LOCALIZED SURFACE PLASMON RESONANCE AND DAMPING MECHANISMS OF UNCONVENTIONAL TRANSITION METALS

Faith sila[1], Benjamin Mbaluka[1], Martin Riara[1] & Ngei Katumo[2]

[1]South Eastern Kenya University, Kenya, [2] Karlsruhe Institute, German

Background

1. Introduction (or educational background)

Noble metal NPs have garnered significant interest due to their unique optical properties, which are heavily influenced by their size, photon energy, electronic structure FWHM and LSPR (Zhang & Chen, 2021). As NP size increases, FWHM broadens due to enhanced radiative damping and multipolar effects. (Kheirandish *et al*., 2023). To extract the plasmonic properties of the resonance, Modified Long Wavelength Approximation(MLWA) is used for the single NP polarizability. Noble metals (Au, Ag) dominate plasmonics: excellent LSPR but expensive and limited in spectral range. Unconventional transition metals (e.g., Zn, Rh, Re, Mo, Ta, Ti, Sc) . Some of these Unconventional transition metals offer lower cost, UV-range operability, Broader spectral tunability.

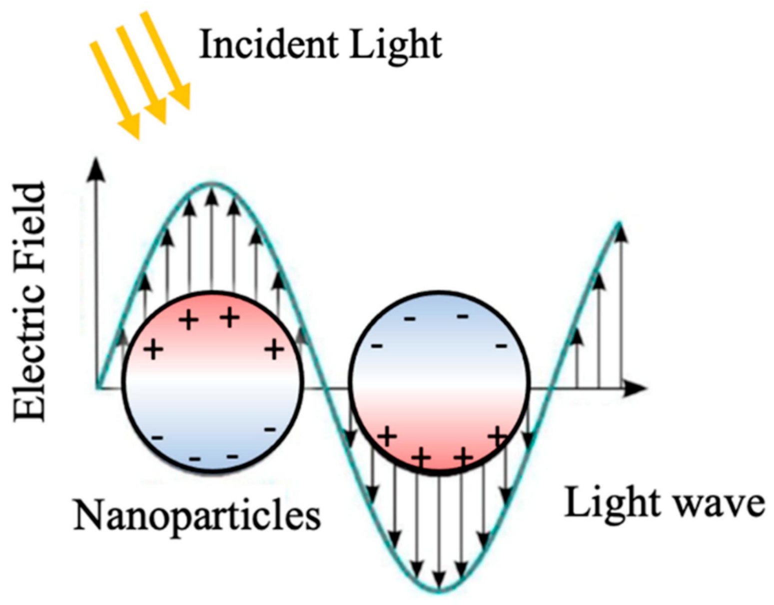

Fig. 1: Schematic description of LSPR in metallic NPs through oscillation of free electrons on the NP surface.

2. Problem statement

Gold is lossy, relatively expensive and not readily available. It's also limited to UV range due to the presence of interband transitions, technological constraints. Oxidation. Silver nanostructures experience aging. This study addresses this research gap by examining how NPs sizes, ranging from 10 nm to 400 nm affects LSPR and FWHM using the Mie theory. Among the studied metals are Zinc ,Gold, Silver, Rhodium , Rhenium , Molybdenum , Tantalum , Titanium , and Scandium

Current Work

1. Objectives

- To extract Mie scattering and absorption data from MieApp.
- To investigate the optical properties (scattering, absorption, LSPR and FWHM) of the unconventional transition metals for broadband application.

2. Methodology

1. This study applies a hybrid methodology that combines literature based data analysis, theoretical modeling and numerical simulation. Mie theory & Modified Long Wavelength Approximation (MLWA) were applied.
2. MATLAB & MieApp were used for simulation (input: digitalized refractive index data).
3. Analysis of LSPR energy, FWHM, scattering/absorption (NP sizes: 10–400 nm). The extracted data was used to determine the electronic properties.

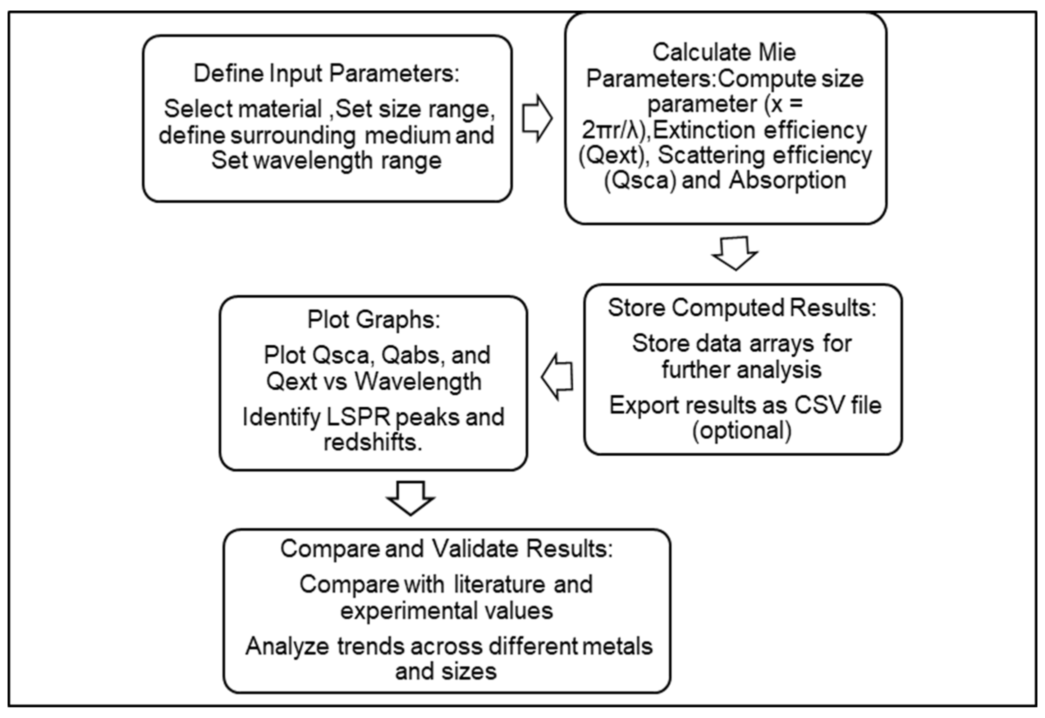

Fig. 2:MATLAB code flow chart

3. Results

- Small NPs (10–30 nm) have high absorption due to LSPR. scattering dominates Large NPs (>80 nm).
- LSPR red-shifts and broadens with size increase due to multipolar modes and retardation.
- LSPR peaks red-shift with increasing NP size. Material-dependent LSPR up to ~275 nm. Material-independent behavior above 275 nm due to dynamic depolarization. Mo & Ti show peak energies >6 eV (UV range).
- Ta lowest FWHM across all sizes. Ti highest FWHM (150–225 nm). Rh, Re, Zn and Sc have narrow peaks (better for sensing)
- Larger NPs (>200 nm) have FWHM narrows for most metals.

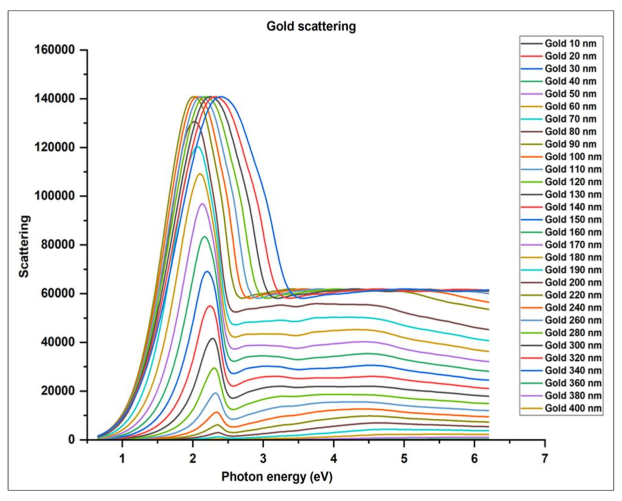

Fig. 3: Scattering of Au NPs

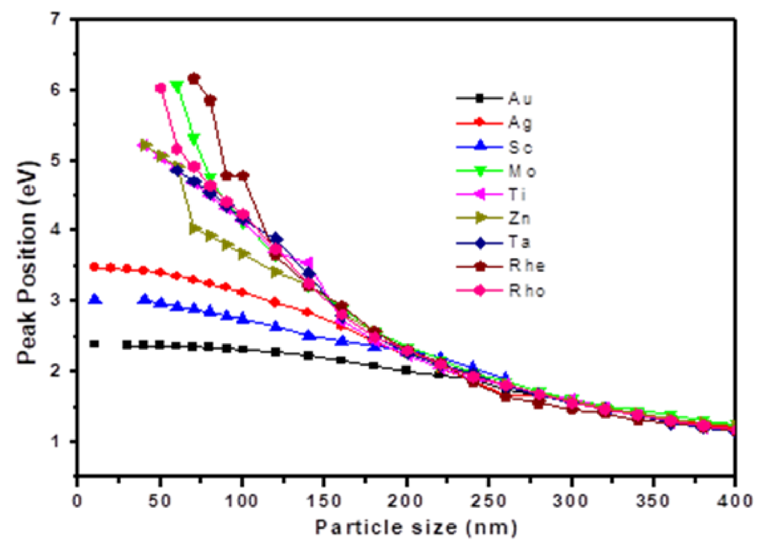

Fig. 4: LSPR vs NP size

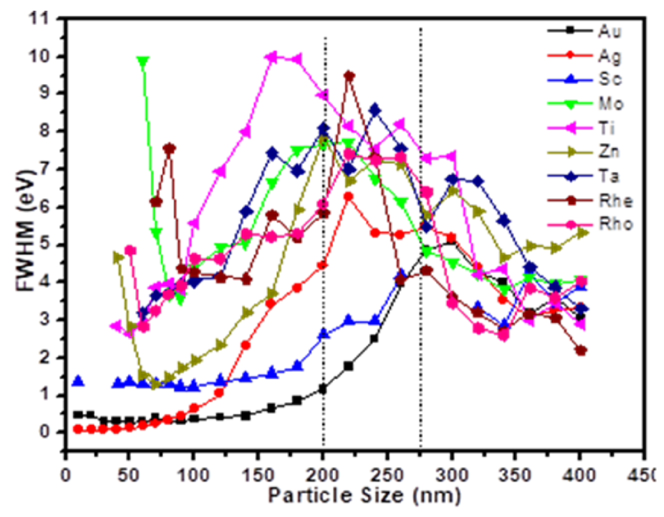

Fig. 5: FWHM vs NP size

Conclusion & Expectations

- NPs have a broad and tunable LSPR across a wide spectral range, making them promising candidates for broadband optical applications.
- Gold and silver NPs showed strong and narrow LSPR peaks with relatively low damping, especially in larger NPs of size 100 nm to 400 nm.
- Larger NPs of size range 100 nm – 400 nm demonstrated a broader spectral response due to increased radiative damping.
- In addition, interband transitions in these unconventional transition metal NPs contributed to LSPR broadening, which enhanced the overlap of plasmonic peaks across the visible and near-infrared regions.

References

- Zhang L. & Chen Y. Alloying Palladium with Gold for Tunable Plasmonic Nanoparticles. *ACS Nano* 14. 2021. P. 5678–5685.
- Kheirandish A., Sepehri Javan N. & Mohammadzadeh, H. Modified Drude model for small gold nanoparticles surface plasmon resonance based on the role of classical confinement. 2023. *Preprint*.

Acknowledgment

I would like to acknowledge Dr. B. Mbaluka , Dr. Martin Riara and Dr. Ngei Katumo for their academic guidance..

Contact: faithsila422@gmail.com.
+254 704 856 502

UNIVERSITY OF NAIROBI