100%. However, the out-coupling efficiency of the best organic light emitting diodes is still at only approximately 80%[6,7]. This manuscript attempts to address the gap in the literature surrounding the upper limit of the out-coupling efficiency achievable through plasmonic scattering materials.

As a first step in that direction, this manuscript calculates the light retention capability of metallic nanoparticles. This is commonly referred to as albedo.

II. METHODS

Studies were conducted with Lumerical FDTD 2016B R2. In each case, the simulation region contained a single spherical nanoparticle of radius 50 nm. The background index was 1.0 and the simulations were carried out for 50 fs, at a temperature of 300K. The simulation region was 2 micronsx2micronsx2microns with the nanoparticle in the center of the simulation region. Mesh accuracy was set to 8 ("very high accuracy") and the dt stability factor was .99. The xmin BC was symmetric, the xmax, ymin, ymax, and zmax BCs were PML, and the zmin BC was antisymmetric. This was suggested by Lumerical for Mie-type analyses. The mesh lattice points were spaced at .6 nm for the x, y and z directions. The source injected light along the y axis as a Gaussian beam from 300 to 800nm.

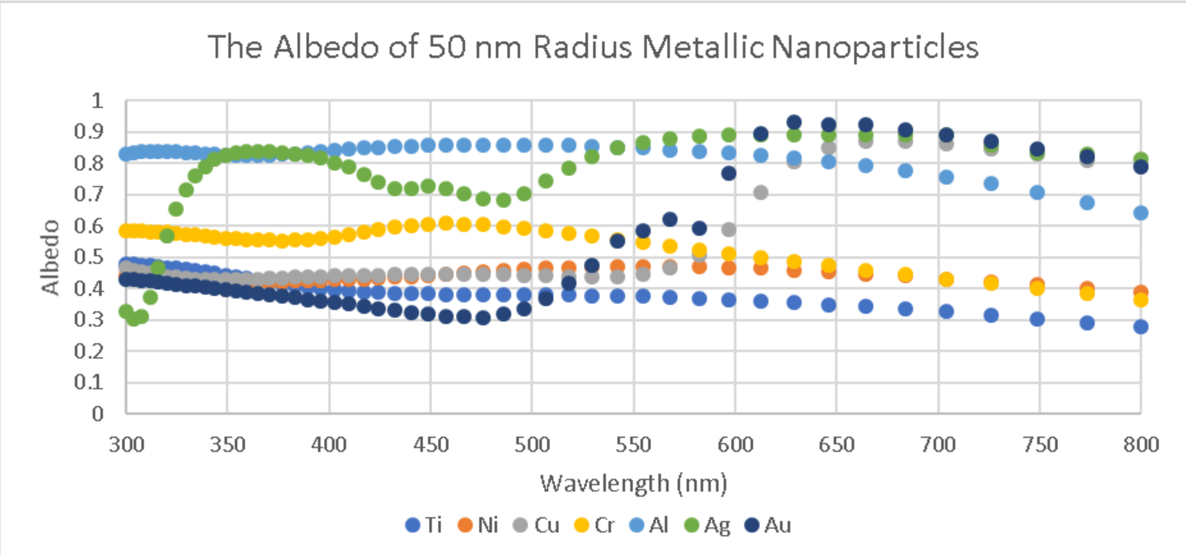

Fig.1: The albedo of 50 nm radius metallic nanoparticles as determined from Lumerical FDTD computations.

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The scattering and absorption cross-sections are computed natively within the software. A script was written to compute the wavelength dependent albedo as the ratio of the scattering cross-section to the sum of the scattering cross-section and the absorption cross-section. The integral of albedo was computed using the trapezoidal rule.

III. RESULTS

For 50 nm radius particles embedded in air the following statistics apply:

Metal	Average Albedo	St. Dev.	Integral of Albedo
Ti	0.33	0.09	70.10
Ni	0.38	0.08	84.77
Cu	0.44	0.10	120.84
Cr	0.50	0.16	101.74
Au	0.42	0.15	120.36
Al	0.76	0.15	170.86
Ag	0.64	0.21	174.50

For 50 radius particles embedded in index 1.8 the following statistics apply:

Metal	Average Albedo	St. Dev.	Integral of Albedo
Ti	0.40	0.05	92.47
Ni	0.44	0.02	109.98
Cu	0.52	0.16	149.62
Cr	0.54	0.06	129.00
Au	0.50	0.21	151.02
Al	0.82	0.05	201.95
Ag	0.75	0.15	200.71

The metal with the highest average albedo throughout the visible is aluminum. Followed by silver, then chromium, then copper, then gold, then nickel, then titanium. The metal with the smallest standard deviation throughout the visible is nickel. Then titanium, then copper, then gold, then aluminum, then chromium, then silver. While aluminum has the highest average albedo, silver has a higher integral of albedo and therefore will have better overall spectral performance when incorporated into OLED devices and optimized for nanoparticle concentration considerations.

IV. CONCLUSIONS

Aluminum has the highest average albedo in the visible but silver has the highest integral of albedo. Silver performs better in the red, while aluminum performs better in the blue. A scattering layer mixed of these two particles may prove better than either one alone. Simulations should be carried out of these materials in higher index environments such as glasses and silicon nitride.

When employing small metallic nanoparticles in display devices silver scatterers should be employed in the red pixels and aluminum in the blue pixels. For lighting and tandem OLED devices, silver nanoparticles are the best 50 nm radius particle available.

Nickel, Chromium, Gold, Aluminum and Silver all have decreases in albedo when embedded in a higher refractive index, primarily in the red. In the blue, overwhelmingly, albedo increases are apparent in these materials.

Again, future studies should seek to explore the size-dependence of the albedo and its value in common dispersive glasses such as ITO. Furthermore, they should seek a method to inter-relate the out-coupling efficiency with the wavelength-dependent albedo, which comes from the material considerations, and the nanoparticle concentration.

While this manuscript indicates the amount of light that is retained, and therefore suggests which plasmonic particles will have the greatest out-coupling efficiency upper limit, it does not tell the angular dependence of the scattering process nor what fraction of the scattering process is due to light triggering the total internal reflection criterion versus Fresnel reflections.

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REFERENCES

[1] N.K. Patel, S. Cinà, J.H. Burroughes, IEEE J. Select. Top. Quant. Electron. 8, 346 (2002).
[2] D.S. Mehta, K. Saxena, in: Proceedings of the Ninth Asian Symposium on Information Display (ASID-06) p. 198 (2006).
[3] M.H. Lu, J.C. Sturn, J. Appl. Phys. 91, 595 (2002).
[4] T. Nakamura, H. Fuji, N. Juni, N. Tsutsumi, Opt. Rev. 13, 104 (2006).
[5] H.J. Peng, Y.L. Ho, C.F. Qiu, M. Wong, H.S. Kwok, SID 04 Digest 158 (2004).
[6] N.K. Patel, S. Cinà, J.H. Burroughes, IEEE J. Select. Top. Quant. Electron. 8 346 (2002).
[7] T. Nakamura, H. Fuji, N. Juni, N. Tsutsumi, Opt. Rev. 13, 104 (2006).