Appendix A

Boundary Element Method Calculations of LDOS and Decay Rates

A.1 Decay Rates in Atomic Units

This appendix provides a brief tutorial for BEM calculations of the total and radiative decay rates, including a sample command file and material data file for BEMAX (program for structures with axial symmetry), and intended to supplement the internal help files that accompany the BEMAX program. As described in Chapters 4 and 6, the total decay rate is proportional to the LDOS, and the radiative decay rate is determined from the far-field radiation [85]. All calculations within the BEM program use atomic units with standard physical quantities defined as follows:

$$\hbar = m_e = e = 4\pi\varepsilon_0 = 1 \tag{A.1a}$$

$$c = 137.036 \tag{A.1b}$$

$$\lambda = \frac{10 \cdot \lambda[\mathrm{nm}]}{0.52918} \tag{A.1c}$$

$$\omega = \frac{\mathrm{E[eV]}}{27.211} = \frac{1240}{27.211 \cdot \lambda[\mathrm{nm}]}. \tag{A.1d}$$

The BEM calculations of the local density of optical states ρ output a value for each orientation (x, y, and z) and a total LDOS, all normalized ρ_0, the LDOS in a homogeneous region of refractive index n, given by

$$\rho_0 = \frac{\omega^2 n}{\pi^2 c^3} \tag{A.2}$$

in atomic units. To distinguish, we define LDOS_x as the value output from the BEM program for the x orientation (command `calc LDOS`), and ρ_x the unnormalized value, such that

$$\text{LDOS}_x = \frac{\rho_x}{\rho_0}. \tag{A.3}$$

Now, we are equipped to calculate decay rates from BEM output. This thesis reports total and radiative decay rates normalized to decay in vacuum, Γ_0,

$$\Gamma_0 = 4\pi^2 \frac{\omega}{\hbar} \frac{\rho_0}{3} |D|^2, \tag{A.4}$$

which in atomic units becomes

$$\Gamma_0 = \frac{4}{3} \left(\frac{\omega}{c}\right)^3. \tag{A.5}$$

Similarly, the total decay rate Γ_{tot} is given by

$$\Gamma_{\text{tot}} = \frac{4\pi^2 \omega |D|^2}{\hbar} \rho_x, \tag{A.6}$$

or in atomic units,

$$\Gamma_{\text{tot}} = 4 \left(\frac{\omega}{c}\right)^3 n\text{LDOS}_x. \tag{A.7}$$

The radiative decay rate is calculated by integrating the far-field Poynting vector for a dipole source, given by

$$\Gamma_{\text{rad}} = \frac{c}{2\pi\omega} \int f^2. \tag{A.8}$$

In this case, $\int f^2$ is the output from the BEM command `calc total-far-field`.

In summary, the quantities from BEM commands can be used directly to calculate decay rates using (A.7) and (A.8), and properly normalized by dividing by (A.5). The following pages provide a sample BEMAX input file for determining the decay rates in a Si-Ag core-shell nanowire resonator, as well as a sample material file for Ag with the dielectric constants of Johnson and Christy [34].

A.2 Example BEM Input File

```
CoreShell_SiAg_a25L150.bem

mmax 3
  // calculations performed for m=-3,-2,-1,0,1,2,3

epsilon 2 Ag // calls material file Ag.eps
epsilon 3 Si // calls material file Si.eps
                    // material 1 is always air (n=1)
photon-wavelength 500 1000 101
  // defines range of wavelengths for calculations
  // (in nm) and number of wavelengths used
  // for calculation (101)

// Define structure
  L=150  // wire length (nm)
  a=25   // core radius
  C=100  // coating thickness
  n1=25  // number of parameterization points, radius
  n2=50  // number of param. points, coating
  n3=150 // number of param. points, length

  // Structure made of straight line segments
  // from (x1,z1) to (x2, z2) with material
  // mu1 to left and mu2 to right
  // add-segment command format:
    // mu1, mu2, x1, z1, x2, z2, # param. points
  add-segment 3 1 0 0 a 0 n1
  add-segment 1 3 0 L a L n1
  add-segment 2 1 a 0 a+C 0 n2
  add-segment 1 2 a L a+C L n2
  add-segment 3 2 a 0 a L n3
  add-segment 2 1 a+C 0 a+C L n3

begin-calculation   // begins calculation loop

// Calculate NF intensity for plane-wave excitation
  // at all wavelengths

  grid 5 5 1 0 0 1 0 150 76
    // grid for NF E2 intensity along z-axis for x=5:
    // command format is grid x1 x2 nx y1 y2 ny z1 z2 nz
```

```
  incident-plane-wave  0 0 0 0
   // incident plane wave at theta=0

  calc E2-near-field nf05th=0.dat
   // output will appear in this file

  grid 5 5 1 0 0 1 0 150 76

  incident-plane-wave  90 0 0 0
   // incident plane wave at theta=90

  calc E2-near-field nf05th=90.dat
   // output will appear in this file

// Components required to calculate decay rates

  // First position
  z=15   R=5
     grid R R 1 0 0 1 z z 1
        // single point at (R,z)
     calc LDOS LDOS_r5z15.dat
        // LDOS used to find total decay rate

     electric-dipole R z 1 0 0 0 0 0
        // dipole source oriented along x at position (R,z)
     calc total-far-field totalff_r5z1_px.dat
        // FF used to find radiative decay rate

  // Second position
  z=75   R=5
     grid R R 1 0 0 1 z z 1
        // single point at (R,z)
     calc LDOS LDOS_r5z75.dat
         // LDOS used to find total decay rate

     electric-dipole R z 1 0 0 0 0 0
        // dipole source oriented along x at position (R,z)
     calc total-far-field totalff_r5z75_px.dat
        // FF used to find radiative decay rate

end-calculation

end
```

A.3 Example BEM Material Data File

```
Ag.eps

63 E(eV) n

0.64 0.24 14.08
0.77 0.15 11.85
0.89 0.13 10.1
1.02 0.09 8.828
1.14 0.04 7.795
1.26 0.04 6.992
1.39 0.04 6.312
1.51 0.04 5.727
1.64 0.03 5.242
1.76 0.04 4.838
1.88 0.05 4.483
2.01 0.06 4.152
2.13 0.05 3.858
2.26 0.06 3.586
2.38 0.05 3.324
2.5 0.05 3.093
2.63 0.05 2.869
2.75 0.04 2.657
2.88 0.04 2.462
3 0.05 2.275
3.12 0.05 2.07
3.25 0.05 1.864
3.37 0.07 1.657
3.5 0.1 1.419
3.62 0.14 1.142
3.74 0.17 0.829
3.87 0.81 0.392
3.99 1.13 0.616
4.12 1.34 0.964
4.24 1.39 1.161
4.36 1.41 1.264
4.49 1.41 1.331
4.61 1.38 1.372
4.74 1.35 1.387
4.86 1.33 1.393
4.98 1.31 1.389
5.11 1.3 1.378
5.23 1.28 1.367
```

```
5.36 1.28 1.357
5.48 1.26 1.344
5.6 1.25 1.342
5.73 1.22 1.336
5.85 1.2 1.325
5.98 1.18 1.312
6.1 1.15 1.296
6.22 1.14 1.277
6.35 1.12 1.255
6.47 1.1 1.232
6.6 1.07 1.212
7.0  0.953    1.01
7.2  0.942   0.951
7.4  0.936   0.892
7.6  0.935   0.832
7.8  0.940   0.770
8.0  0.962   0.706
8.2  0.993   0.653
8.4  1.032   0.610
8.6  1.073   0.581
8.8  1.112   0.563
9.0  1.149   0.552
9.2  1.182   0.550
9.7  1.229   0.566
10.0 1.241   0.568

w(eV) n k

First line specfies: number of points (63),
energy E(eV) or wavelength l(nm),
and n & k (n) or eps1 & eps2 (e)

Ag dielectric function from Johnson and Christy (1972)
0.64 eV < w < 6.6 eV ->
187.9 nm < lambda < 1937 nm
```