Excerpt from the Proceedings of the 2011 COMSOL Conference in Tokyo

Light scattering simulation of nano-objects on the surface of silicon wafer by 3D finite element method

Y. Oshikane, T. Higashi, N. Taniguchi, M. Nakano and H. Inoue

Dept. of Prec. Sci. and Technol. , Grad. School of Eng. , Osaka University,
2-1 Yamada-oka, Suita, Osaka 565-0871, Japan
Email: oshikane@prec.eng.osaka-u.ac.jp
Phone&Fax: +81–6–6879–7278

1. Simulation of light scattering by nano structure

Nanotechnology is rated as a key technology of the 21st century. In the field of nano-optics already at present, state-of-the-art scientific experiments and industrial applications exhibit nanometer to sub-nanometer design tolerances. This motivates the development and application of fast and accurate simulation tools for these fields or electromagnetic (EM) field. But there would be no end or no answer if we start spending too much time on it, and accumulation of technical knowledge about EM simulation will give us powerful nearly-completed tool. We have adopted a program package for numerical simulations of Maxwell's equations based on advanced finite-element methods (FEM) [1,2]. We give a short introduction to the package and report on the current status of light scattering simulation, incorporating semi-infinite air, semi-infinite silicon, nano structure lying on boundary between them, and polarized oblique-incident plane light wave at visible region.

2. Light scattering simulation by finite element method

2.1 Simulation model and method

Fig. 1 shows a principle of visible light illumination of nano structure on the surface of mirror-polished silicon wafer in an actual experiment. P-polarized illumination laser light, which is plane wave, at incident angle of around 76 degrees mostly penetrate into bulk silicon by refraction of light. Reflected light from the surface is less than one percent. Therefore distracting stray light for detection of the nano structure is suppressed effectively. Numerical model for FEM simulation, as shown in fig. 2, reflects the experimental fundamentals. The model has an upper vacuum domain and lower silicon domain. The effective simulation regions are circumscribed by the walls of perfectly matched layer (PML) to prevent both multiple reflection and interference of outgoing light, which come out from simulation region. Each tetrahedral finite element is about one-tenth the size of light wavelength in medium. To replicate semi-infinite layers or periodic structure, boundary conditions of side surfaces parallel to

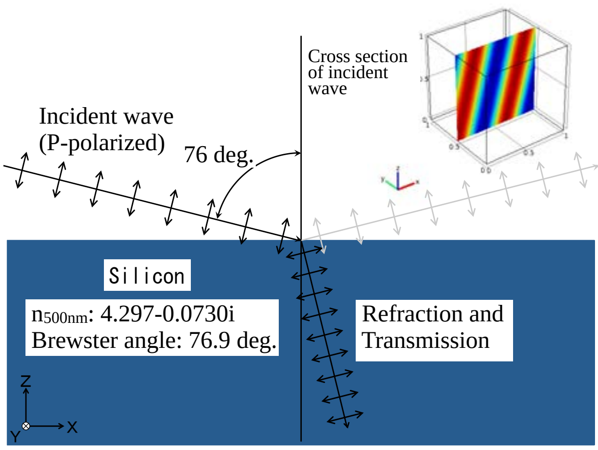

Fig. 1. Incident angle of light wave is set at 76 degrees. The illumination light wave is p-polarized and is refracted into bulk silicon.

YZ plane are determined by Floquet's theorem. Complex refractive index of material is determined by reference to a comprehensive book by E. D. Palik [4]. As a result, Snell's law of illumination light at the boundary of vacuum and silicon is reappeared in fig. 2.

2.2 Light scattering by subwavelength spherical nano particle

Light scattering by a spherical nano sphere as shown in the center of fig. 2 is calculated after the reproduction of background light field distribution without the sphere. Hence, in brief, Maxwell's equations determined in the whole region of model are solved explicitly by a sparse linear solver [3] in twice for about 40 minutes using dual Xeon Quad-Core with 40 gigabytes of memory.

3. Simulation result

Typical far-field pattern of scattering field $|\mathbf{E}_{scat}|$ by a 52-nm polystyrene latex (PSL) sphere in all directions at each wavelength of light is shown in fig. 3. The wavelength-dependent pattern is projected on to the model surface as indicated in fig. 2. Scattering characteristic depends strongly on wavelength of light, and both specular-like forward scattering and backward scattering are dominant.

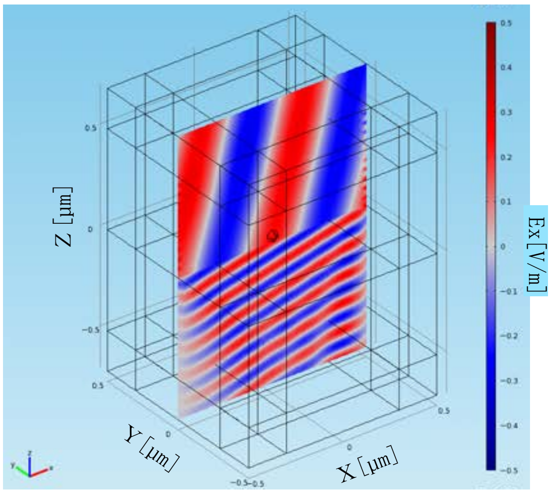

Fig. 2. Wireframe image of simulation model, and cross-sectional imaging of typical light wave propagation inside the model. Outermost hexahedral and cubic elements are defined as PMLs when light scattering calculation is done.

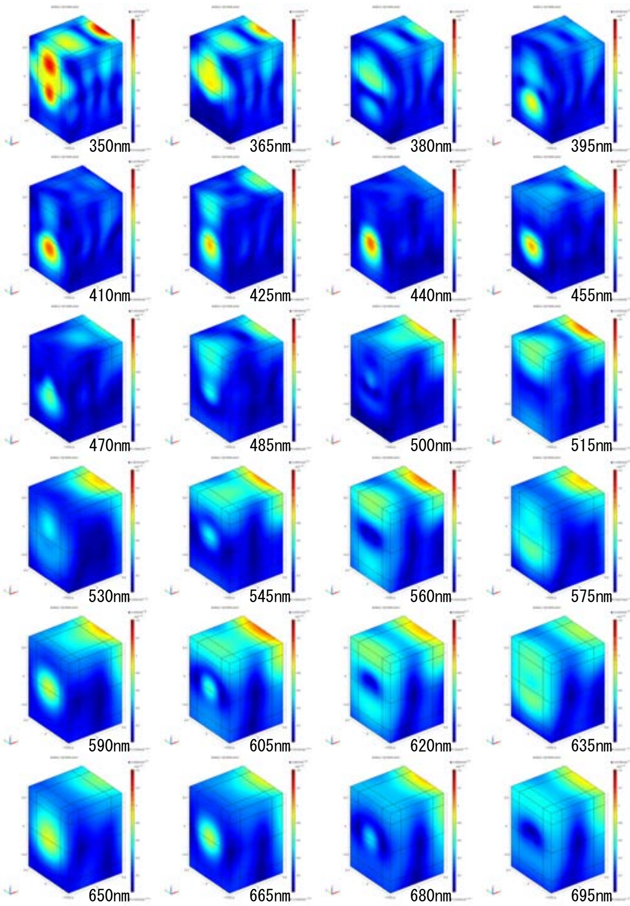

Fig. 3. Simulated $|\mathbf{E}_{scat}|$ distribution of scattering light by PSL sphere, 52nm in diameter, in all directions. Scattering characteristic depends strongly on wavelength of illumination light from 350 nm to 695 nm. Sharply-directed radiation pattern is observed at shorter wavelengths. In most cases, forward and backward scattering are prominent.

References

[1] J. Jin, *The Finite Element Method in Electromagnetics 2nd edition*, New York: John Wiley & Sons (2002).

[2] http://www.comsol.com/

[3] http://www.pardiso-project.org/

[4] E. D. Palik (ed.), *Handbook of Optical Constants of Solids*, San Diego: Academic Press (1985).