Plasmon Resonance Modelling of Nanostars

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STARSTEM

INTRODUCTION

Finite Difference Time Domain (FDTD) method is a numerical modelling method that involves solving the time dependent Maxwell Equations.

FDTD is a useful method when trying to simulate nanostructures with complex features that are comparable in size to the incident wavelength of light used.

The Localised Surface Plasmon Resonance (LSPR) of a structure can be modelled using FDTD to give an insight into the structure's effectiveness for optical sensing. [1]

Here, we demonstrate the effectiveness of nanostars for optical sensing and how the geometry of the nanostar can be altered to tune the peak absorption to a desired wavelength range.

MOTIVATION

Regenerative medicine, particularly stem cell therapy has shown great potential in the treatment of a wide range of illnesses.

However, it is not clear yet how stem cell treatment works inside the body and therefore makes it difficult for new therapies involving them to be approved.

Optoacoustic Imaging (OAI) takes advantage of the photothermal effect and is inherently non-invasive. OAI matched with the electrodynamic fields of nanoparticles could give sophisticated images of stem cells and insights into their healing process.

LOCALISED SURFACE PLASMON RESONANCE (LSPR)

LSPR occurs when incident light's electric field induce coherent oscillations of the free conducting electrons on the surface of a nanoparticle.

While bulk material's optical properties can be described in terms of their dielectric constant, nanomaterials optical properties are dictated by the LSPR of the material.

It is important to understand how this electron cloud interacts with incident light and other parameters as the change in a couple of nanometres of the size can drastically affect properties of the material such as the peak absorption. [2]

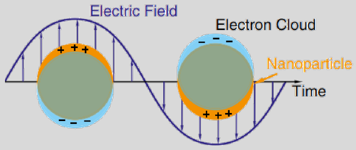

Fig. 1. Schematic of LSPR. The induced oscillating electric dipole greatly increases the scattering and absorption at the resonant wavelength. [3]

REFERENCES

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SIMULATION SET UP

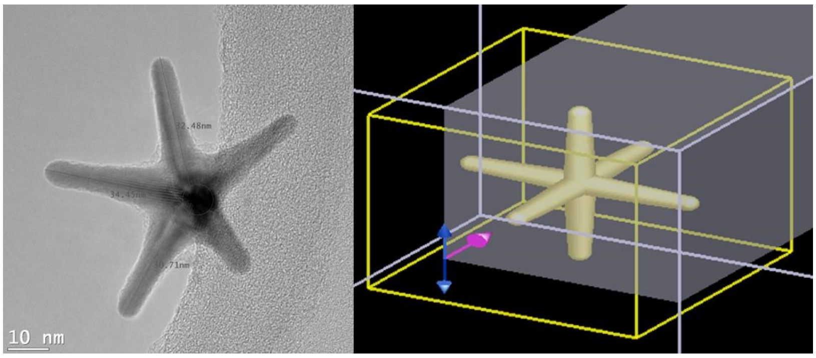

Fig. 2. **Left)** HRTEM image of synthetised nanostar. **Right)** Simulated 3-D model of nanostar in FDTD.

Simulations were run in FDTD software by Lumerical Inc. Parameters that were kept constant throughout the simulations were the material used, Au (Gold) Johnson and Christy, and the incident light source is centred at 1064 nm matching the emission peak of a Nd:YAG laser.

RESULTS AND DISCUSSION

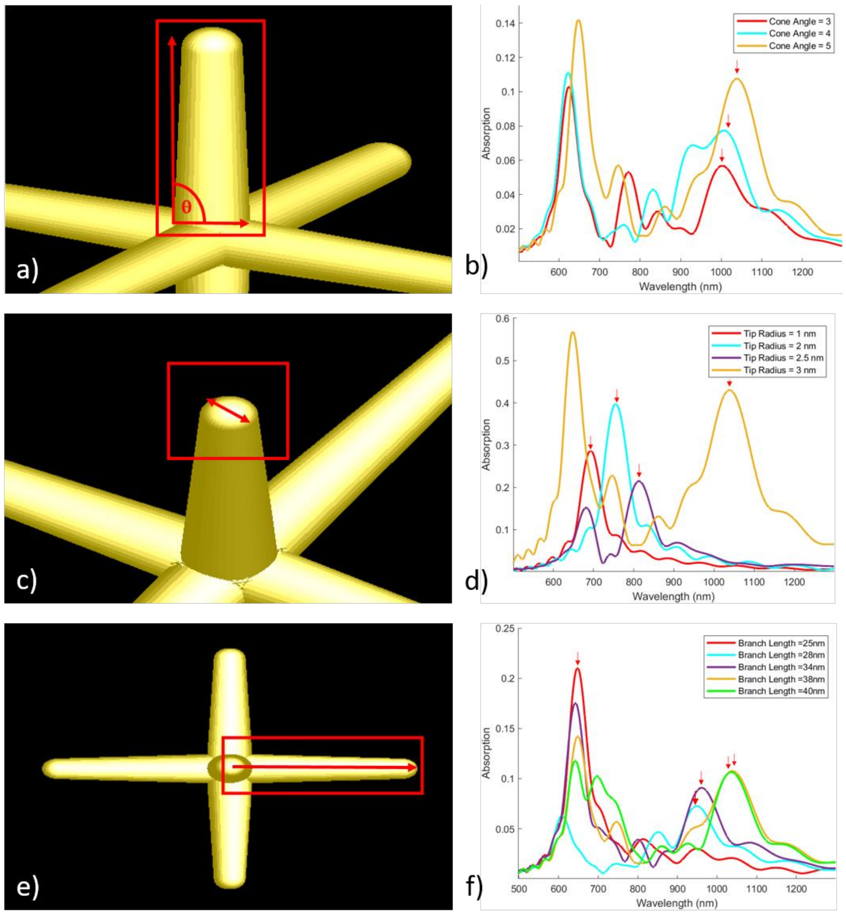

Fig. 3 **a)-b)** Model and absorption spectra of nanostar with varying cone angle. **c)-d)** Model and absorption spectra of nanostar with varying tip radius. **e)-f)** Model and absorption spectra of nanostar with varying branch length.

- Desired absorption for the nanostar is 1064 nm, roughly the emission peak of a commercially available Nd:YAG laser.
- Figure 3 show simulated absorption spectra of the nanostars showing red-shift of the resonance peak in the NIR range with increasing cone angle, from 3° to 5°, with increasing tip radius, from 1 nm to 3nm and also an increase in branch length, from 25 nm to 40 nm.
- Maximum resonance peak in the NIR range was found with a cone angle of 5°, a tip radius of 3 nm and a branch length of 38 nm (plotted in gold above).
- Results show that aspects of the absorption can be controlled by adjusting the above geometrical features. Further adjustments to the geometrical shape of the nanostar can be simulated to fine tune the absorption to as close 1064 nm as possible.

TOMI Tissue optics & microcirculation imaging

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