Shape Optimization of a Nanoparticle for Plasmonic Enhancement in a Small Gap

Hak Yong Lee[1], Jeonghoon Yoo[1]

[1]Yonsei University, Korea

Abstract

Film-coupled nanoparticle is a structure composed of a thin gold (Au) film and Au nanoparticles on top of it. Between the Au nanoparticles and Au film, there are very thin self-assembled monolayers (SAMs) of amineterminated alkanethiolds. Due to the existence of the thin spacer layer of SAMs, a small gap exists between the Au nanoparticle and the Au film. When an electromagnetic (EM) wave hits the film-coupled nanoparticle structure, a dramatic enhancement of an electric field occurs in the small gap due to the localized surface plasmon resonance (LSPR) effect. The electric field strength increases intensively as the size of the small gap decreases.

In this study, we focus on the shape design of the Au nanoparticle to increase the electric field strength in the small gap. Structural optimization based on the phase field method was applied as a systematic design procedure for the nanoparticle. For reliable results, the size of the small gap is considered as 2 nm. A double well potential function was applied to constrict the optimization process of the phase field method to become a shape optimization. A smooth Heaviside function is proposed as a new filtering scheme and it was applied to design the nanoparticle. The resulting nanoparticle shape has a concave part in the lower right part, and the electric field strength has increased as 3.48 times compared to the strength in case of using initial circular shaped nanoparticle.

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