Nanophotonic Modeling
Lecture 3.6: FDTD Dispersion Modeling with QCRF

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Quadratic Complex Rational Function (QCRF) Model

\[ \varepsilon_r(\omega) = \frac{A_0 + A_1(j\omega) + A_2(j\omega)^2}{1 + B_1(j\omega) + B_2(j\omega)^2} \]

- Accurate in the frequency of interest [1].
- Computationally efficient.
- Recently, it is implemented to FDTD scheme [2,3].

The coefficients are found by applying the complex-curve fitting [6-8].

\[ \lambda_h = \sum_{k=0}^{m} \omega_k^h \]
\[ S_h = \sum_{k=0}^{m} \omega_k^h R_k \]
\[ T_h = \sum_{k=0}^{m} -\omega_k^h I_k \]
\[ U_h = \sum_{k=0}^{m} \omega_k^h (R_k^2 + I_k^2) \]

\[ \omega_k \text{: Sampled } \omega \]
\[ R_k \text{: Sampled } \text{Re}(\varepsilon_r) \]
\[ I_k \text{: Sampled } \text{Im}(\varepsilon_r) \]

\[
\begin{bmatrix}
A_0 \\
A_1 \\
A_2 \\
B_1 \\
B_2
\end{bmatrix} = \begin{bmatrix}
\lambda_0 & 0 & -\lambda_2 & T_1 & S_2 \\
0 & \lambda_2 & 0 & -S_2 & T_3 \\
\lambda_2 & 0 & -\lambda_4 & T_5 & S_4 \\
T_1 & -S_2 & -T_3 & U_2 & 0 \\
S_2 & T_3 & -S_4 & 0 & U_4
\end{bmatrix}^{-1} \begin{bmatrix}
S_0 \\
T_1 \\
S_2 \\
0 \\
U_2
\end{bmatrix}
\]

Complex curve fitting via QCRF model

Analytic absorption vs simulated absorption

- 3-D QCRF based FDTD takes 75 hours for full-spectrum analysis
- 3-D single frequency FDTD takes approximately $75 \times 200 = 15,000$ hours

RMS error = 3.9671%
Material dispersion fitting for Finite Difference Time Domain (FDTD) simulations

Better fitting guarantees more accurate calculations.

Analytic calculation

\[ R = \left| r^2 \right| = \frac{r_1^2 + r_2^2 + 2r_1r_2 \cos 2\theta}{1 + r_1^2r_2^2 + 2r_1r_2 \cos 2\theta} \]
The left figure indicates the experimental absorption rate for a 1500 nm thick c-Si solar cell. It is adapted from recently published research [4]. The right figure indicates the absorption rate obtained by the simulation.

- 3-D QCRF-FDTD simulation is performed using the same geometry in order to prove its accuracy.

Random surface texturing algorithm

\[ Z_{n+1} = f \cdot Z_n - \sqrt{1 - f^2} \cdot r_n \]

- Where \( Z_1 = r_1 \), \( r_n \) is an independent sampling from a random distribution of Gaussian variables with zero mean and unit variance.

- We expended this algorithm to 2-D and applied periodic boundary condition for each edge.

- Add double-sided correlation equation.

- Two variables:
  - Maximum texturing height
  - Correlation factor
From the flat structure to the totally random structure via random surface texturing algorithm

Higher correlation

Lower correlation


[5] Plan view SEM image of porous silica AR layer formed by vapour-etch method [56].