

## Computational Design of Nano-Optical Components Consisting of Nanoparticle Arrays

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Thanks to inherently strong plasmonic interactions, arrays of nanoparticles can be used for various purposes in diverse nano-optical applications. Recently, we have demonstrated that such well-designed arrangements can be employed as efficient couplers in nanowire transmission systems [1] and as beam-shaping structures to generate directive radiations from isotropic sources [2]. In this work, we further present computational design and optimization of compact components, such as diodes, which can be used in nano-optical systems.

A designed component in this study typically involves several hundreds of nanoparticles, such as nanocubes, with an optimal configuration in accordance with the desired electromagnetic response. The nanoparticles are analyzed as three-dimensional bodies, often together with the base system (e.g., a nanowire system), which are all formulated via surface integral equations. A stable formulation, which was particularly developed for plasmonic media, is employed to obtain accurate results. Discretization of the formulation leads to dense matrix equations, which are solved iteratively via a stable and efficient implementation of the multilevel fast multipole algorithm (MLFMA). The MLFMA solver is integrated into a module of genetic algorithms via dynamic accuracy control for efficient optimization of components [3]. We usually apply on-off optimization to arrange nanoparticles, as its success has been demonstrated many times in the context of coupling and beam steering applications. Once a design is obtained, it is exposed to various sensitivity analysis (using the same solver) to test its robustness against possible fabrication errors, such as geometric deformations, missing particles, and positioning/periodicity faults.

As an example, Fig. 1 presents the results of an optimization involving an 11x11 grid of 120x120x120 nm nanocubes to be used as a nano-optical diode. The grid is integrated onto a 5+5  $\mu\text{m}$  pair of nanowires, while on-off optimization is performed to determine the nanocubes to be kept/extracted for the best diode performance. Both nanowires and nanocubes are made of Ag, while the frequency is fixed to 250 THz. As excitations, pairs of Hertzian dipoles are placed in the vicinity of the nanowire ends. As shown in Fig. 1, depending on the placement of the excitation, the nanocube array successfully prevents or allows the transmission along the nanowires. It is remarkable that this type of an operation is achieved by using only around 100 nanocubes and with simple materials (without any material anisotropy).

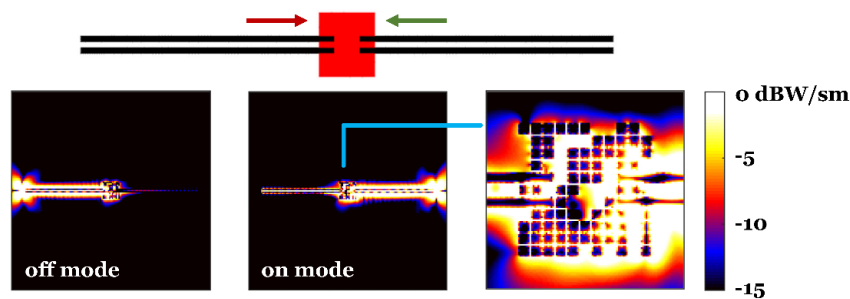


Figure 1. Power density distributions in the vicinity of a system involving a nano-optical diode (optimized array of nanocubes) integrated onto straight nanowires. Transmission through the diode is directional.

### References

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