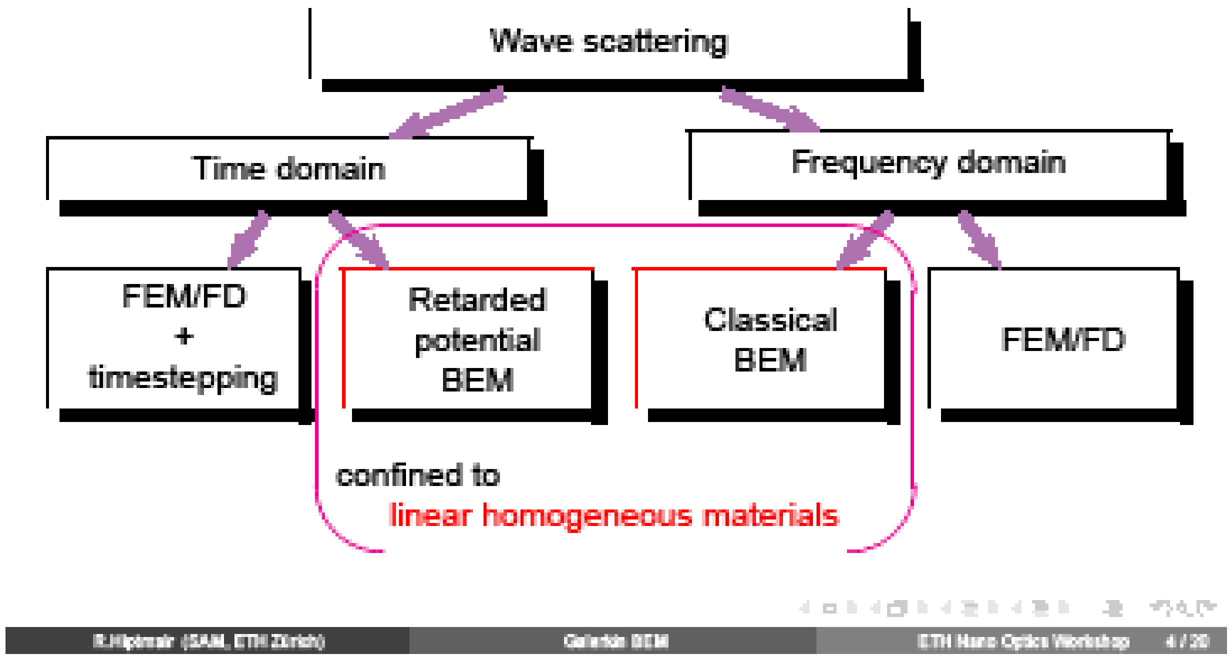
ΥΠΟΛΟΓΙΣΤΙΚΗ ΜΕΛΕΤΗ ΝΑΝΟΥΛΙΚΩΝ

Υπολογισμοί διάδοσης ηλεκτρομαγνητικών κυμάτων σε νανοδομημένα υλικά



Υπολογιστικές Μέθοδοι

Finite difference Time Domain
Finite Element
Multiple Scattering
Boundary Elements

Όλες αυτές οι μέθοδοι χρησιμοποιούν το ε και τη δομή των νανοδομημένων υλικών και υπολογίσουν τα T, R, A.

Finite difference time domain (FDTD) method:

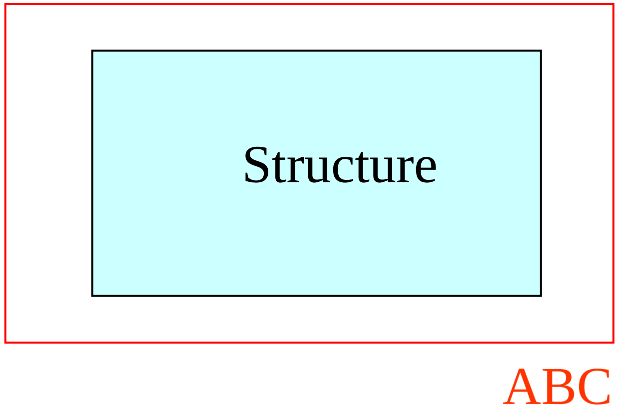
-Approximate the space and time derivatives in Maxwell's equations with finite differences.

-Use absorbing boundary conditions (ABC) to close the space.

-Use an initial pulse excitation (point source, a waveguide mode or a plane wave).

-Solve Maxwell's equations as a function of time.

-Do a Fourier transform to get spectral information out.



Maxwell's Equations

$$\frac{\partial \vec{E}}{\partial t} = \frac{1}{\varepsilon_0} \vec{\nabla} \times \vec{H}$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu_0} \vec{\nabla} \times \vec{E}$$

In 1D, they become:

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon_0} \frac{\partial H_y}{\partial z}$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}$$

Finite difference approximations of the partial derivatives in space and time:

$$\frac{\partial E_x(z,t)}{\partial t} = \frac{E_x^{n+1/2}(k) - E_x^{n-1/2}(k)}{\Delta t}$$

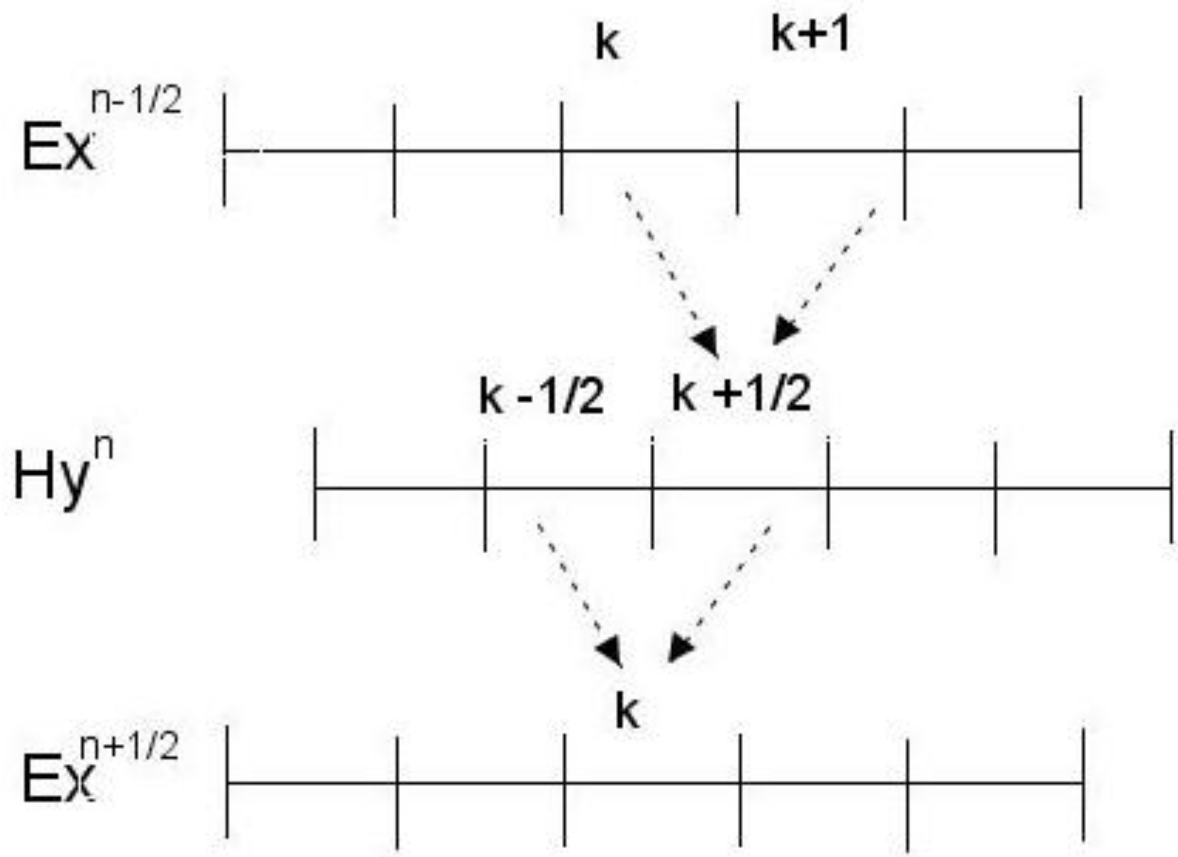
$$\frac{\partial H_y(z,t)}{\partial z} = \frac{H_y^{n}(k+1/2) - H_y^{n}(k-1/2)}{\Delta z}$$

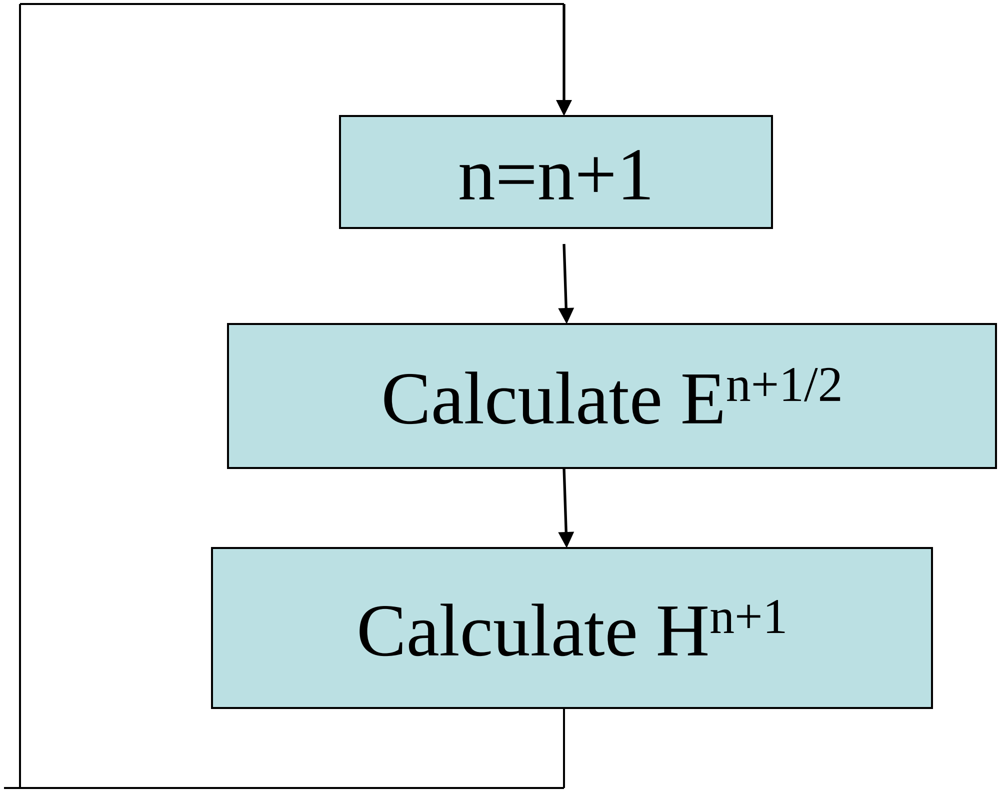
Each new value of the fields (E, H) is determined by the previous values:

$$E_x^{n+1/2}(k) = E_x^{n-1/2}(k) - \frac{\Delta t}{\varepsilon_0 \Delta z}\left[H_y^n(k+1/2) - H_y^n(k-1/2)\right]$$

$$H_y^{n+1}(k+1/2) = H_y^n(k+1/2) - \frac{\Delta t}{\mu_0 \Delta z}\left[E_x^{n+1/2}(k+1) - E_x^{n+1/2}(k)\right]$$

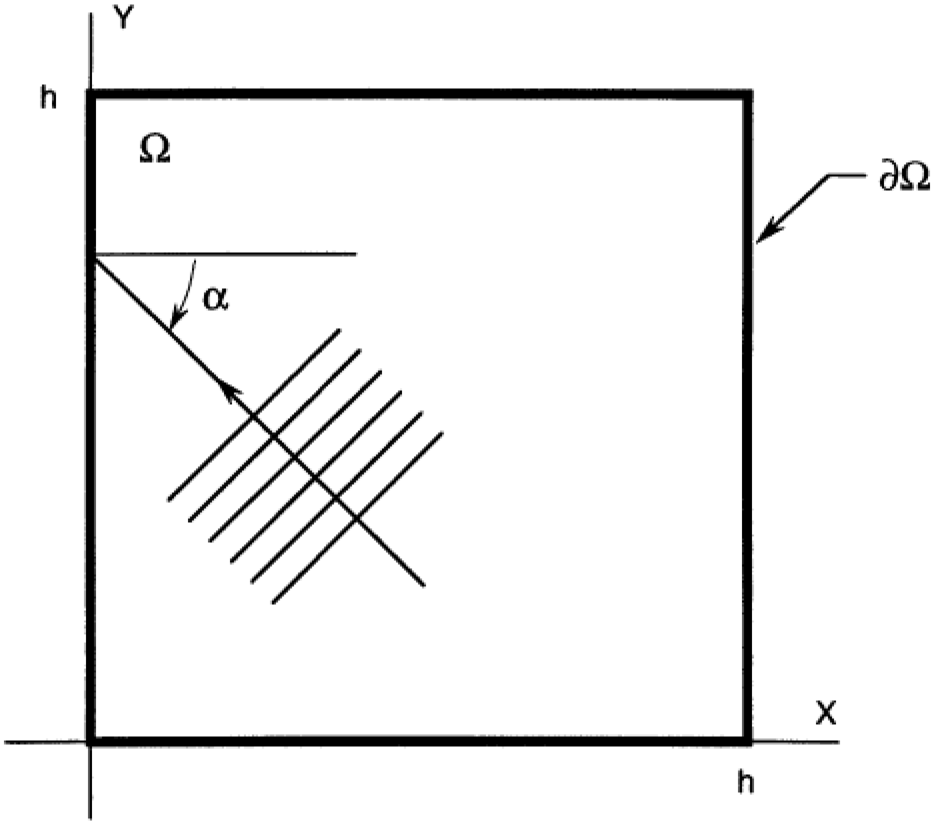
The k represents the location in the discrete space, while n represents the time:





Each time step represents an increment in the total time $T = n\,\Delta t$.

Absorbing Boundary Conditions

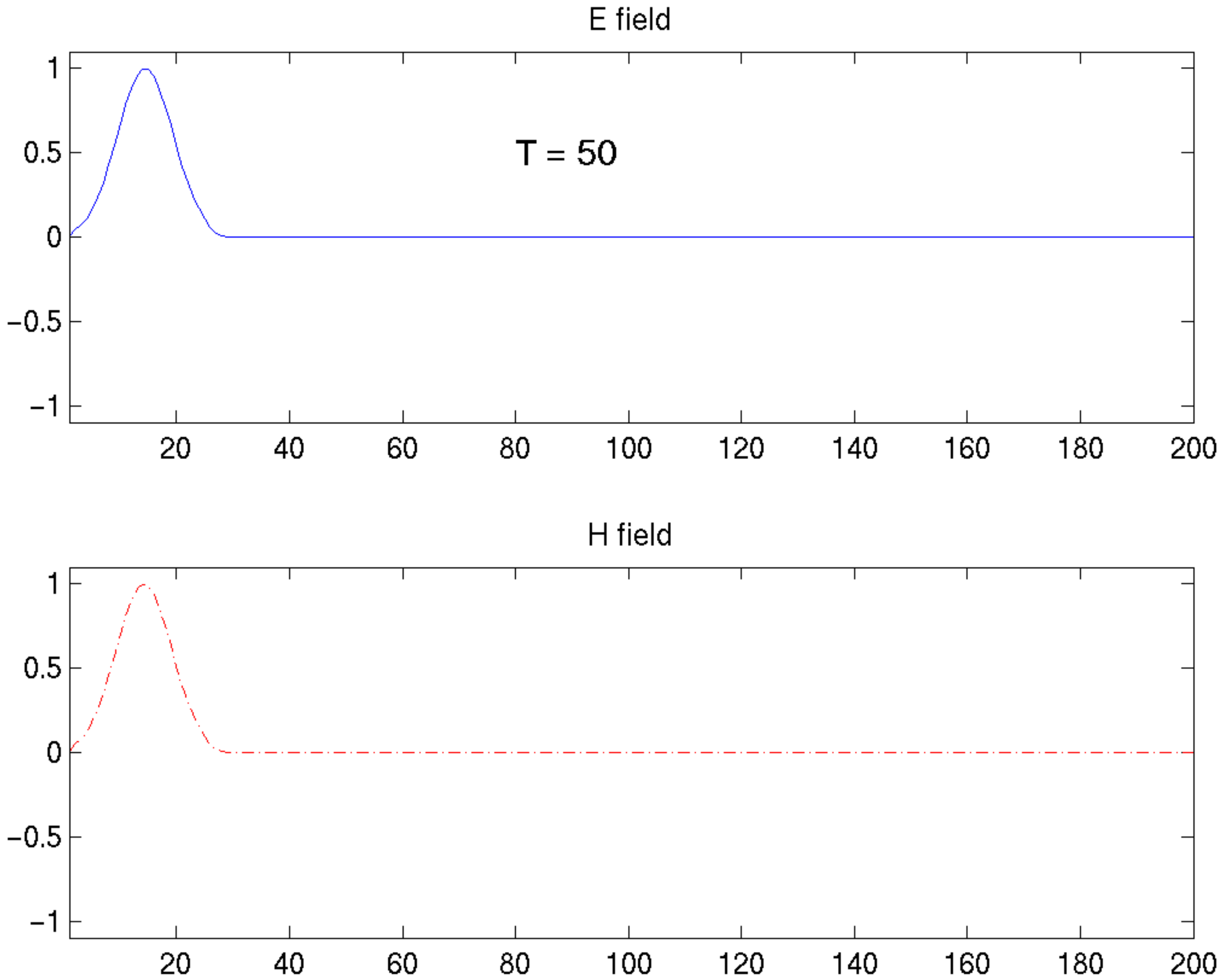


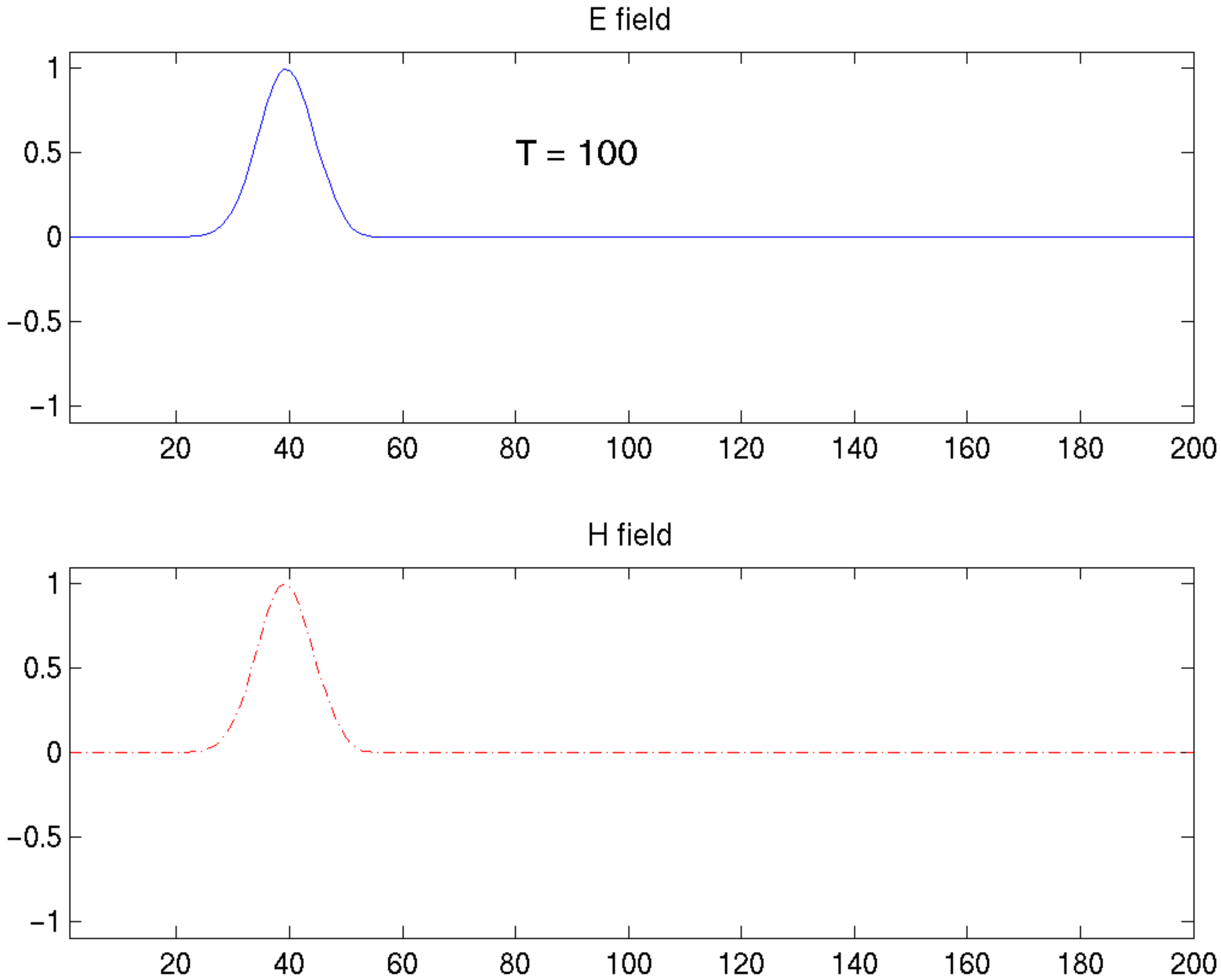
1st order Mur's ABC in 1D

$$E_x^{n+1/2}(0) = E_x^{n-1/2}(1) - \frac{c\Delta t - \Delta z}{c\Delta t + \Delta z}\left[E_x^{n+1/2}(1) - E_x^{n-1/2}(0)\right]$$

The following is a one-dimensional simulation of an EM pulse propagation in free space.
(T represents the number of time steps.)

``FDTD method for hyperthermia simulations,'' D. Sullivan (U. of Idaho)


E field
T = 50
H field
1
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200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−1
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40
60
80
100
120
140
160
180
200
H field
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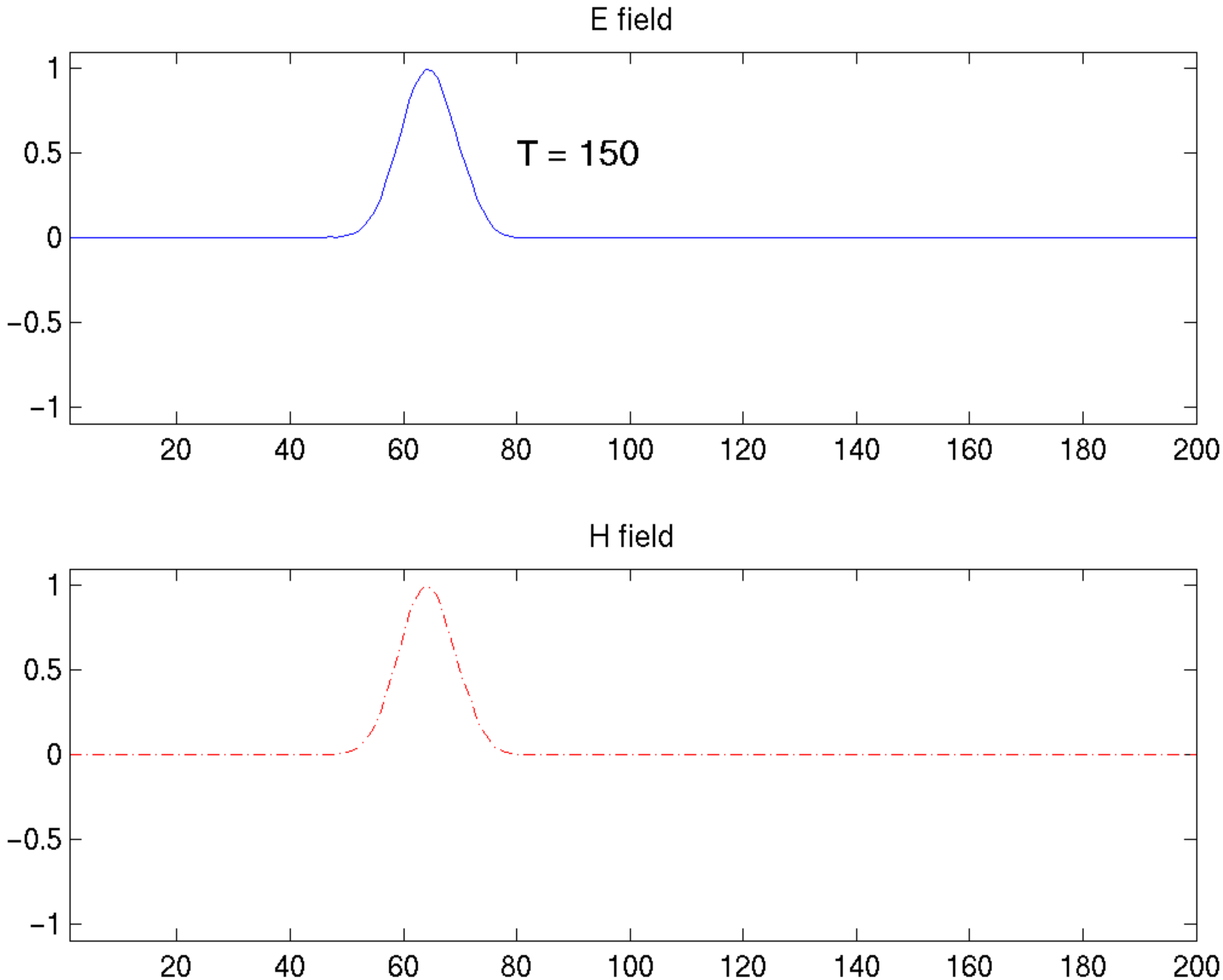
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200



E field
T = 150
1
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200
H field
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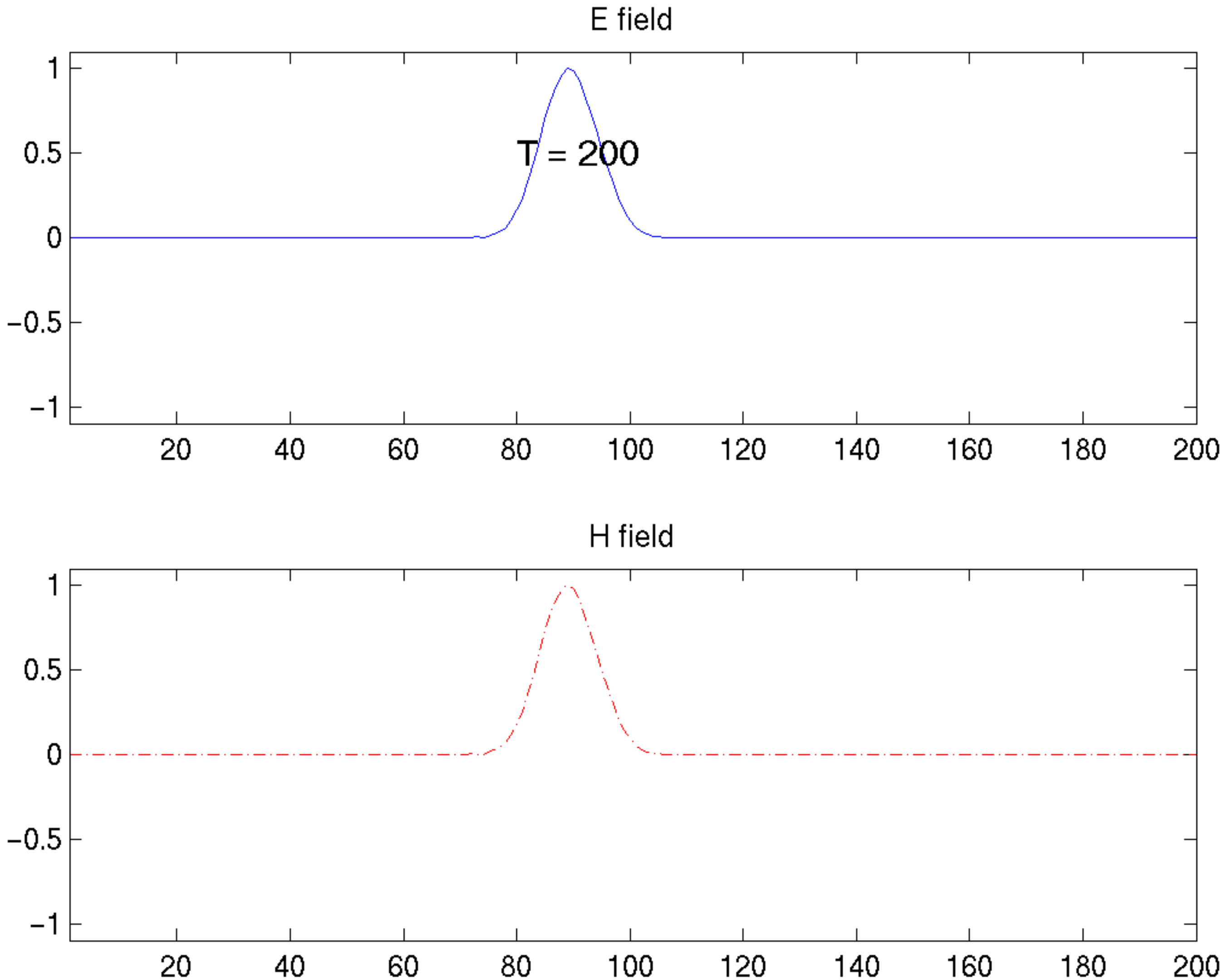
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200


E field
T = 200
1
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200
H field
1
0.5
0
−0.5
−1
20
40
60
80
100
120
140
160
180
200

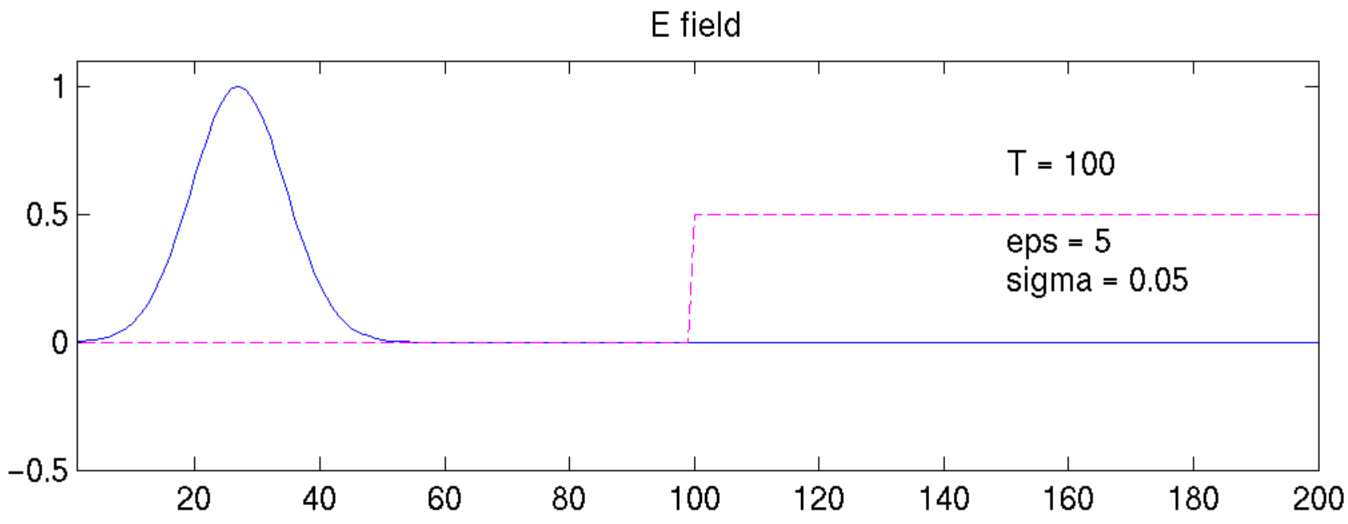
For lossy media:

$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\varepsilon_0 \varepsilon_r} \nabla \times \boldsymbol{H} - \frac{\sigma}{\varepsilon_0 \varepsilon_r} \boldsymbol{E}$$

$$\tilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}} E$$

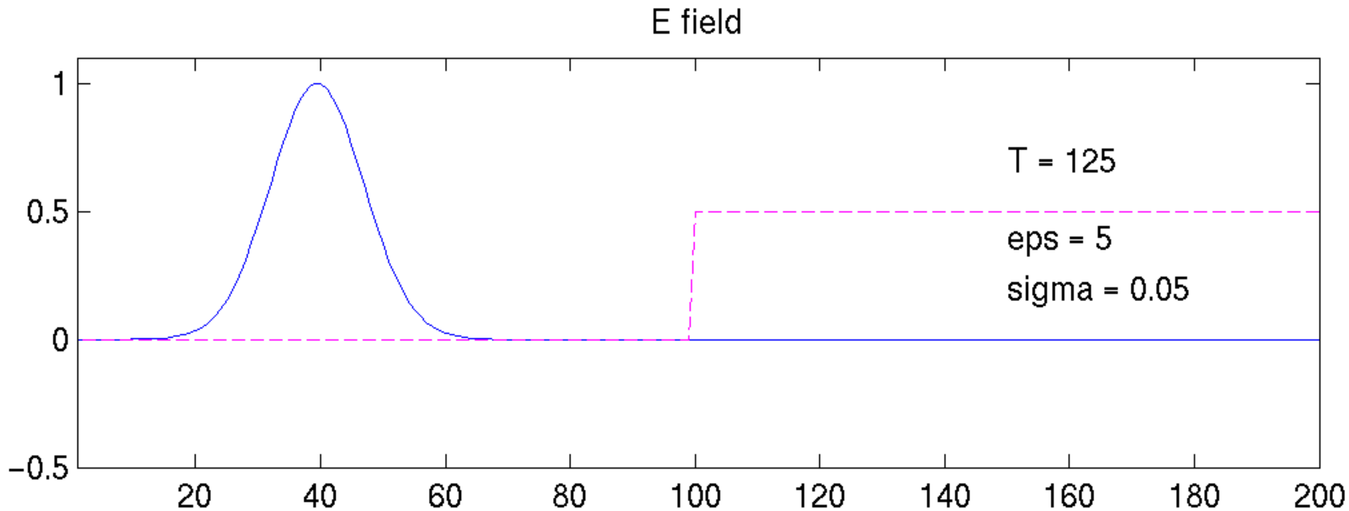
$$\tilde{E}_x^{\,n+1/2}(k) = \frac{\left(1 - \dfrac{\Delta t \cdot \sigma}{2\varepsilon_r \varepsilon_0}\right)}{\left(1 + \dfrac{\Delta t \cdot \sigma}{2\varepsilon_r \varepsilon_0}\right)} \tilde{E}_x^{\,n-1/2}(k) + \frac{1/2}{\varepsilon_r \cdot \left(1 + \dfrac{\Delta t \cdot \sigma}{2\varepsilon_r \varepsilon_0}\right)} \left[H_y^{\,n}(k+1/2) - H_y^{\,n}(k-1/2)\right]$$

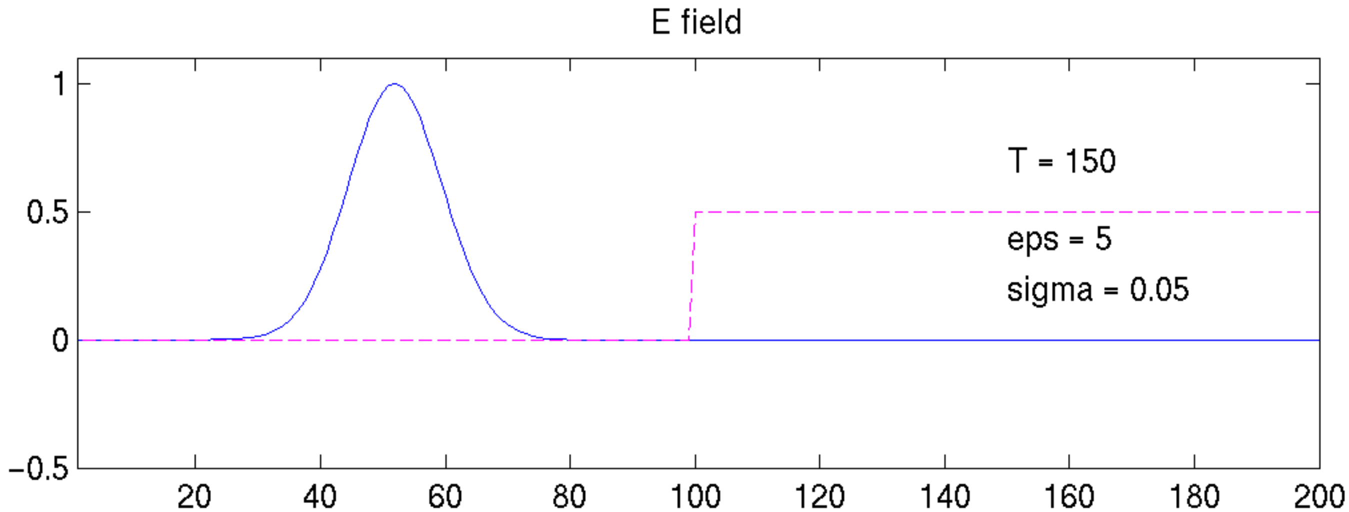
The following simulation shows an EM pulse propagating in free space and then striking a material with $\varepsilon = 5$, $\sigma = 0.05$.

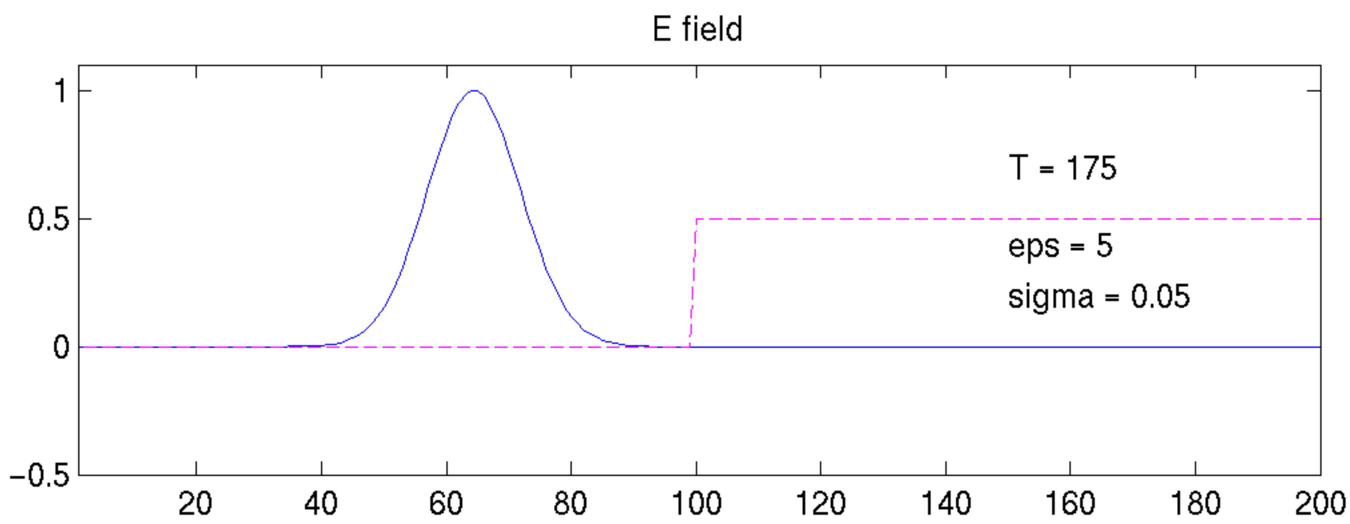


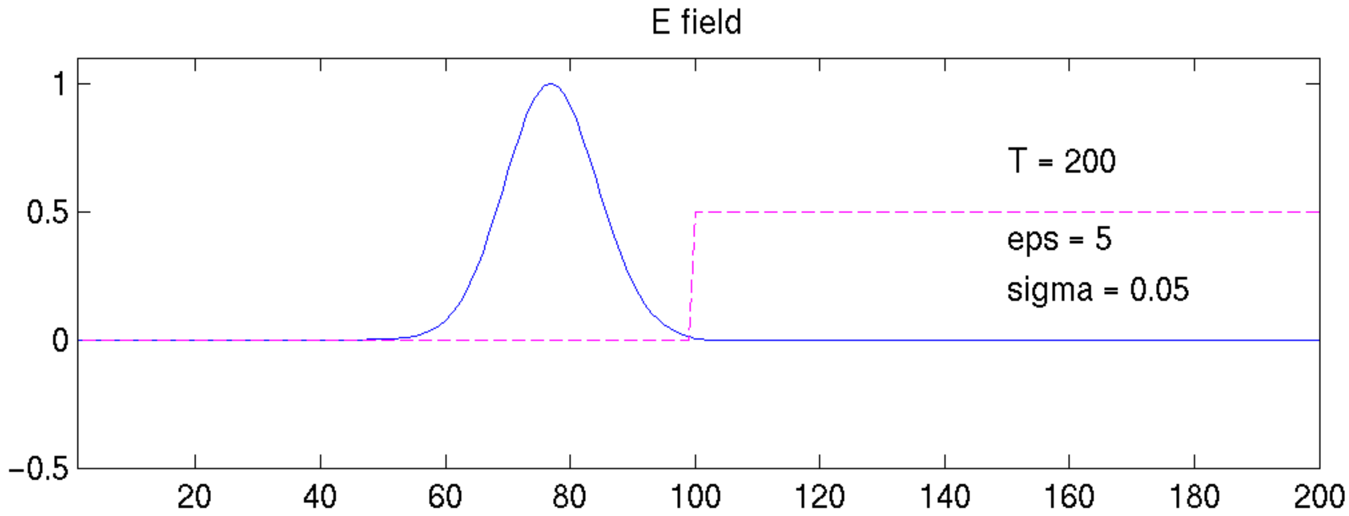
The cells between 100 and 200 have been assigned the properties

$$\varepsilon_r = 5 \qquad \sigma = .05$$


E field
T = 125
eps = 5
sigma = 0.05
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200


E field
T = 150
eps = 5
sigma = 0.05
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200


E field
T = 175
eps = 5
sigma = 0.05
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200



E field
T = 200
eps = 5
sigma = 0.05
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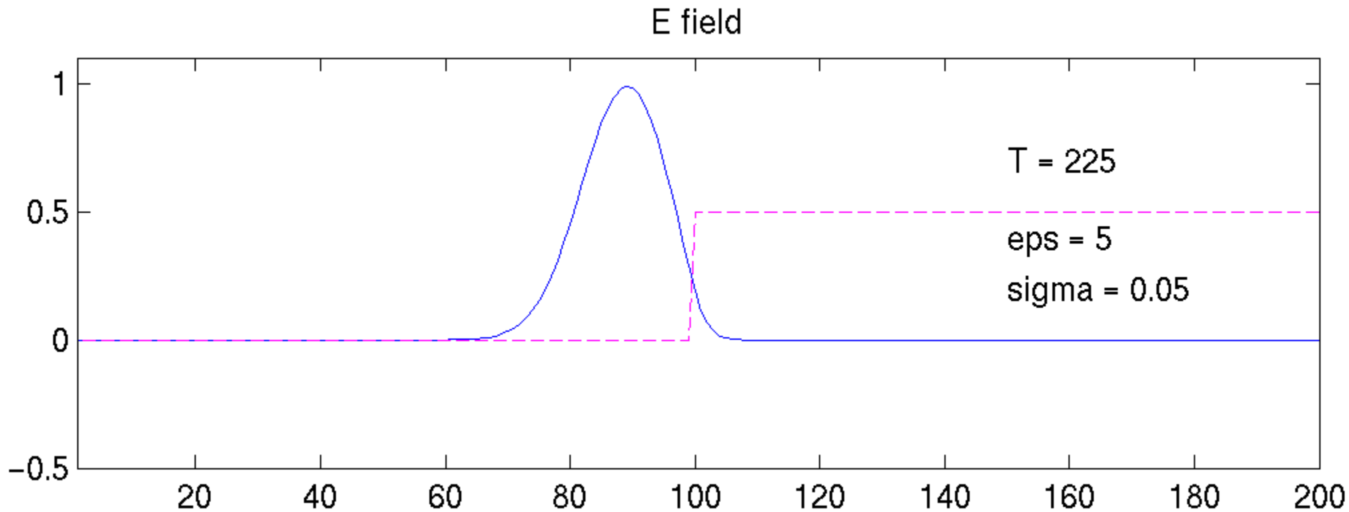
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200



E field
T = 225
eps = 5
sigma = 0.05
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0.5
0
−0.5
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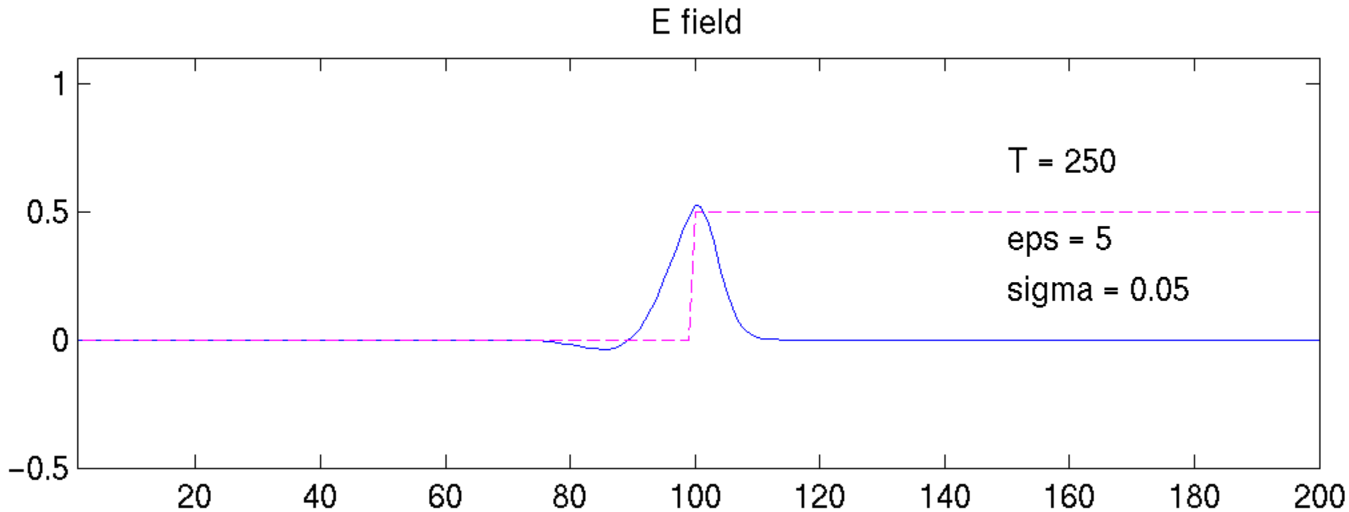
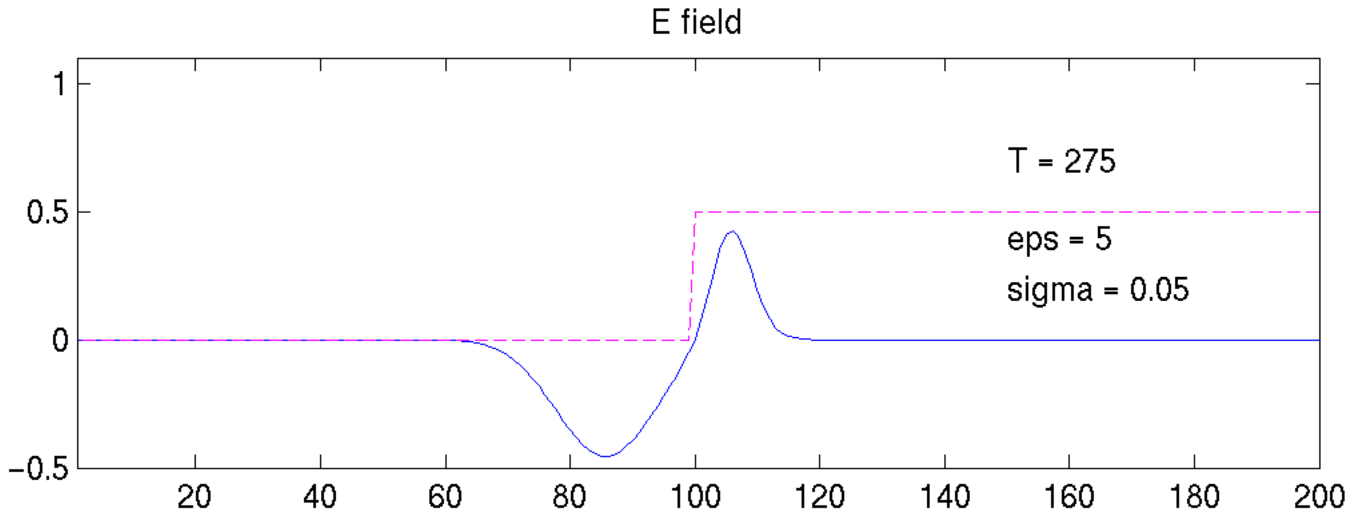
60
80
100
120
140
160
180
200


E field
T = 250
eps = 5
sigma = 0.05
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200


E field
T = 275
eps = 5
sigma = 0.05
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0.5
0
−0.5
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60
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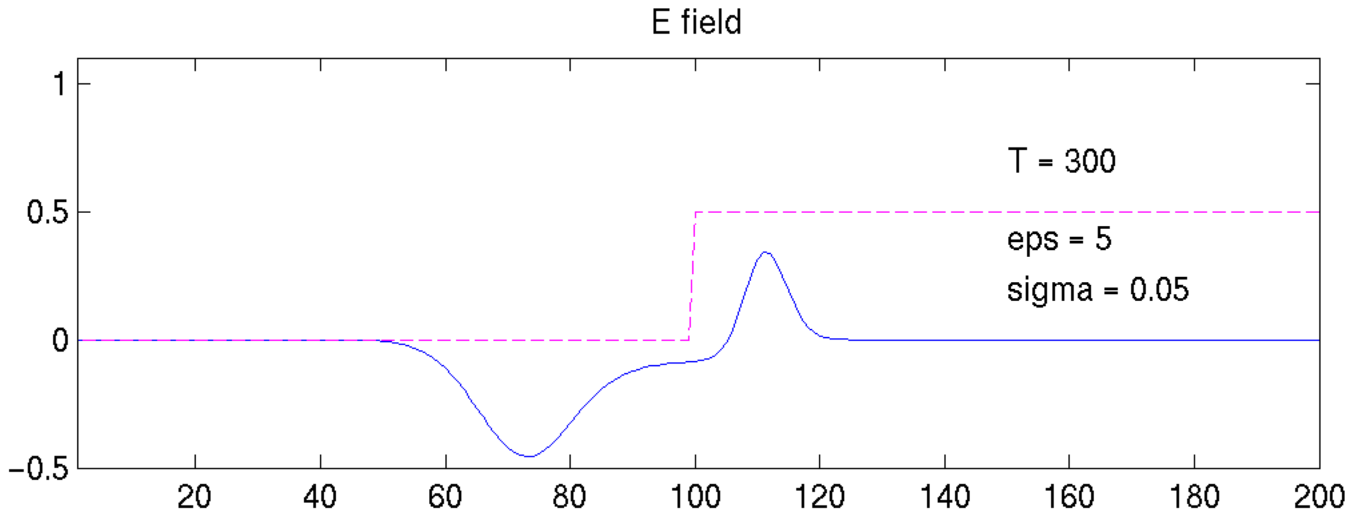
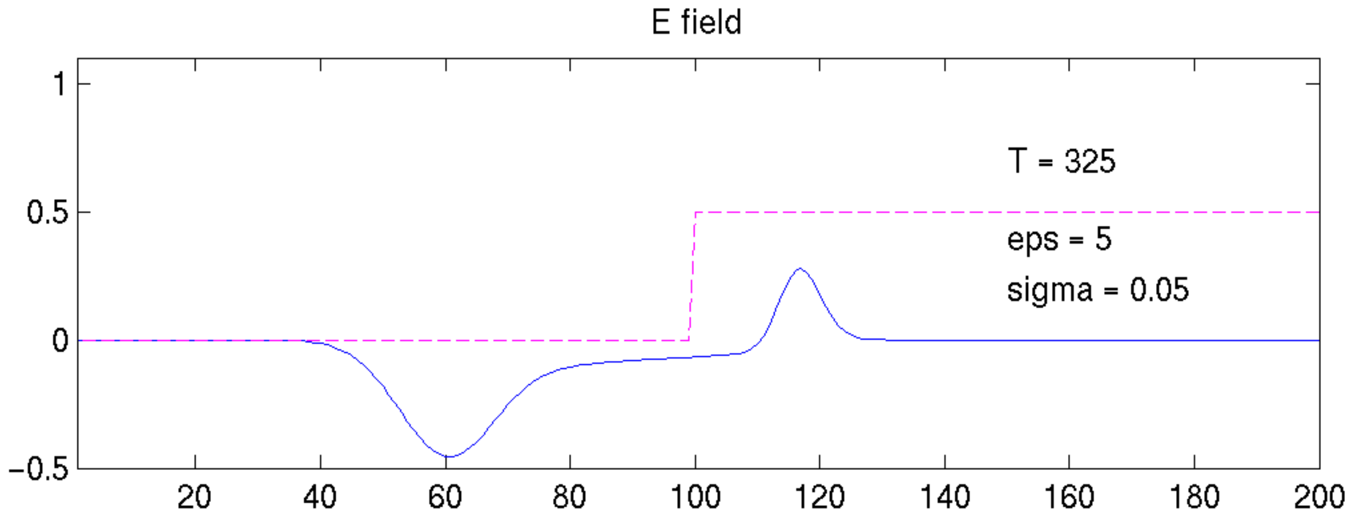
140
160
180
200


E field
T = 300
eps = 5
sigma = 0.05
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200



E field
T = 325
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sigma = 0.05
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0.5
0
−0.5
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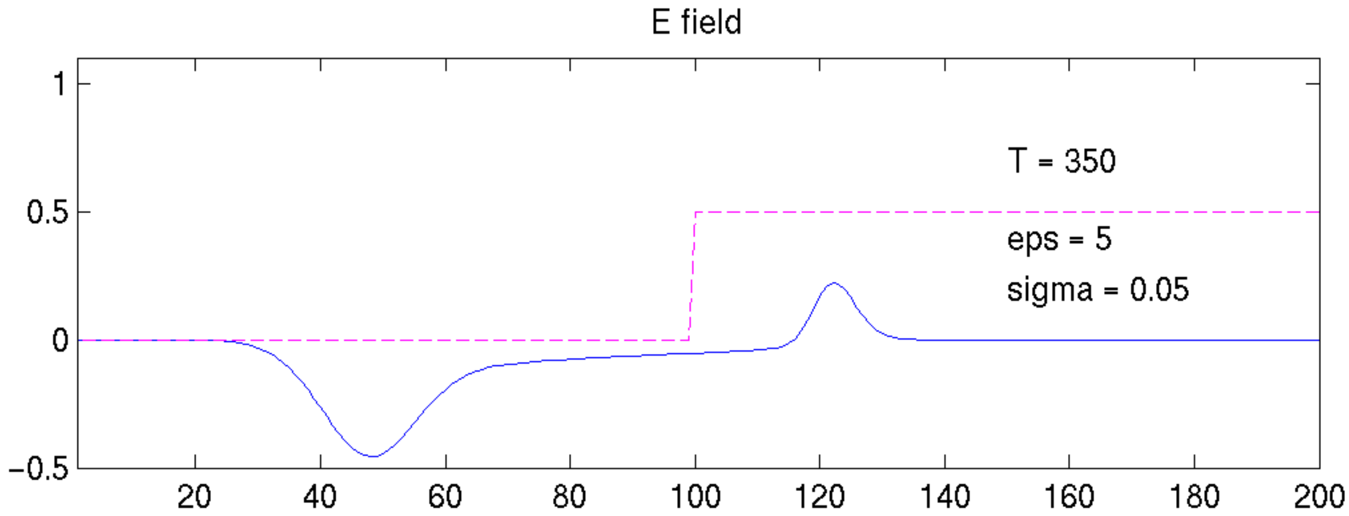
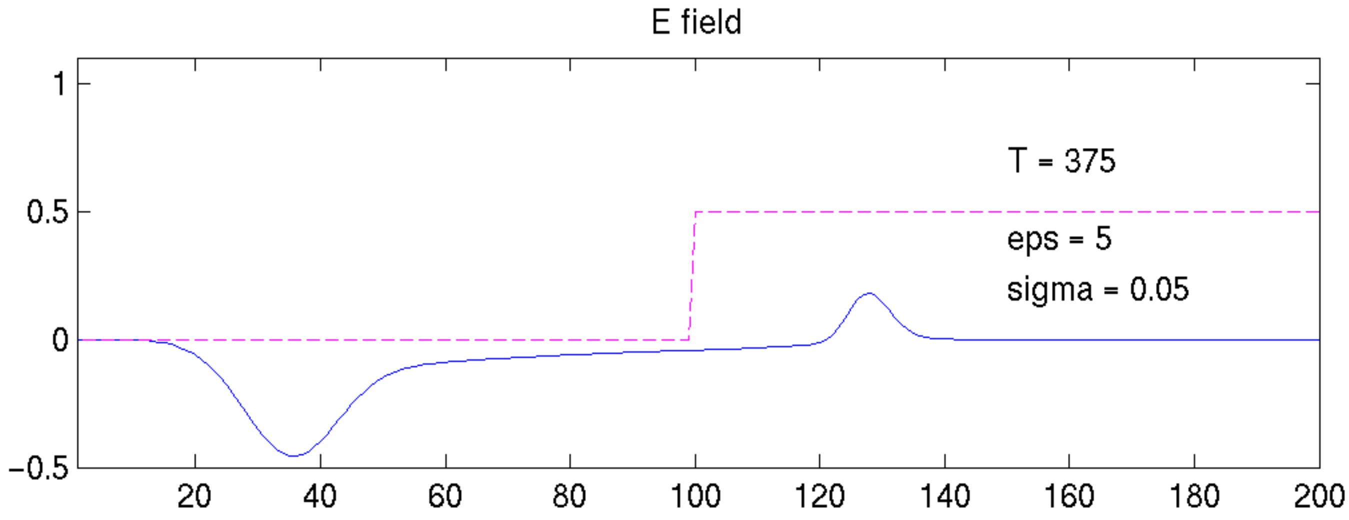
60
80
100
120
140
160
180
200


E field
1
0.5
0
−0.5
20
40
60
80
100
120
140
160
180
200
T = 350
eps = 5
sigma = 0.05



E field
T = 375
eps = 5
sigma = 0.05
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0.5
0
−0.5
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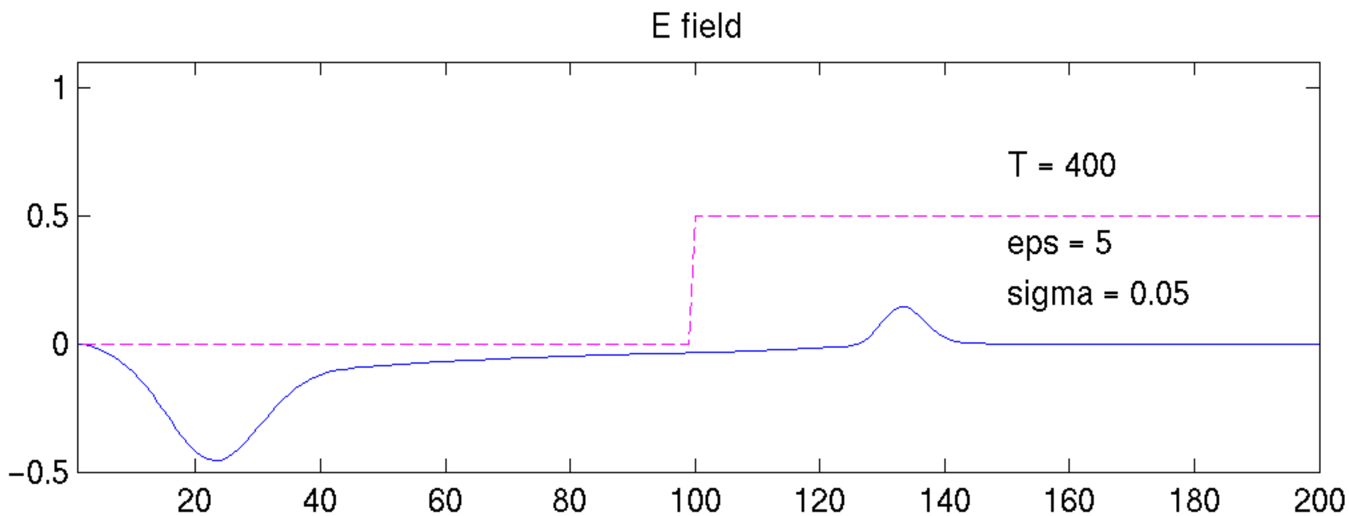
40
60
80
100
120
140
160
180
200


E field
T = 400
eps = 5
sigma = 0.05
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0.5
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60
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100
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140
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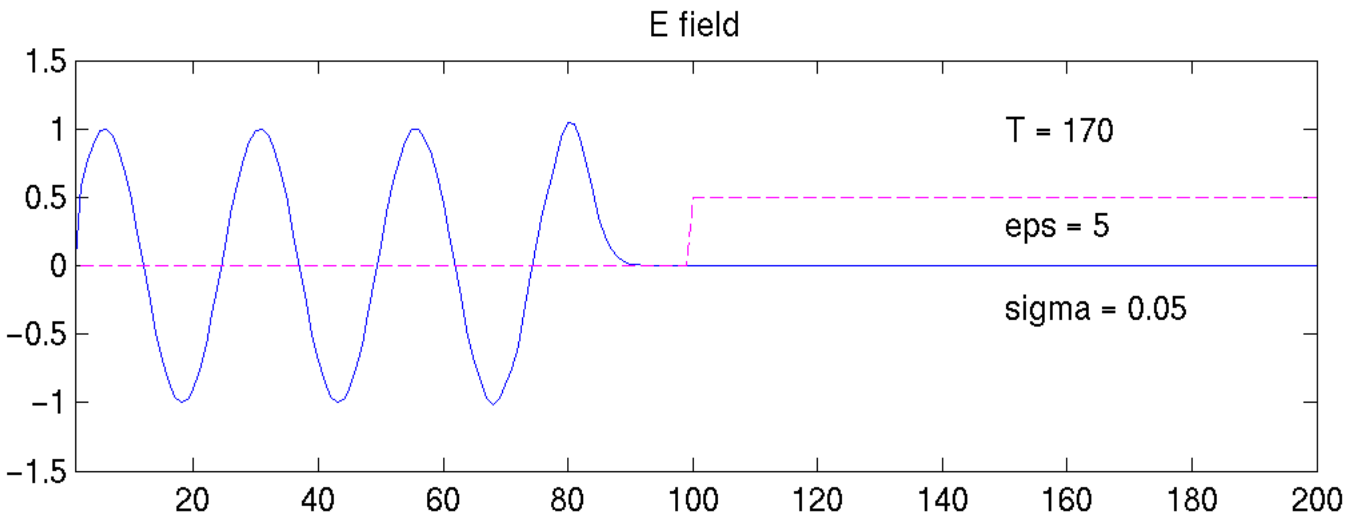
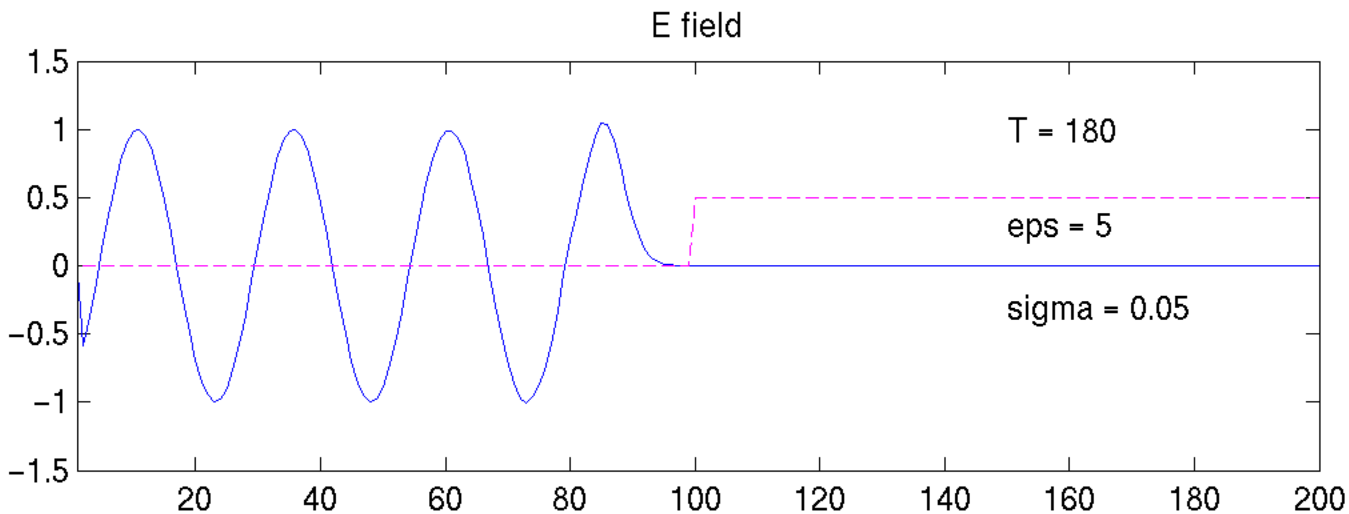
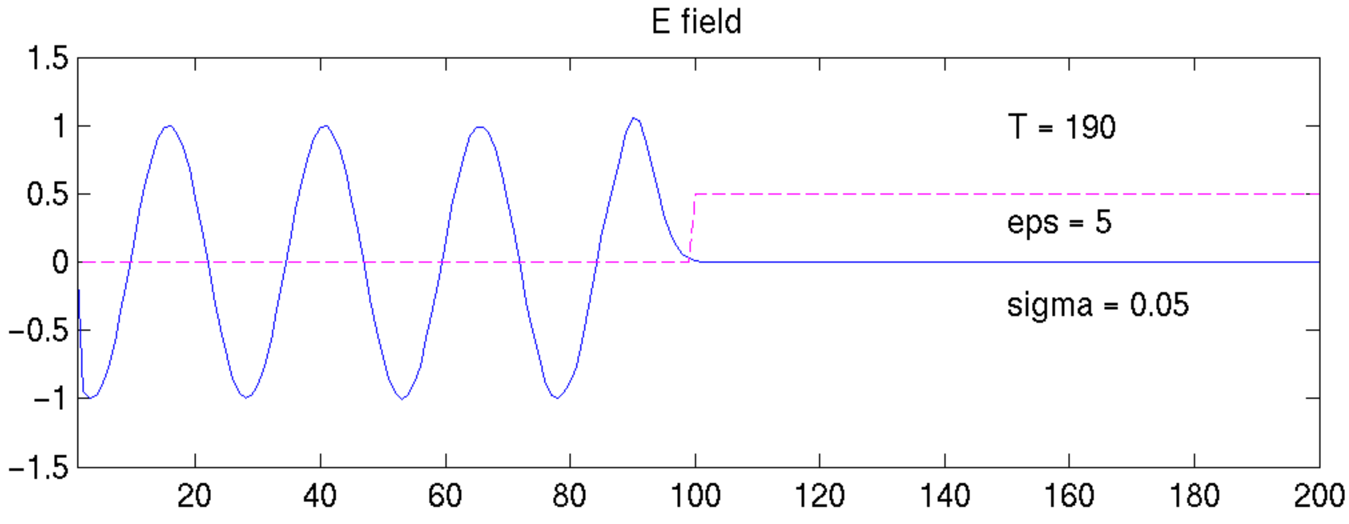
180
200

For sinusoidal radiation:




E field
1.5
1
0.5
0
−0.5
−1
−1.5
20
40
60
80
100
120
140
160
180
200
T = 180
eps = 5
sigma = 0.05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T = 190
eps = 5
sigma = 0.05
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−1.5
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60
80
100
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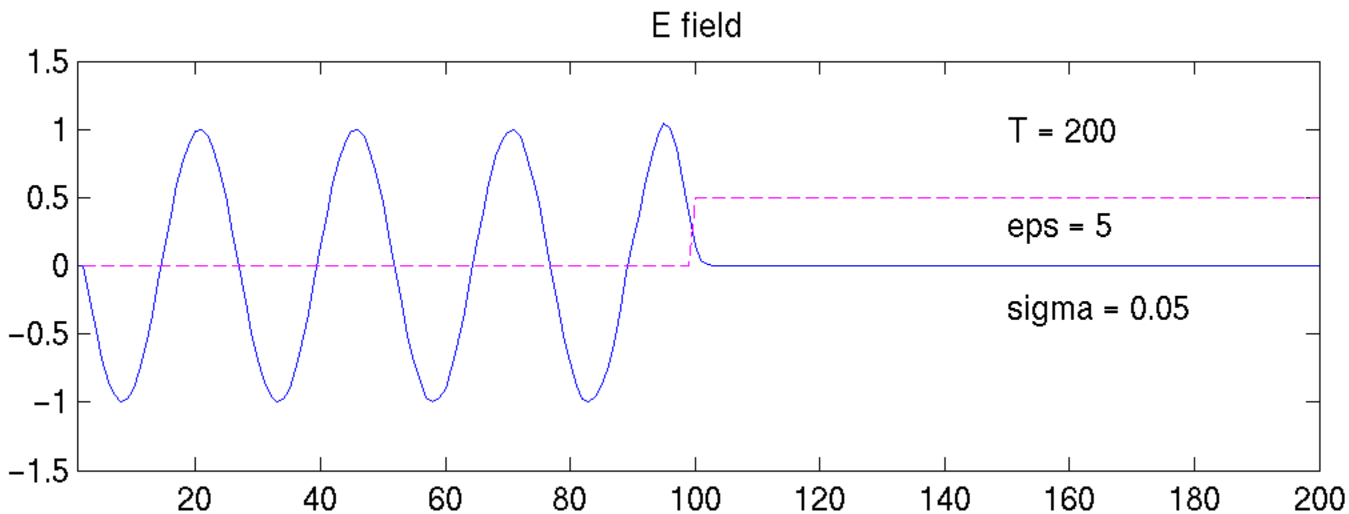
140
160
180
200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T = 200
eps = 5
sigma = 0.05
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60
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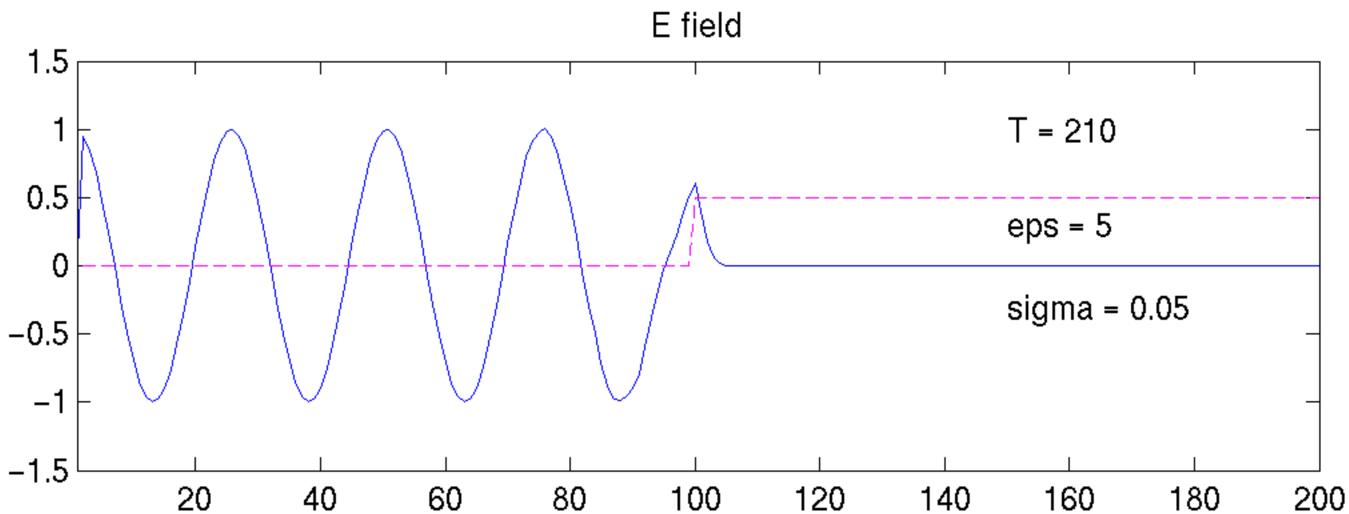
180
200



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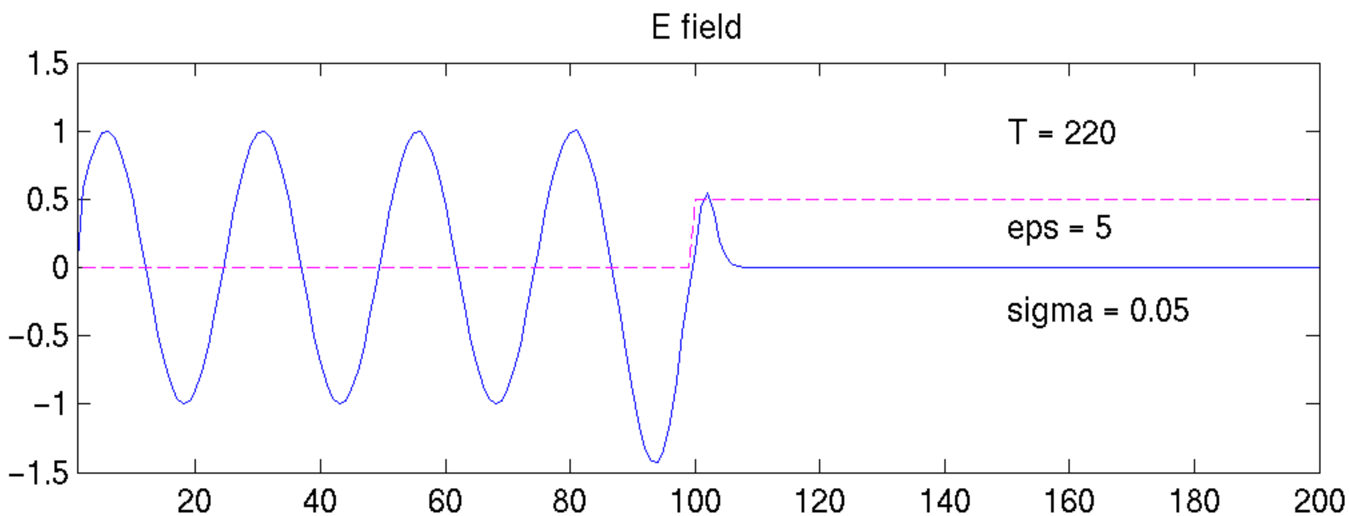

E field
1.5
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−1
−1.5
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100
120
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180
200
T = 220
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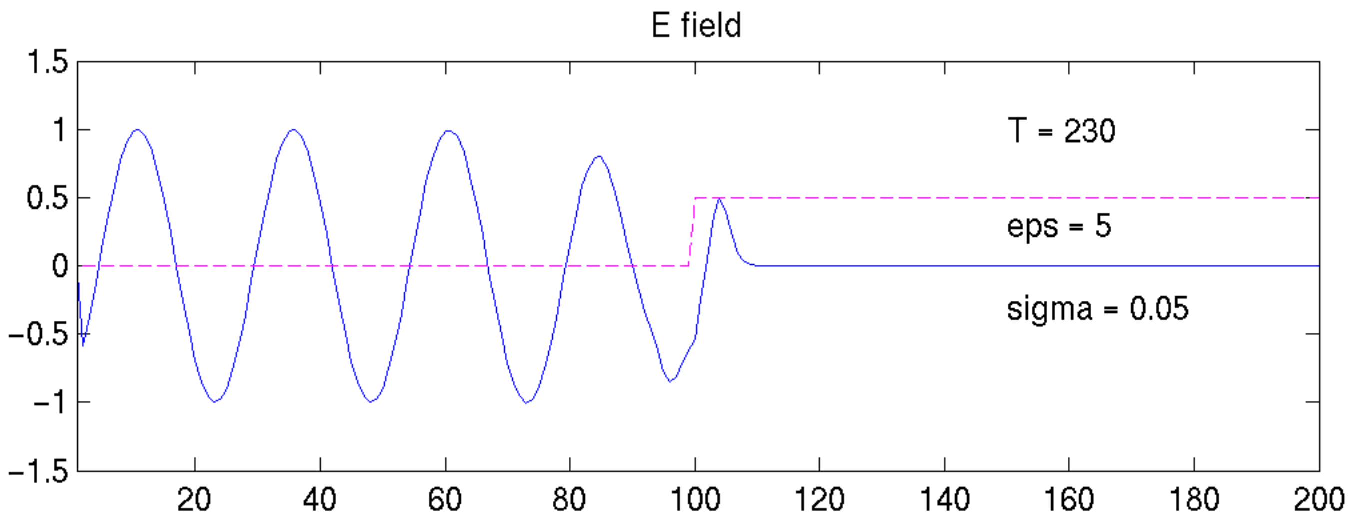
sigma = 0.05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sigma = 0.05
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180
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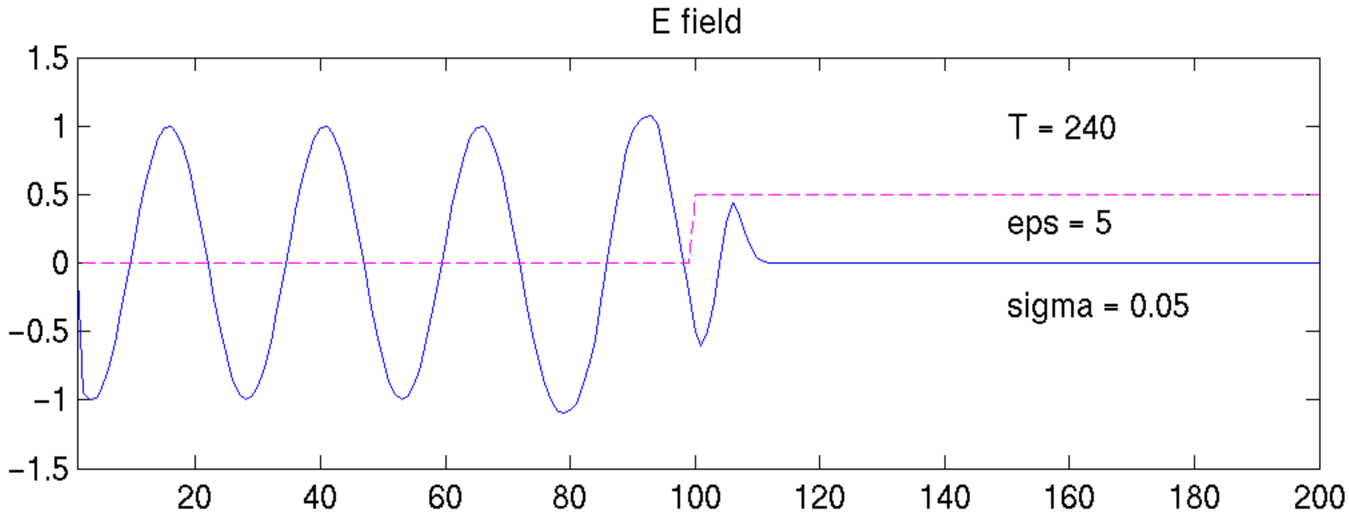

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sigma = 0.05
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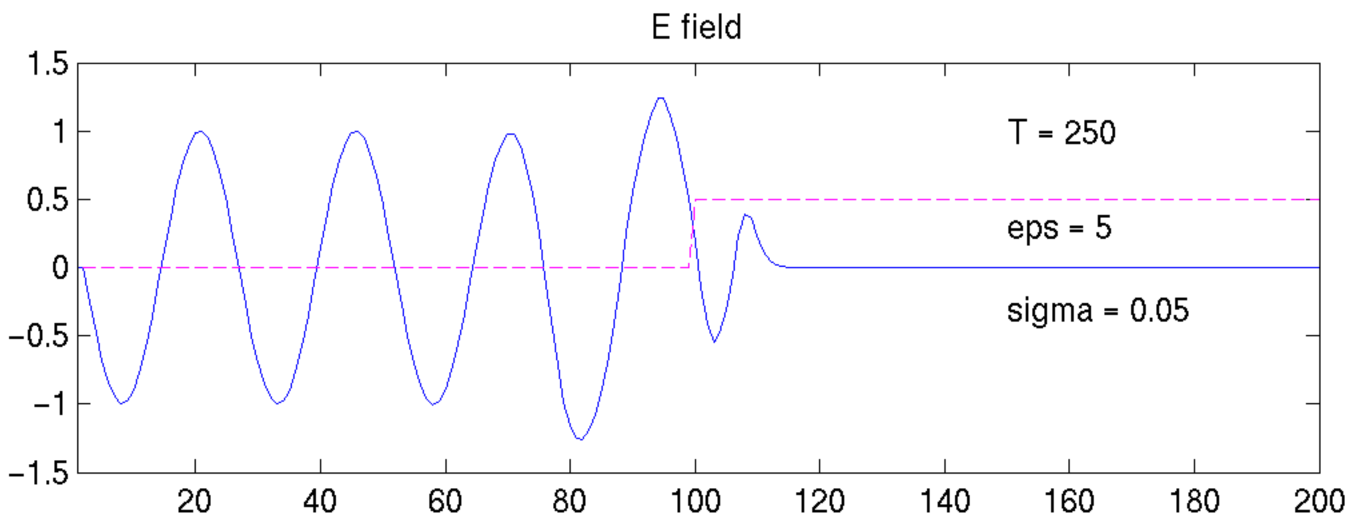
E field
T = 250
eps = 5
sigma = 0.05
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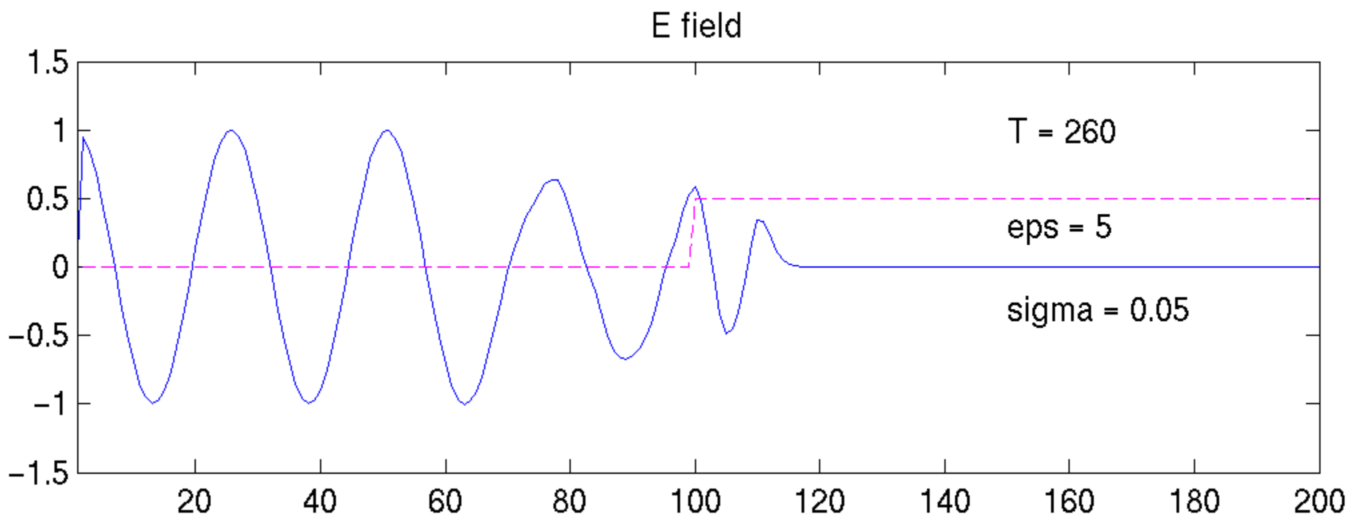
E field
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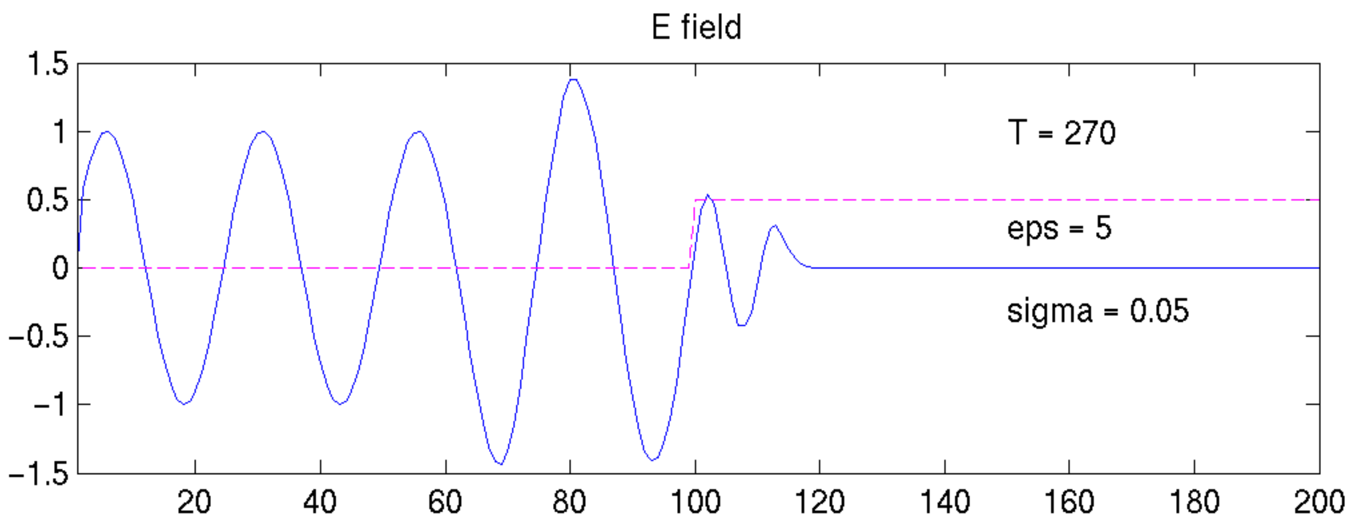
100
120
140
160
180
200
T = 260
eps = 5
sigma = 0.05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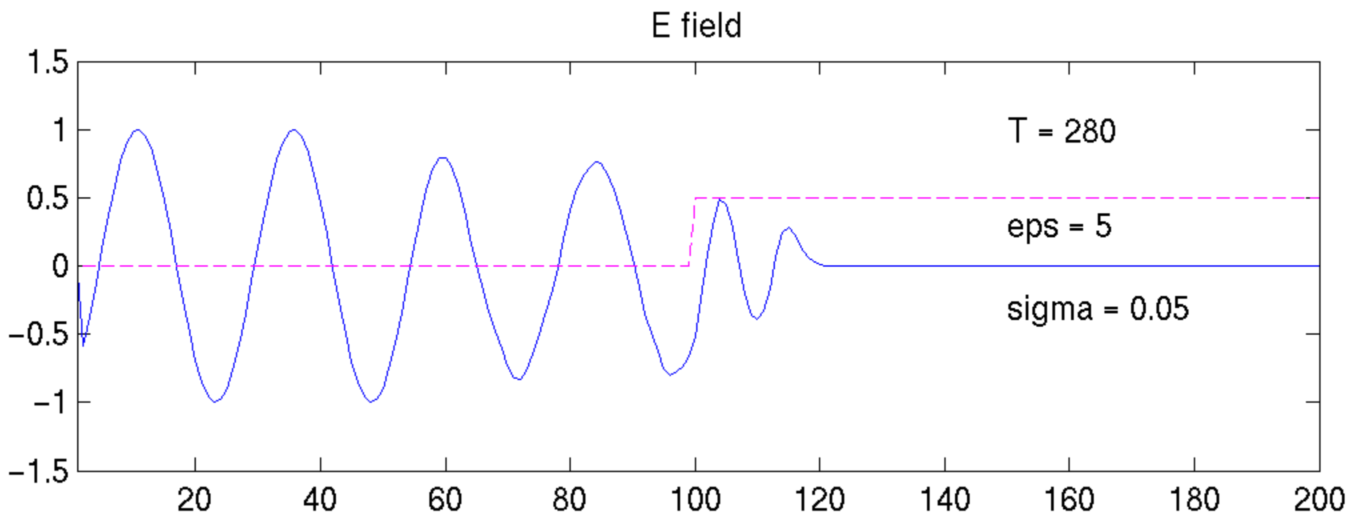
160
180
200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−1.5
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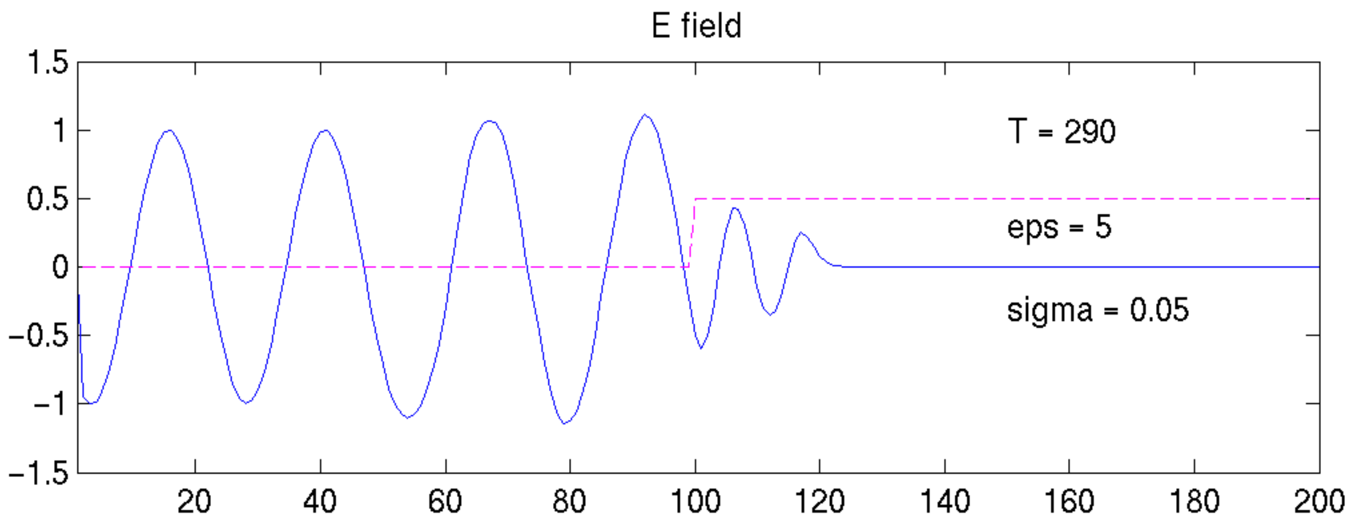
200


E field
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60
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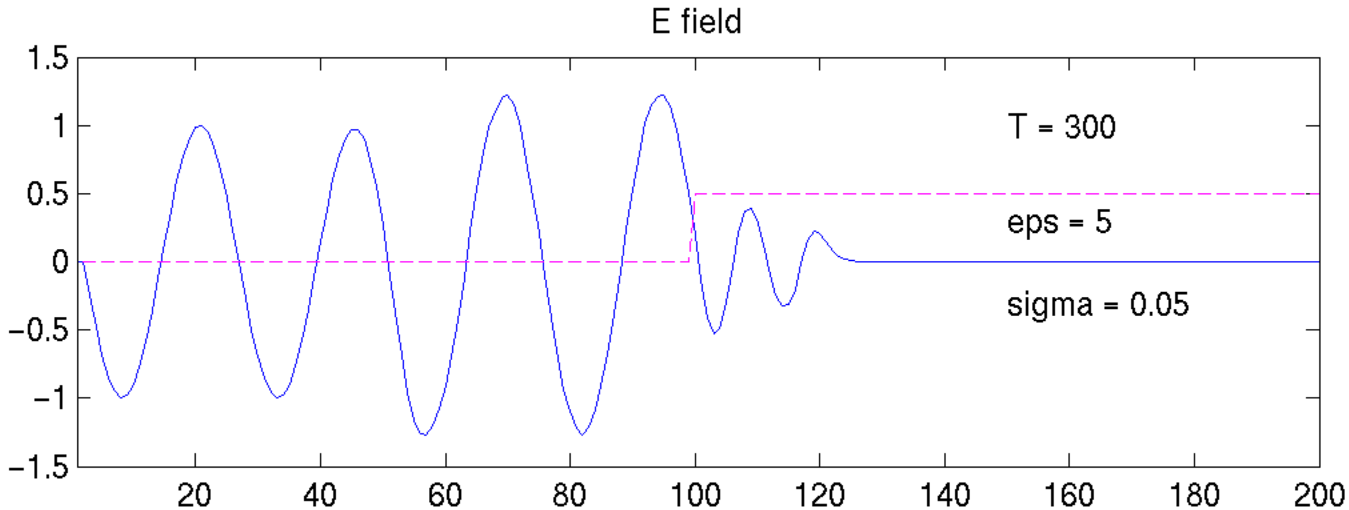
E field
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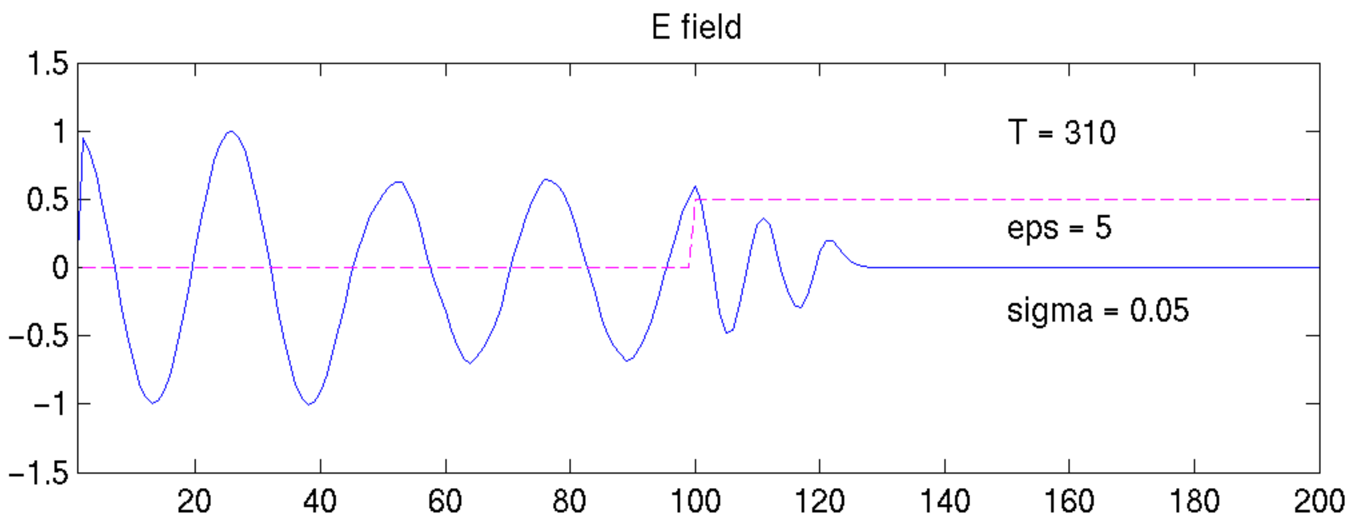
0
−0.5
−1
−1.5
20
40
60
80
100
120
140
160
180
200
T = 300
eps = 5
sigma = 0.05



E field
T = 310
eps = 5
sigma = 0.05
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−1.5
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60
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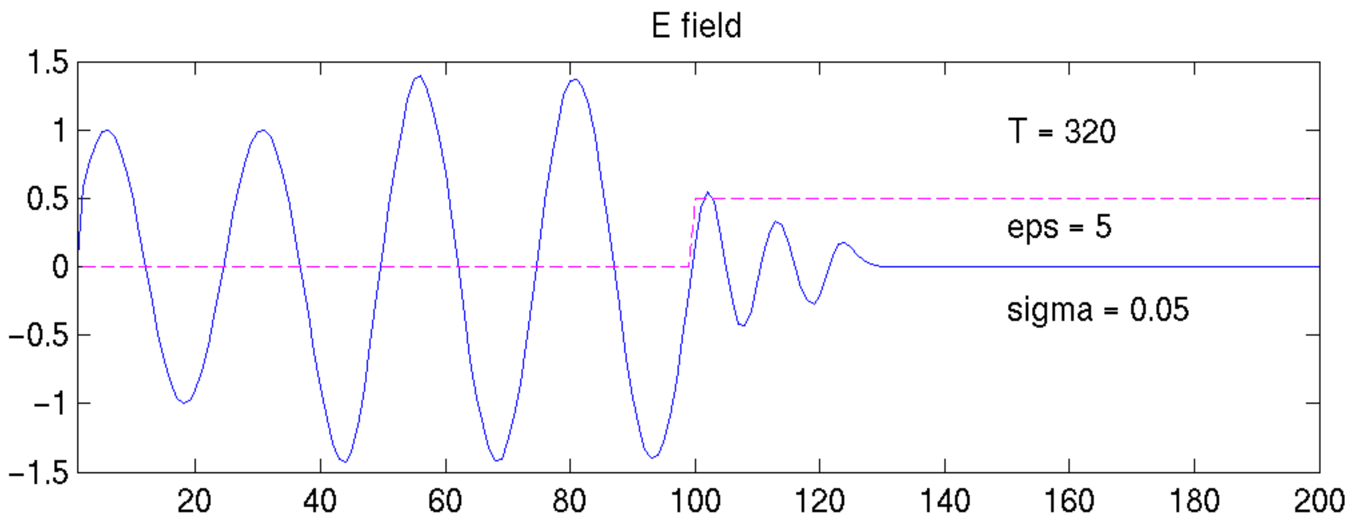
180
200


E field
T = 320
eps = 5
sigma = 0.05
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0.5
0
−0.5
−1
−1.5
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60
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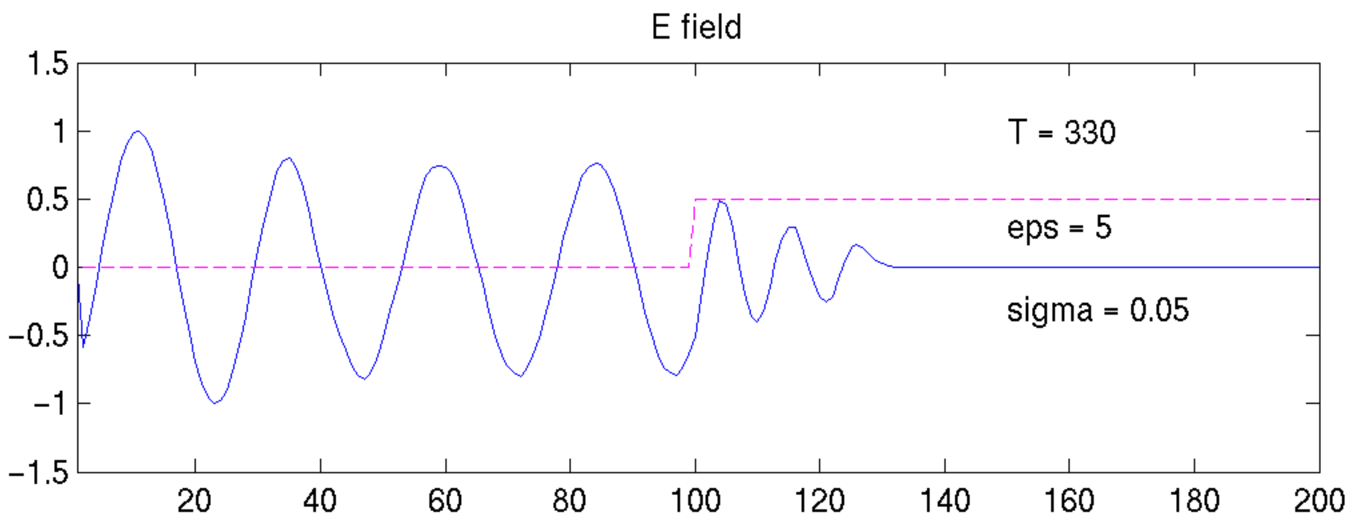
180
200



E field
T = 330
eps = 5
sigma = 0.05
1.5
1
0.5
0
−0.5
−1
−1.5
20
40
60
80
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120
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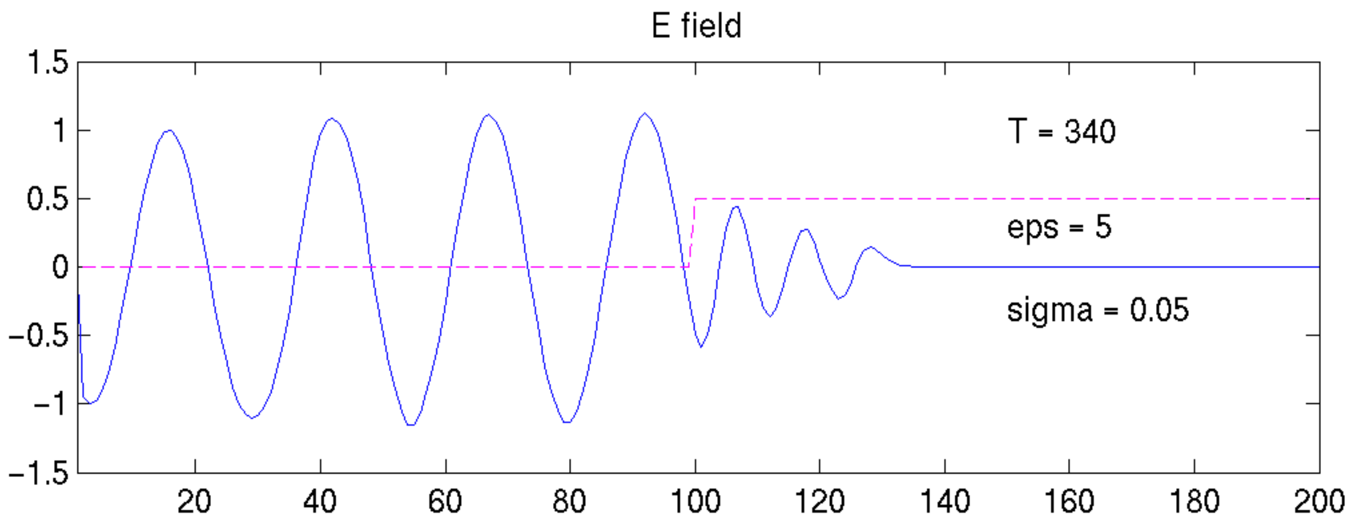
160
180
200


E field
1.5
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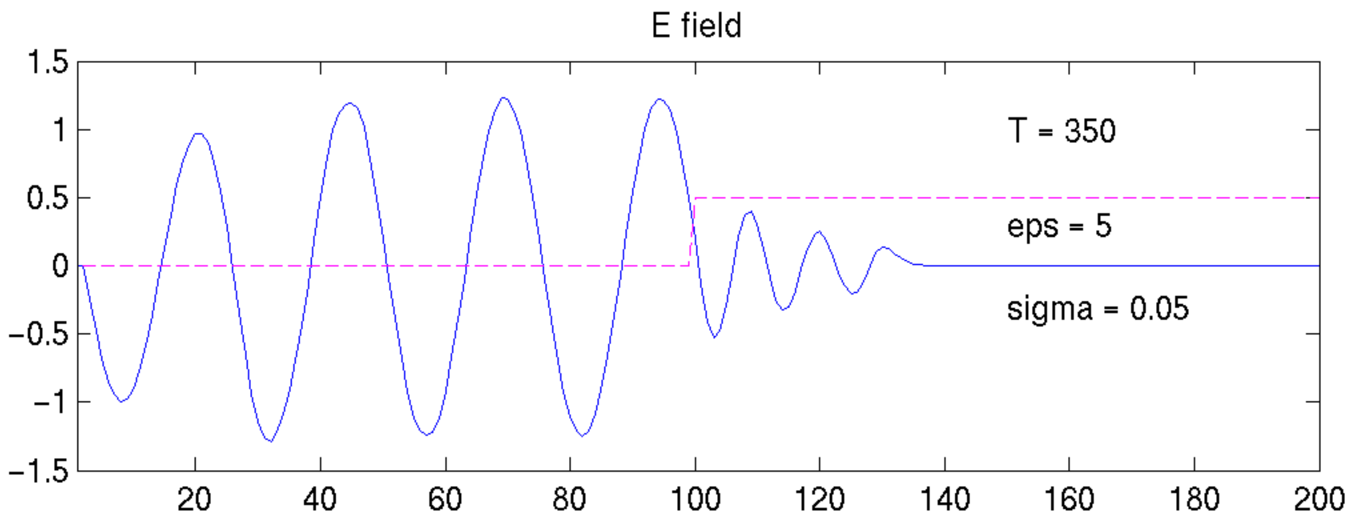
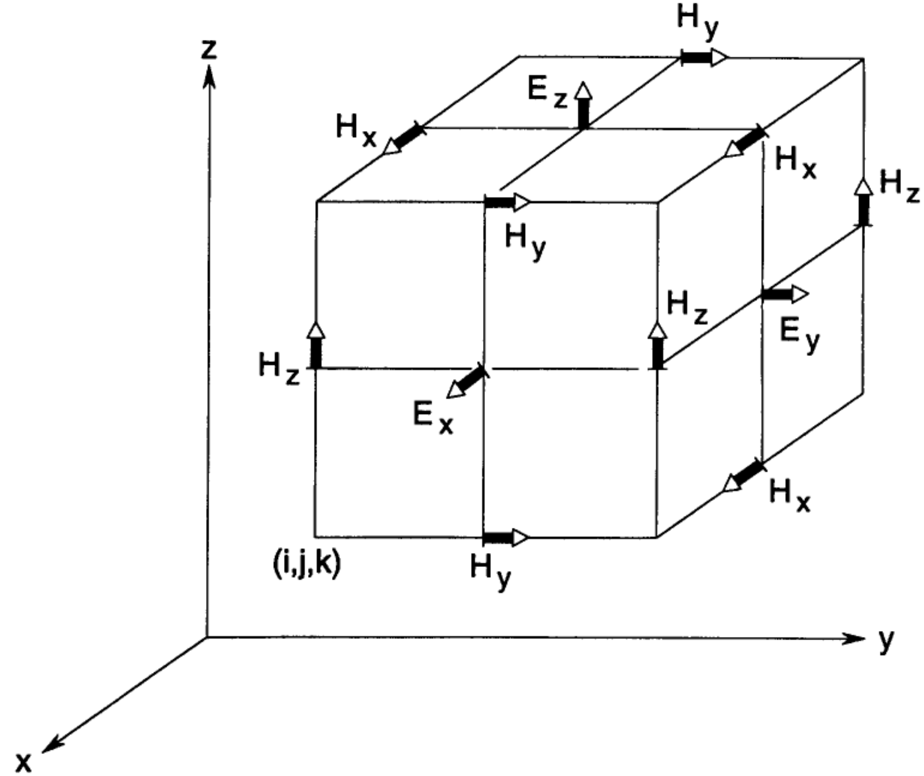
0.5
0
−0.5
−1
−1.5
20
40
60
80
100
120
140
160
180
200
T = 340
eps = 5
sigma = 0.05


E field
T = 350
eps = 5
sigma = 0.05
1.5
1
0.5
0
−0.5
−1
−1.5
20
40
60
80
100
120
140
160
180
200

3D FDTD Yee formalism

``Computational electrodynamics: The FDTD method,''
A. Taflove and S. Hagness



$$
E_x\Big|^{n+1/2}_{i,\,j+1/2,\,k+1/2} - E_x\Big|^{n-1/2}_{i,\,j+1/2,\,k+1/2} =
$$

$$
\frac{\Delta t}{\varepsilon_{i,\,j+1/2,\,k+1/2}} \cdot \left[\frac{H_z\Big|^{n}_{i,\,j+1,\,k+1/2} - H_z\Big|^{n}_{i,\,j,\,k+1/2}}{\Delta y} - \frac{H_y\Big|^{n}_{i,\,j+1/2,\,k+1} - H_y\Big|^{n}_{i,\,j+1/2,\,k}}{\Delta z} - J_{\text{source}_x}\Big|^{n}_{i,\,j+1/2,\,k+1/2} - \sigma_{i,\,j+1/2,\,k+1/2} \cdot \left(\frac{E_x\Big|^{n+1/2}_{i,j+1/2,k+1/2} + E_x\Big|^{n-1/2}_{i,j+1/2,k+1/2}}{2} \right) \right]
$$

Metal nanoparticles have been suggested as light trapping agents in solar cells

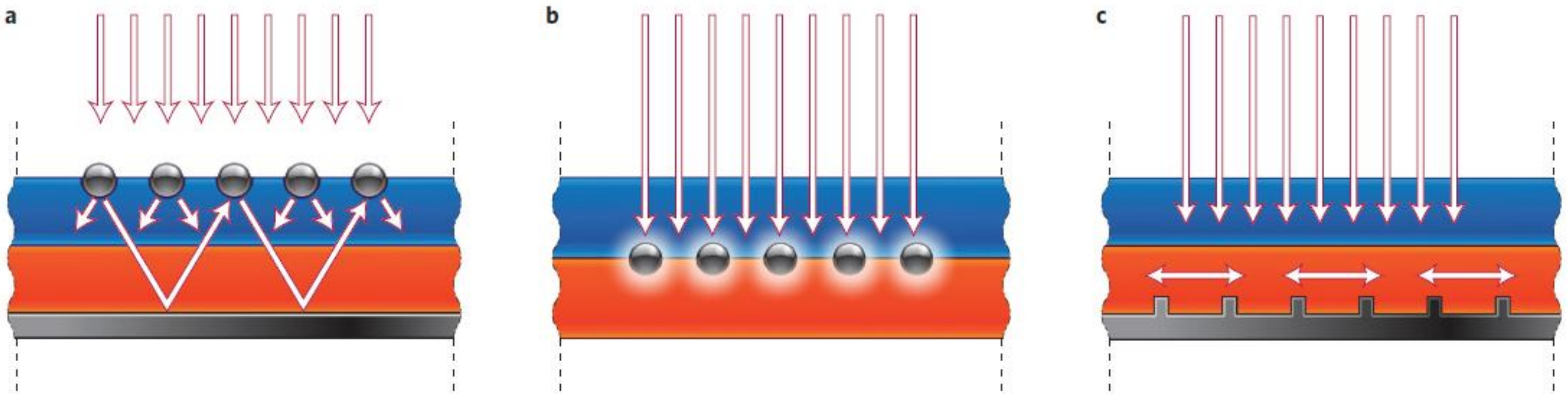
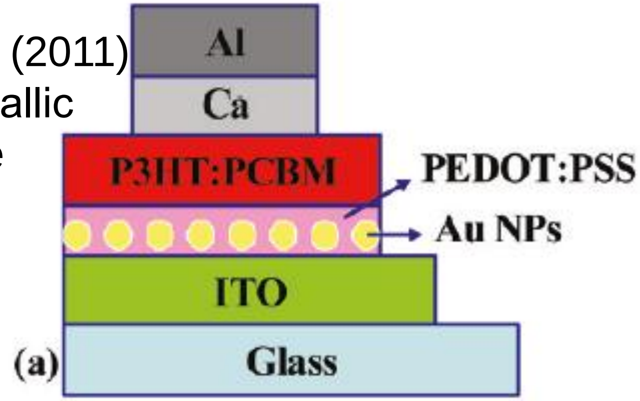


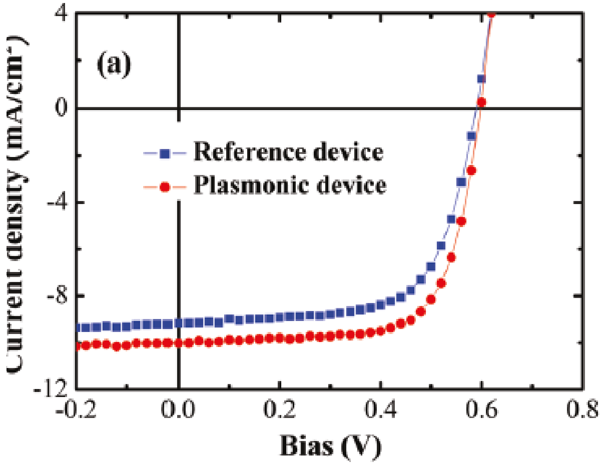
Figure 2 | Plasmonic light-trapping geometries for thin-film solar cells. a, Light trapping by scattering from metal nanoparticles at the surface of the solar cell. Light is preferentially scattered and trapped into the semiconductor thin film by multiple and high-angle scattering, causing an increase in the effective optical path length in the cell. **b**, Light trapping by the excitation of localized surface plasmons in metal nanoparticles embedded in the semiconductor. The excited particles' near-field causes the creation of electron–hole pairs in the semiconductor. **c**, Light trapping by the excitation of surface plasmon polaritons at the metal/semiconductor interface. A corrugated metal back surface couples light to surface plasmon polariton or photonic modes that propagate in the plane of the semiconductor layer.

H. A. Atwater, A. Polman, ``Plasmonics for improved photovoltaic devices,'' Nat. Mater. 9, 205 (2010).

Measurements support theoretical predictions

J.-L. Wu, et. al., ACS Nano 5, 959 (2011)
"Surface Plasmonic Effects of Metallic Nanoparticles on the Performance of Polymer Bulk Heterojunction Solar Cells"

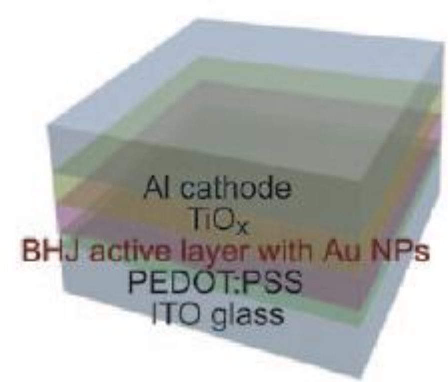


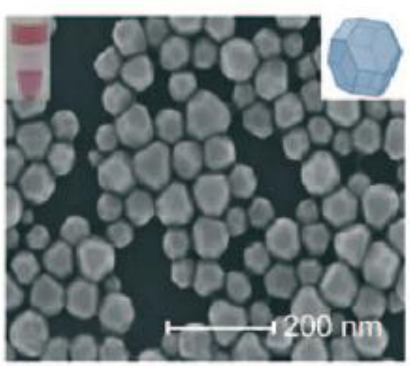


The power conversion efficiency (PCE) of the OPV device incorporating the Au NPs improved to 4.24% from a value of 3.57% for the device fabricated without Au NPs.

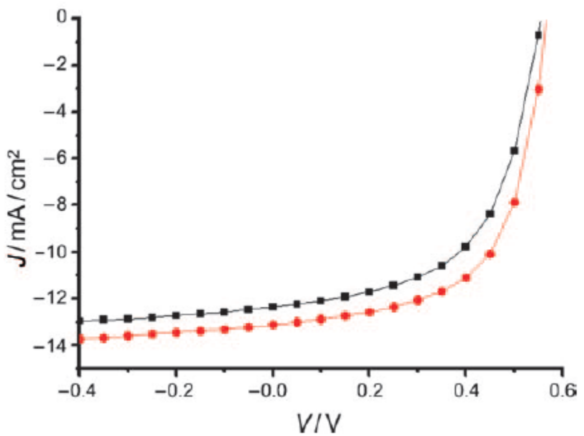
D. H. Wang, et. al., Agnew. Chem. 50 (2011)
Enhancement of Donor–Acceptor Polymer Bulk Heterojunction Solar Cell Power Conversion Efficiencies by Addition of Au Nanoparticles

For P3HT/$PC_{70}BM$, the PCE increased from 3.54% to 4.36%; for PCDTBT/$PC_{70}BM$, the PCE increased from 5.77% to 6.45%, and for Si-PCPDTBT/$PC_{70}BM$, the PCE increased from 3.92% to 4.54%.





truncated octahedral Au



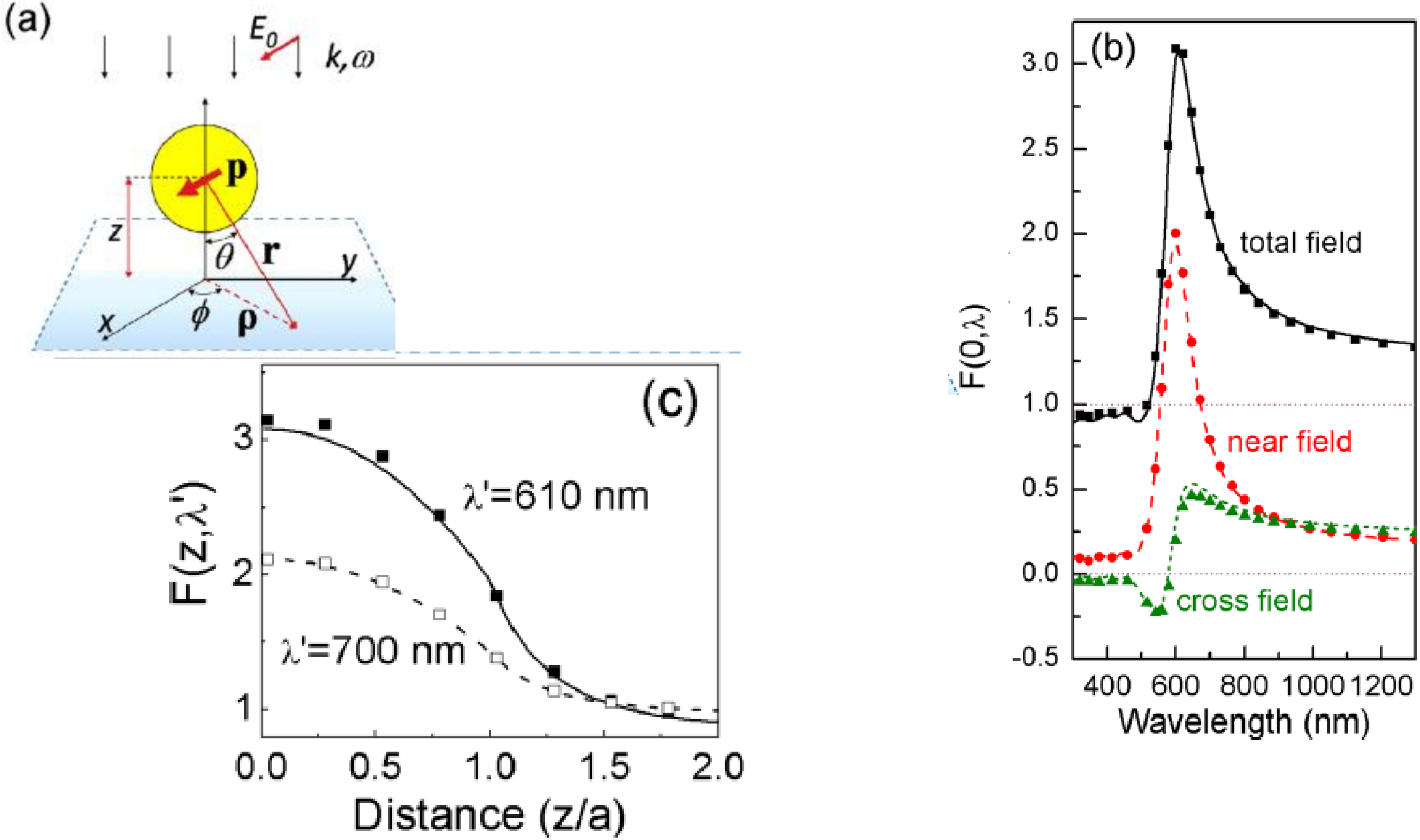


FIG. 1. (Color online) (a) Schematic of the geometry considered. (b) Comparison between Eq. (9) (lines) and accurate FDTD simulations (symbols), for a square array of $a = 4$ nm Au MNPs in a $n_h = 2$ host at periodicity $L = 21.5$ nm ($f = 2.7\%$). The enhancement is calculated on a plane going through the nanoparticle center ($z = 0$). Total, near, and cross field contributions are shown. (c) Total enhancement vs z at $\lambda = 610$ nm (peak enhancement) and $\lambda = 700$ nm.

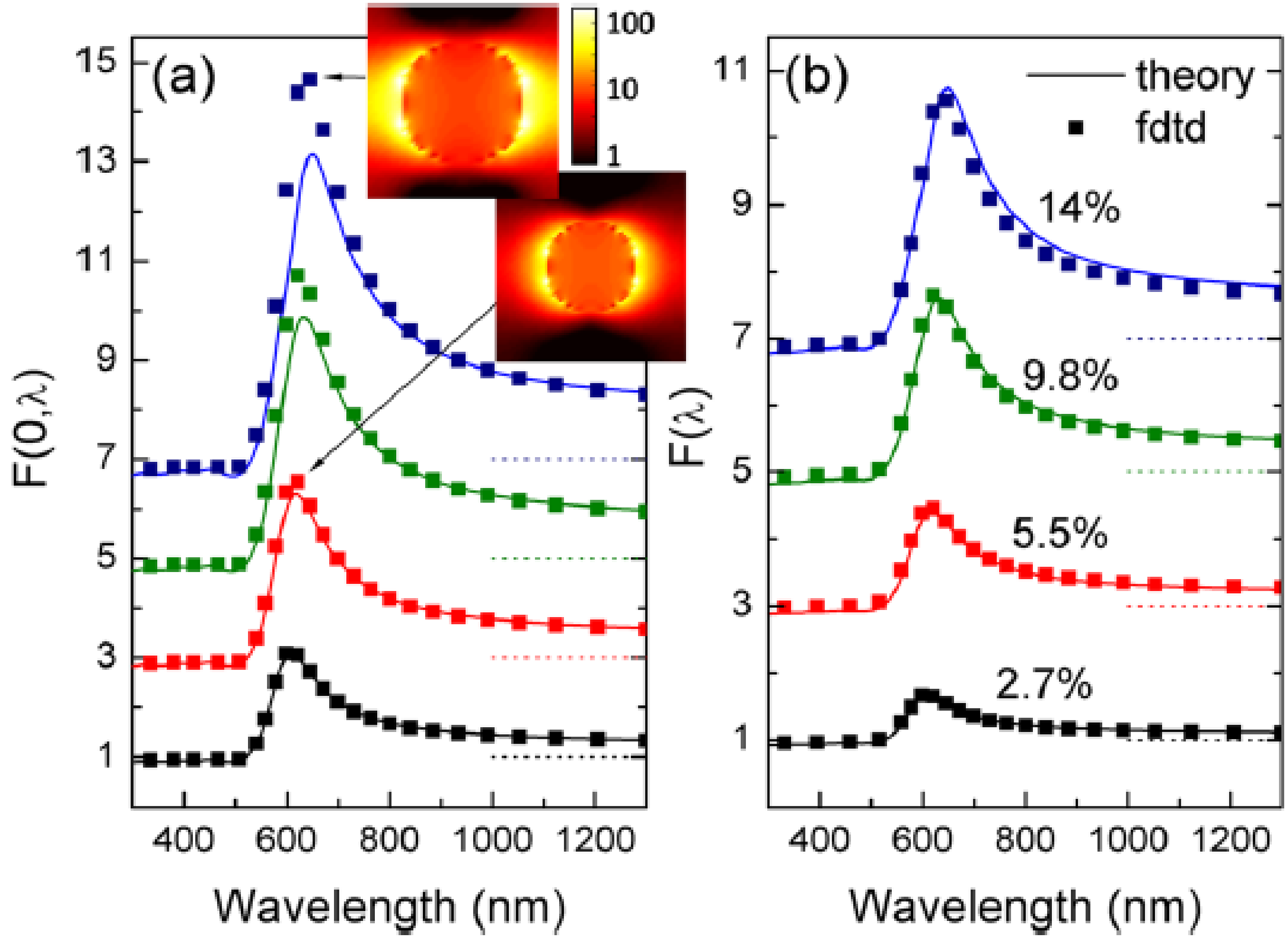


FIG. 2. (Color online) (a) Total enhancement vs wavelength on a plane through the Au MNP center, for four MNP arrays: $L = 21.5$ nm ($f = 2.7\%$), $L = 17$ nm ($f = 5.5\%$), $L = 14$ nm ($f = 9.8\%$) and $L = 12.5$ nm ($f = 14\%$). Lines for analytical and symbols for numerical results (vertically shifted by 2 for clarity). The insets plot the total intensity on a $z = 0$ plane at $f = 14\%$ and $f = 5.5\%$. (b) Total enhancement vs wavelength over all volume for the arrays considered in (a).

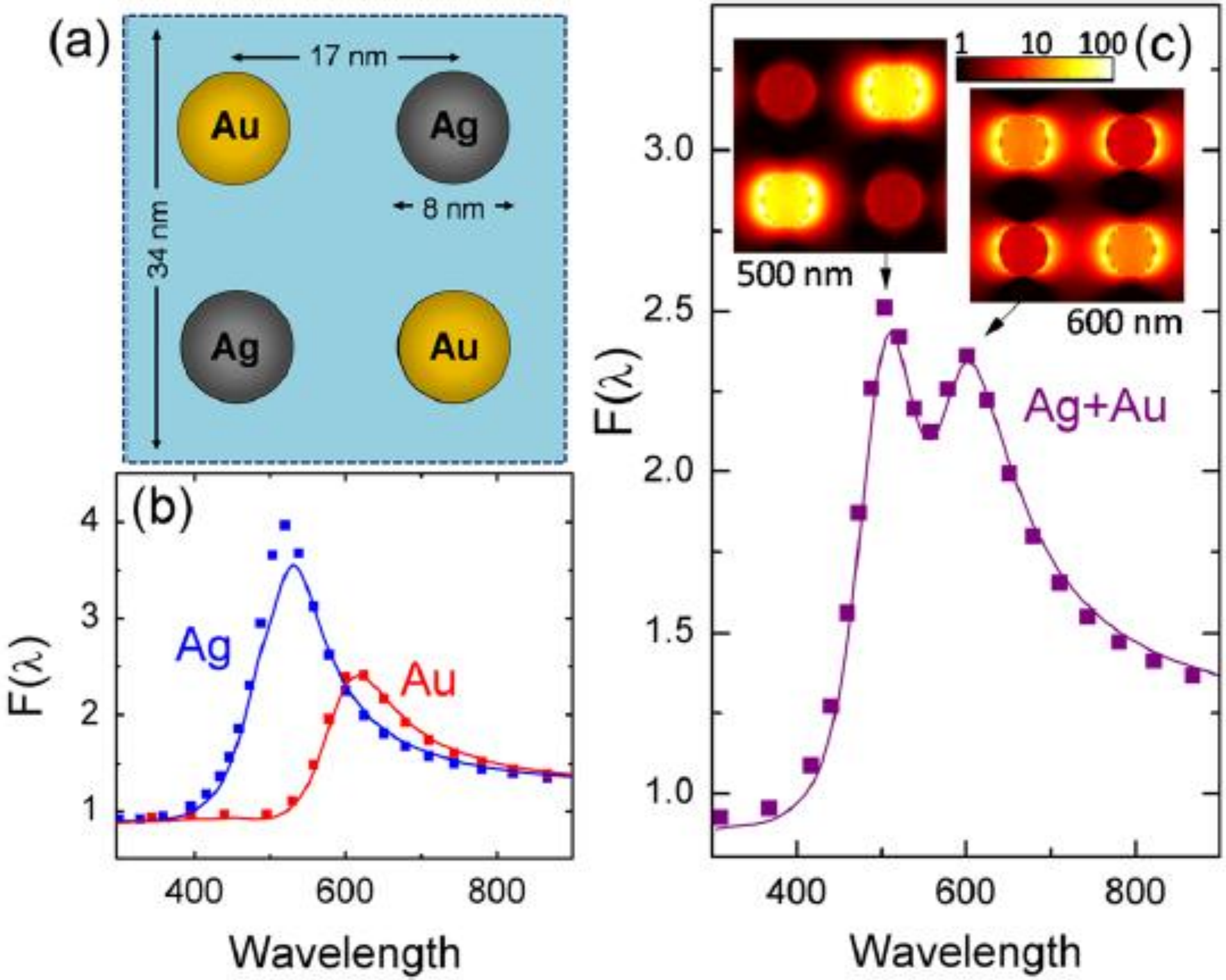


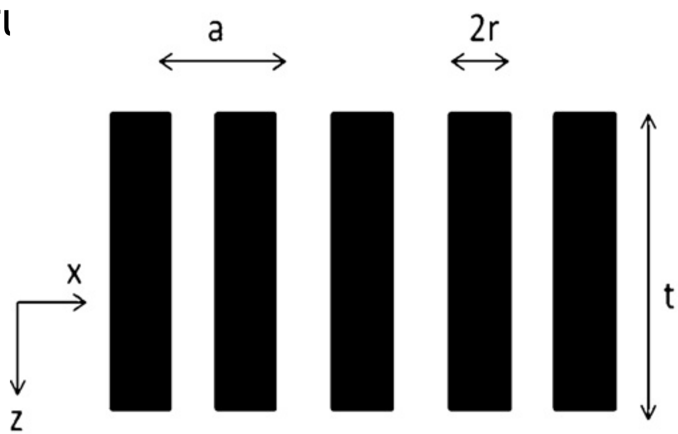
FIG. 3. (Color online) Schematic of a test case with mixed Au and Ag MNPs with $L = 17$ nm ($f = 5.5\%$). (b) Individual enhancement over all space of each MNP type at $f = 5.5\%$ (c) Enhancement of the composite over all space. Lines for analytical and symbols for numerical results. The insets plot the field intensity at $\lambda = 500$ nm (Ag SPR) and $\lambda = 600$ nm (Au SPR).

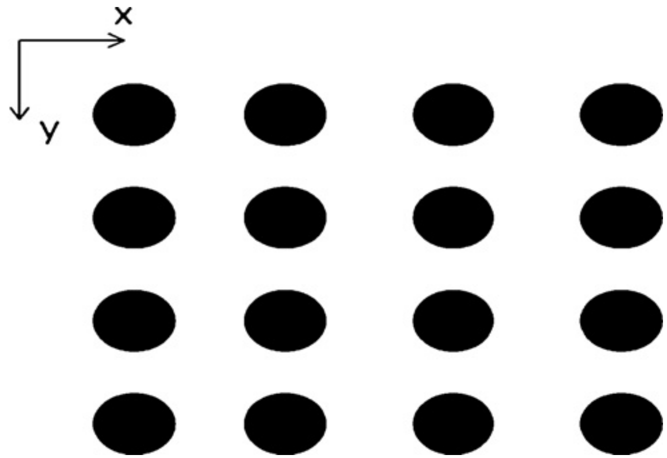
The optical absorption of nanowire arrays

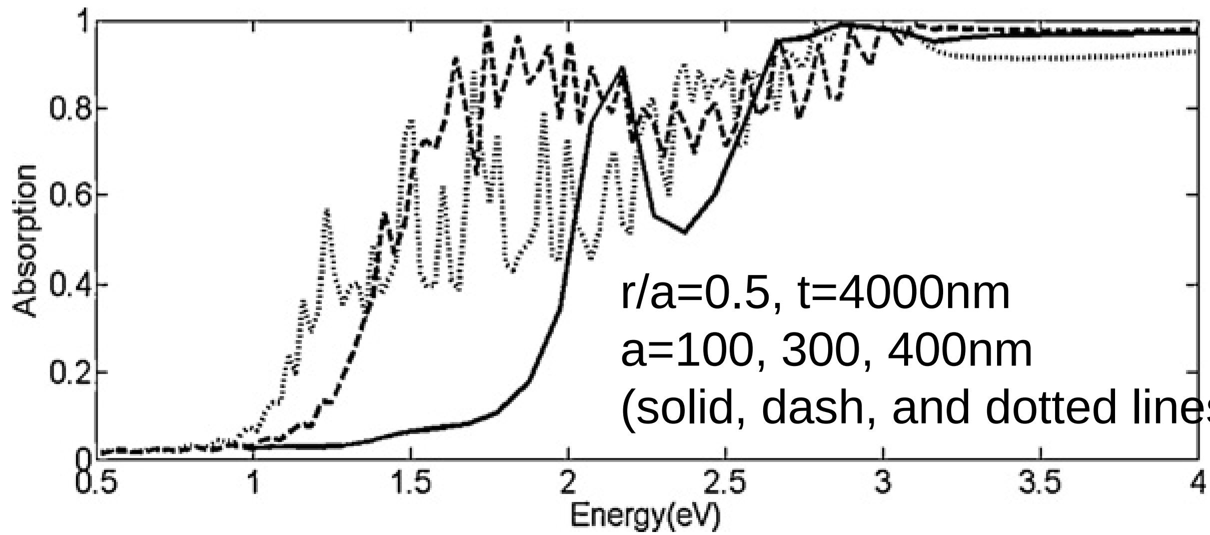
N. Lagos, M. M. Sigalas, D. Niarchos, Photonics and Nanostructures (2011).

Calculations of Si (and other semiconductor) nanowires using the Rigorous Coupled-Wave Analysis (RCWA).

Find the optimum conditions for getting the maximum absorption of visible light spectr





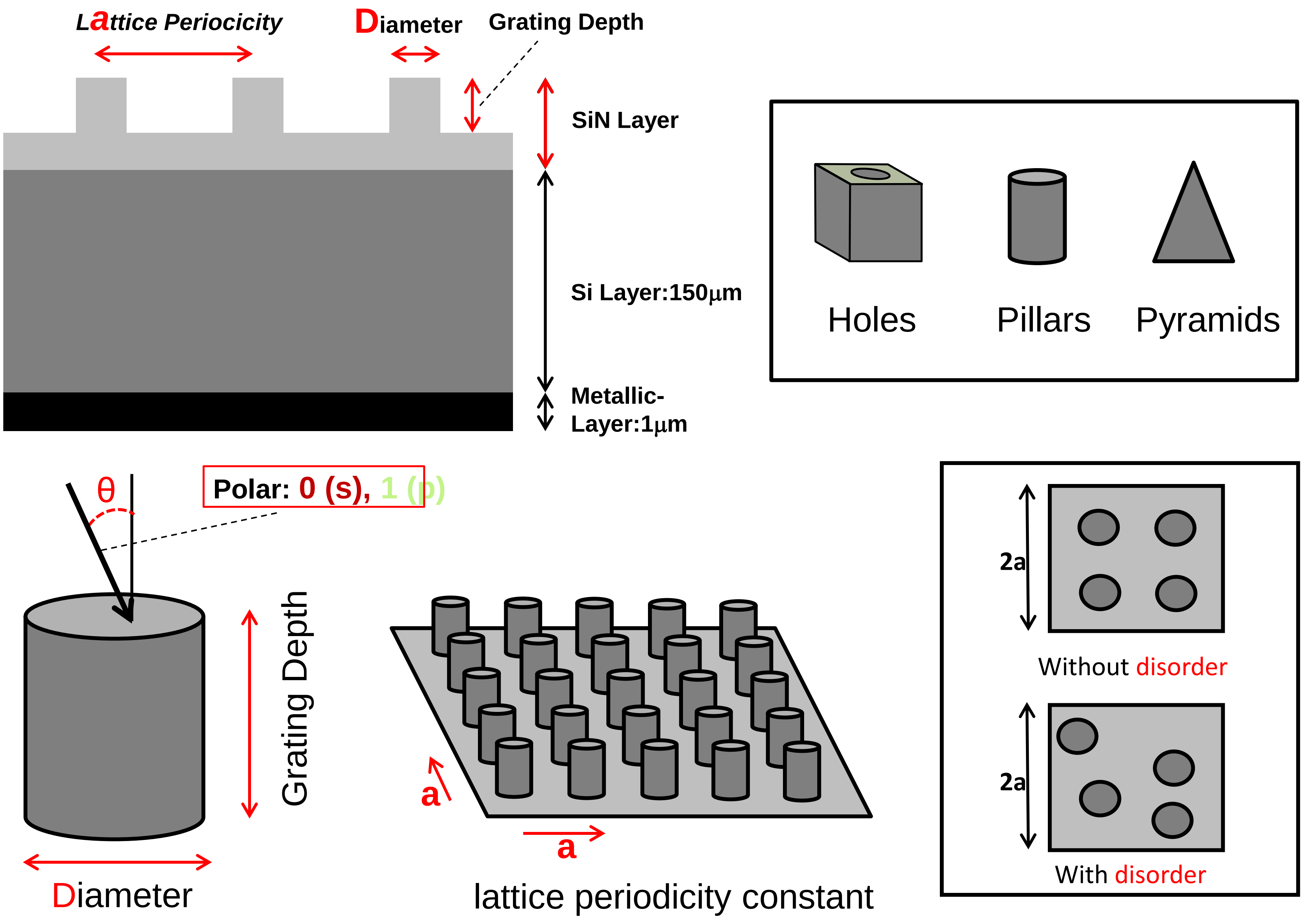


r/a=0.5, t=4000nm
a=100, 300, 400nm
(solid, dash, and dotted lines, respectively)

The absorption for different values of the separation between the nanowires.

The effects of diameter, thickness, orientation and disorder have been also studied.

RCWA Simulation Parameters (1)



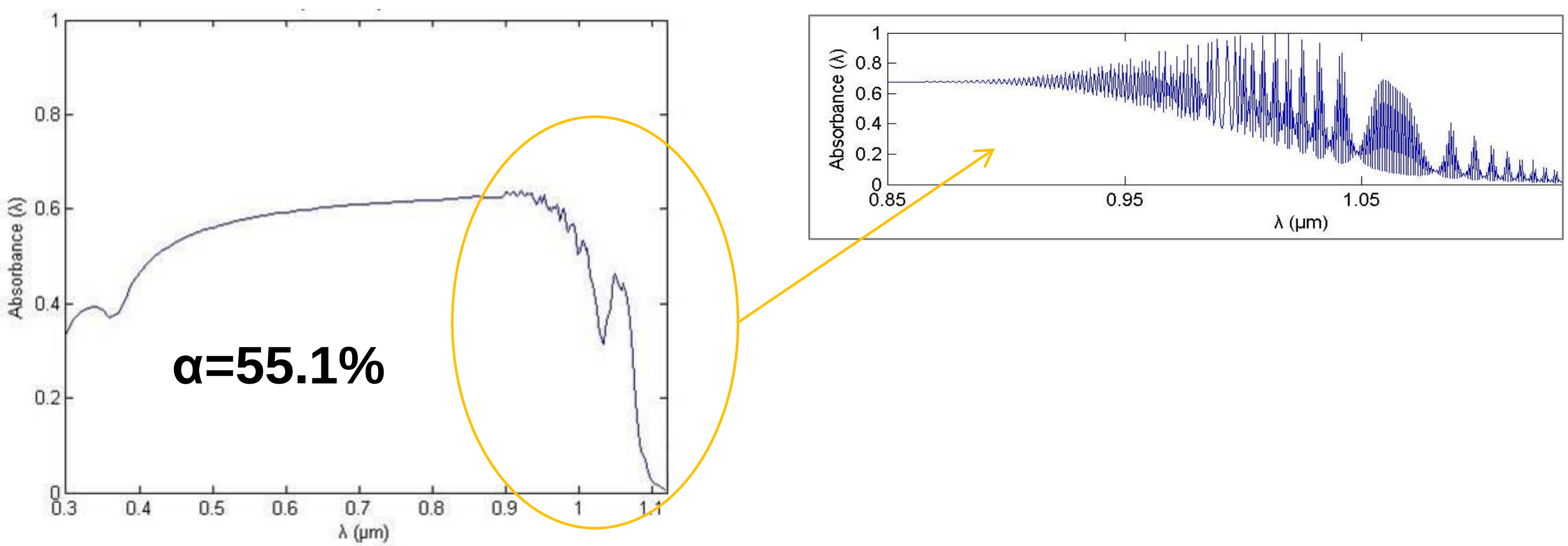
RCWA Simulation Parameters (2)

Si=150µm

REAL(**Ag**)=1µm

$$\alpha = \frac{\int_{0.3}^{1.117} abs_{\lambda} AM1.5_{\lambda} \lambda \, d\lambda}{\int_{0.3}^{1.117} AM1.5_{\lambda} \lambda \, d\lambda}$$

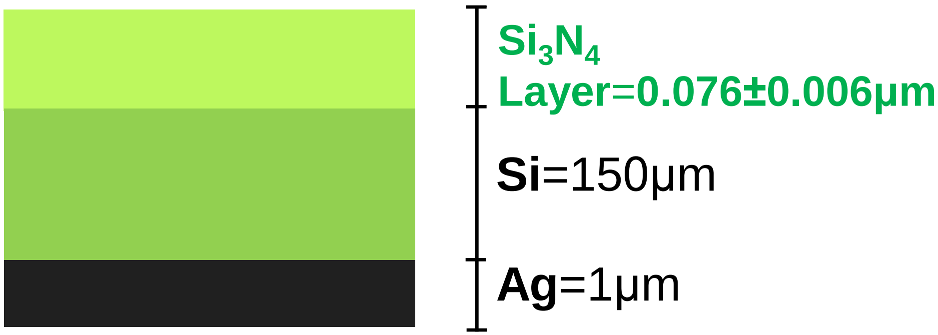
were AM15(λ) is the Solar Spectral Irradiance

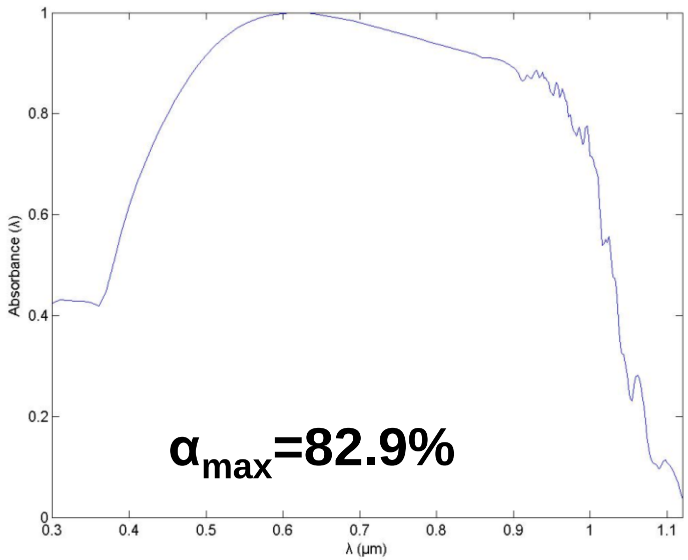


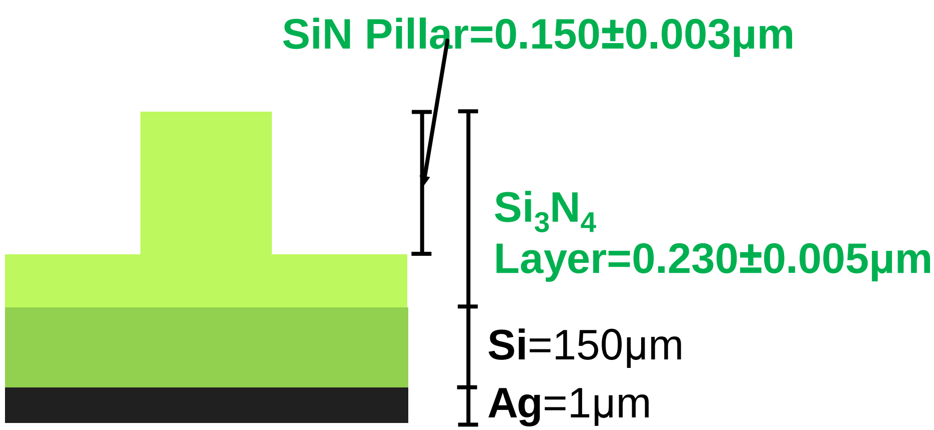
The absorption spectra for Si-wafers (150µm thickness) with metallic substrate using the Aspnes (modified), refractive index. The absorption spectrum has been smoothened as well to eliminate interference effects.*

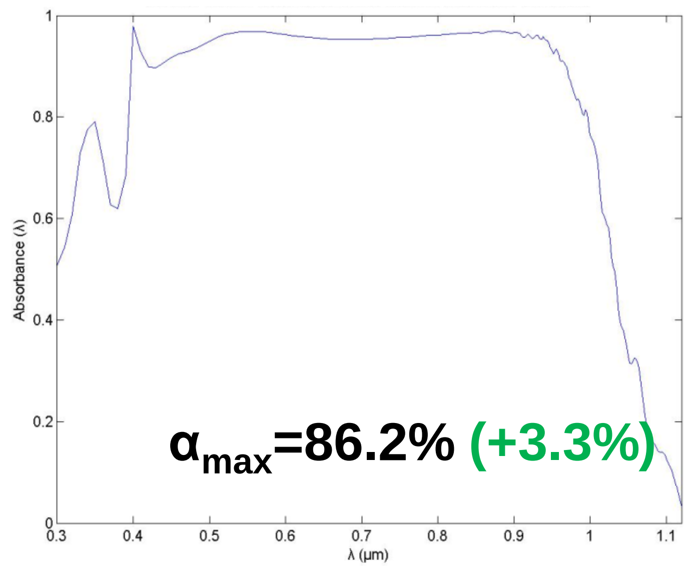
*Aspnes and Stunda, *Phys. Rev. B* **27**, 985 (1983).

Grating on Si/Si_3N_4

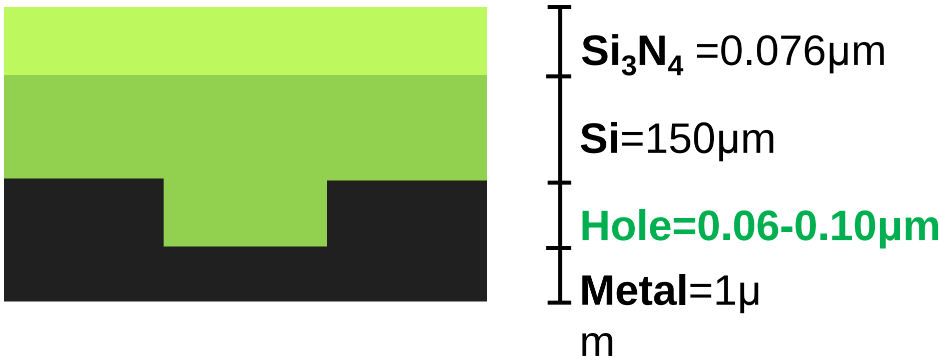


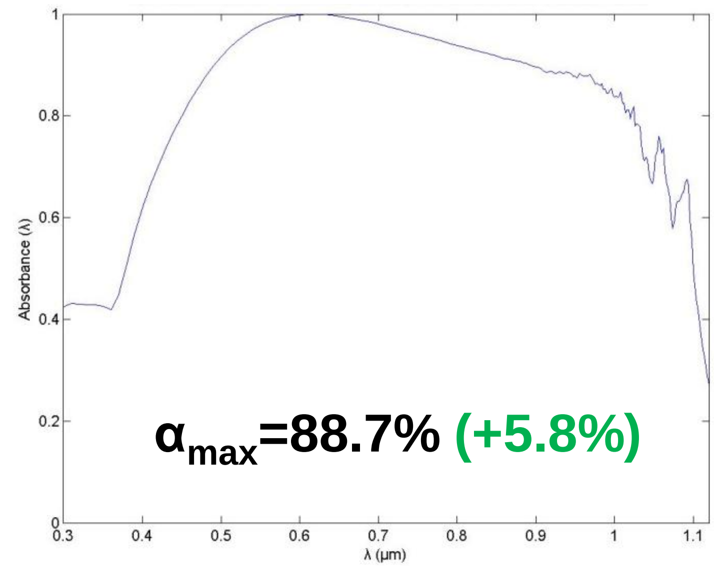


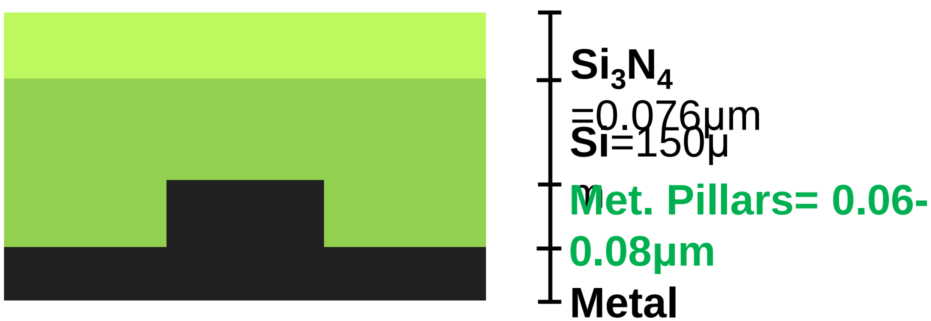


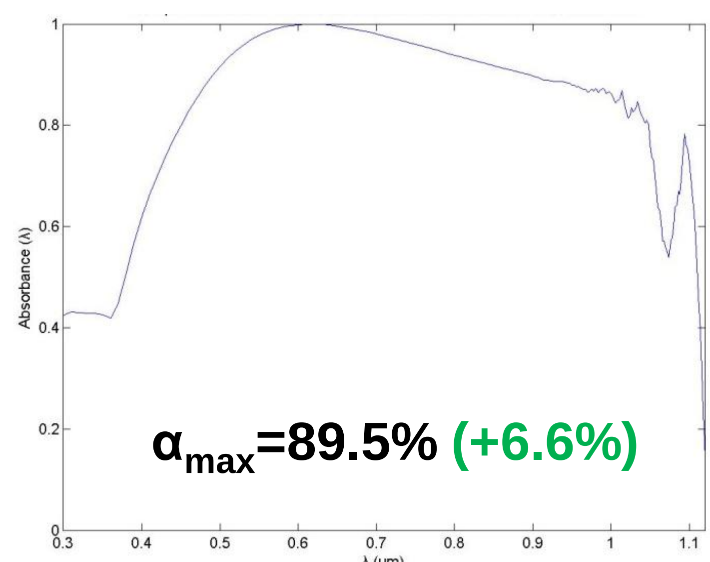


Grating on Si/Si_3N_4









(P079) Polysterene on 101 nm Nitride on Si

Sotiropoulos, Speliotis, Niarchos, Spiratou, Raptis, Misiakos, Lidorikis

Πηγές:

Nanoscience
C. Dupas, P. Houdy, and M. Lahmani

Computational Electrodynamics: The Finite Difference Time Domain Method
A. Taflove, S. C. Hagness