

Modeling of the Electrostatic (Plasmon) Resonances in Metallic and Semiconductor Nanoparticles

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It is known that small dielectric objects can exhibit resonant behavior at certain frequencies for which the object permittivity is negative and the free-space wavelength is large in comparison with object dimensions [1]. This phenomenon usually occurs at nanoscale and at optical frequencies where the above two conditions can be simultaneously satisfied. These resonances are electrostatic in nature, and they result in powerful localized sources of light, which may find applications in nano-lithography, nanophotonics, surface-enhanced Raman scattering, biosensors, and optical data storage. These resonances in semiconductor nanoparticles are of special interest because they can be controlled through optical manipulation of carrier densities. This optical controllability can be utilized for the development of nanoscale light switches and all-optical transistors.

Currently these resonances in nanoparticles are found experimentally (or numerically) by probing dielectric objects of complex shapes with radiation of various frequencies, i.e. by using a “trial-and-error” method. There has not existed any technique for direct calculation of the negative values of dielectric permittivities, and the corresponding frequencies of electromagnetic radiation at which these resonances occur. In the paper, we present a new technique for direct calculation of resonance frequencies and to study unique physical features of these resonances for 3D nanoparticles. It is demonstrated that the resonance values of permittivity, and hence the resonance frequencies, can be directly (i.e. without laborious probing) found by computing the eigenvalues of a specific boundary integral equation. Once the resonance permittivity is known, the resonance frequency can be obtained by invoking appropriate dispersion relations. This approach also reveals the unique physical property of plasmon resonances: resonance frequencies depend on dielectric object shapes, but they are scale invariant with respect to object dimensions, provided that they remain appreciably smaller than the free-space wavelength.

It turns out that the integral operator in the integral equation is compact, and hence the plasmon spectrum is discrete. General properties of this spectrum have been studied along with the excitation conditions for plasmon resonances. A novel algorithm and robust codes have been developed to solve the corresponding eigenvalue problem. This algorithm and codes have been tested for spherical particles (see Table) where exact analytical solutions are available (Mie theory). Our computations have also reproduced (with sufficient accuracy) the experimental results (see Figure) for golden nano-rings recently published in [2]. In the paper, extensive numerical results will be presented and the optical controllability of plasmon resonances for semiconductor nanoparticles will be discussed.

Reference:

- [1] D. R. Fredkin and I. D. Mayergoyz, “Resonance Behavior of Dielectric Objects (Electrostatic Resonances)”, *Physical Review Letter*, Vol. 91, No. 25, Dec. 2003
- [2] J. Aizpura, P. Hanarp et al., “Optical Properties of Gold Nanorings”, *Physical Review Letter*, Vol. 90, No. 5, Feb. 2003

A full journal publication of this work will be published in the *Journal of Computational Electronics*.

Index	Eigenvalue	Mie	Index	Eigenvalue	Mie
1	2.999191	3	21	9.038890	9
2	2.999193	3	22	9.049236	9
3	2.999194	3	23	9.049301	9
4	4.980130	5	24	9.049312	9
5	4.980130	5	25	10.86267	11
6	4.980148	5	26	10.86268	11
7	5.022817	5	27	10.86291	11
8	5.022828	5	28	10.94108	11
9	6.927911	7	29	10.94200	11
10	6.981790	7	30	11.03838	11
11	6.981884	7	31	11.03839	11
12	6.981885	7	32	11.03846	11
13	7.027287	7	33	11.06465	11
14	7.027289	7	34	11.06497	11
15	7.027393	7	35	11.06500	11
16	8.915480	9	36	12.75603	13
17	8.915606	9	37	12.84736	13
18	8.915633	9	38	12.84819	13
19	8.979679	9	39	12.84824	13
20	8.979774	9	40	12.93150	13

Table: Eigenvalues of a single nano-sphere. The comparison of our numerical results with the theoretical ones (Mie theory).

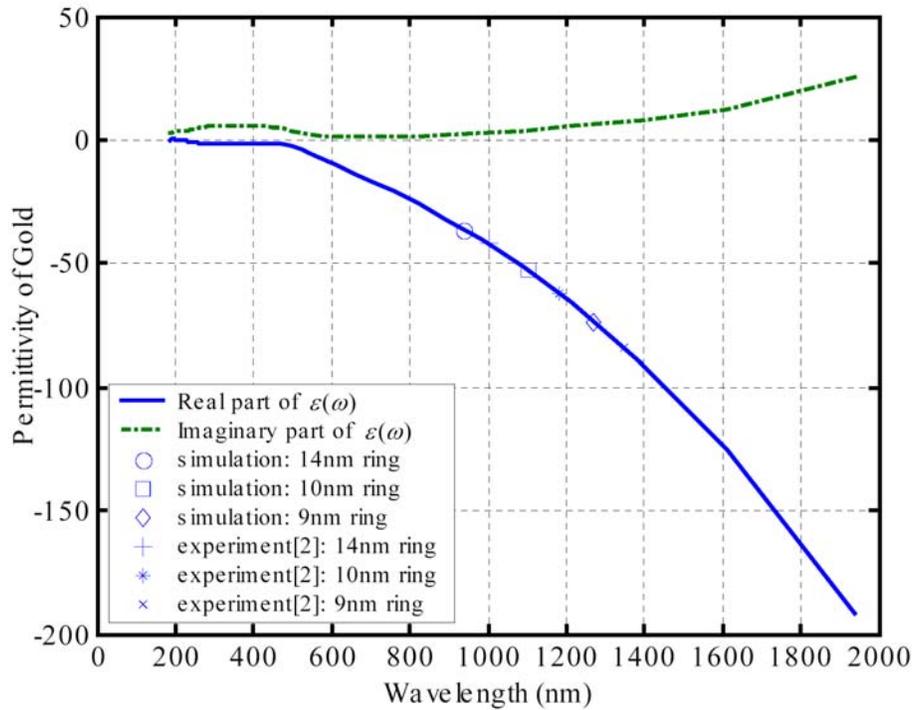


Figure: Resonant frequencies of golden nano-rings. The Comparison of our numerical results with recent experimental results in PRL paper [2].