Influence of sinter necks on the spectral behaviour of ITO aggregates

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Abstract

Different degrees of sintering between nanoparticles lead to different interparticle rigidity and thereby to different material properties. Here, we extend our recent study regarding nano-scaled sintered dimers of ITO to monodisperse fractal-like aggregates and investigate possible approaches for a fast measurement method to characterize the size of connections between the primary particles.

1 Introduction

Fractal-like aggregates are commonly modelled as assemblies of primary particles (spheres) positioned in point contact only. On the other hand, sintered nano-particles can be divided into two groups [1]: 'soft agglomerates' which are characterized by weak van der Waals forces holding the particles together and 'hard agglomerates' (aggregates) where the particles are bound chemically. Depending on their state such agglomerates or aggregates can show quite different behaviour for conductivity, appearance, stability, etc. It follows that the necking can be expected to have a significant impact and should not be neglected. Now, the morphological parameters of fractal-like aggregates can be characterized using different light scattering methods [2]. Here, we would like to present actual results for light scattering simulations for aggregates of Indium Tin Oxide (ITO).

2 Optical properties of ITO

Fig. 1 shows the refractive index, the reflectance and the permittivity (see e.g. [3]) for ITO. The material data is taken from Franzen [4] (Drude model parameters). One can see that the real part of the refractive index n constantly drops until ≈1200nm while the imaginary part k steeply increases starting from ≈1000nm. As a result the reflectance of the bulk material goes up starting from 1000nm, reaching its maximum around ≈1500nm. Now, as a rule of thumb plasmonic resonance for nanospheres occur around $\varepsilon_{real} \approx -2$, and for nanorods at more negative values (see e.g. Cortie et al. [5]). For ITO, $\varepsilon_{real} \approx -2$ is found at ≈1300nm. As a result one can expect interesting spectral behaviour of ITO in the wavelength area from 1000nm to roughly 1700nm.

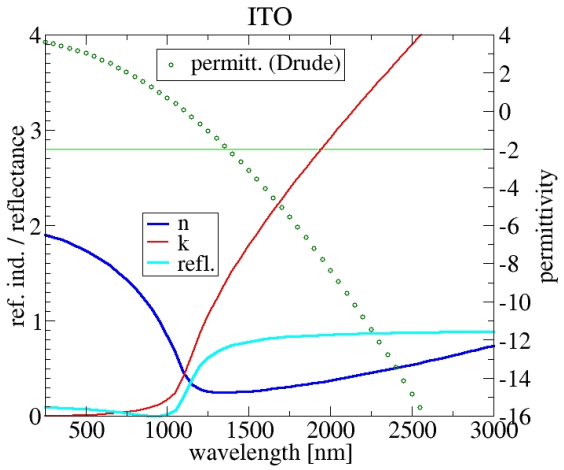

Figure 1 *Optical properties of ITO.*

3 Investigated geometries

Starting from sintered nano-scaled dimers we successively increase the number of particles to create fractal-like aggregates. For the investigations of sintered dimers we use a Cassini-oval curve to describe the shape [6]. For the clusters we assume that the primary particles are bonded by a cylinder-like neck between them. This is outlined in Fig. 2.

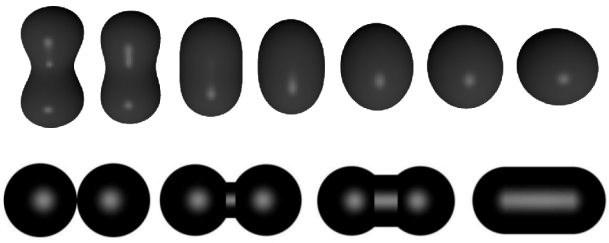

Figure 2 *Particle shapes. Top: Cassini-oval based dimers. Bottom: primary particles connected together by a cylindrical neck. The diameter of the cylinder in relation to the primary particle diameter is (from left to right) Y_{con}=0.00, Y_{con}=0.50, Y_{con}=0.75 and Y_{con}=1.00. The volume of the structure is constant for the calculations (the scaling of the presentations here differs).*

A factor Y_{con} defines the relation between the diameter of the connecting cylinder to the diameter of the primary particle: $Y_{con} = d_{cyl} / d_{particle}$. Therefore Y_{con}=0.0 means point-contact while Y_{con} =1.0 describes a cylinder with rounded ends.

The fractal-like aggregates were generated by the Cluster-Cluster algorithm proposed by Filippov et al. [7]. An exemplarily structure is presented in Fig. 3.

Figure 3 *Fractal-like aggregate models. Parameters: Rp=25nm, Np=50, D f=1.8 and Kf=1.3. The size of the connections presented here: Y_{con}=0.0, Y_{con}=0.5 and Y_{con}=1.0. The volume of the structure is constant for the calculations.*

4 Light scattering calculations

For the light scattering calculations for the sintered dimers we use the Nullfield Method with Discrete Sources (NFM-DS) [8]. This is a variant of the conventional Nullfield Method [9] that allows overcoming the usual numerical restrictions regarding the scatterer's aspect ratio and concave shape [10].

For the light scattering calculations for fractal-like aggregates we use the Discrete Dipole Approximation (DDA) [11]. Here, the DDScat code by Draine and Flatau [12] was applied to the investigations.

5 Results

In the following we would like to present results for the Cassini-based dimers (Fig. 2) as well as the cluster structure (Fig. 3) with cylinder-shaped necks.

5.1 Cassini-oval based dimers

The two original primary particles for this investigations have a diameter of d=50nm. Fig. 4 shows the spectral intensity for a wavelength range of 250-3000nm. These are the orientation averaged results for parallel polarization in forward direction.

One can observe a shift to longer wavelengths the more concave the shape gets. This happens between wavelengths from ≈1400nm to ≈1800nm and thereby corresponds with the expectation regarding the optical properties of the bulk material (see section 2). Note that the curve for the most concave shape shows a pattern that implies that this calculation was on the border of what is numerically possible [10].

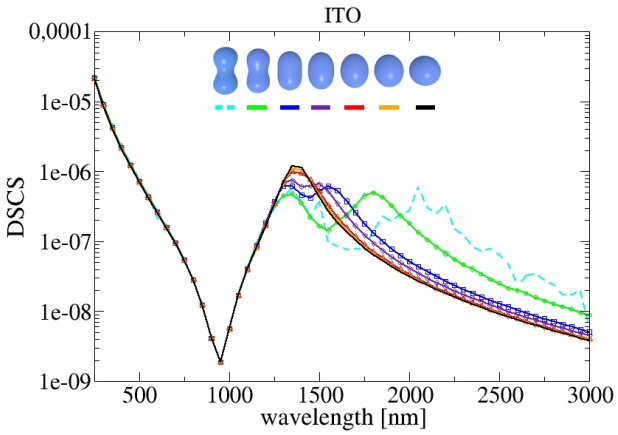

Figure 4 *Results for Cassini-based dimers. The primary particle diameter is d=50nm, orientation averaged results for the Differential Scattering Cross Section (DSCS).*

5.2 Fractal-like aggregates

In Fig. 5 the results for the cluster outlined in Fig. 3 are presented. The investigated necks are Y_{con}=0.5 and Y_{con}=1.0, the primary particle diameter is d=50nm again. Plotted are the orientation averaged extinction, scattering and absorption cross sections.

One can see that the thickness of the sinter-neck has a significant influence on the spectral behaviour in the domain of plasmon resonances, driven by the absorption.

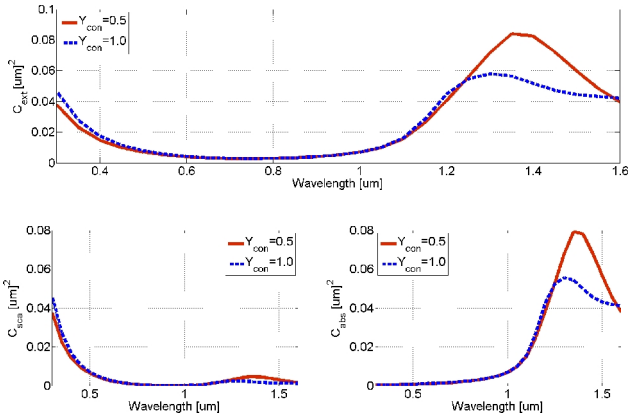

Figure 5 *Results for a cluster (Fig. 3) with Y_{con}=0.5 and Y_{con}=1.0, primary particle diameter d=50nm. Shown are the orientation averaged extinction (top), scattering (bottom left) and absorption cross sections (bottom right).*

6 Outlook

The observed effects for the spectral behaviour might be of interest for the development of a fast, in situ measurement method for the degree of sintering during a

production process. For example the intensity difference for specifically chosen wavelengths could be used for this.

7 Acknowledgement

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8 References

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