Appendix A: Getting started

- Login
- In your home directory, create a directory (e.g., exercisedir)
- Place the achieve file into this directory and uncompress it, in the console, this may read: /~/…./exercisedir$ unzip XXX.zip
- start matlab
- open the script main_densityVsTemperature_lean.m
- run the script

Appendix B: Overview functions

The zip file contains the sample script (main_densityVsTemperature_lean.m) and useful functions

Choose the semiconductor		
AssignSemiconductor.m		

Construct a density of states		
InitializeEnergyAndDOS.m		
InitializeDOSAdministration.m		
AddConductionBandToDOS.m AddValenceBandToDOS.m	AddGaussToDOS.m	AddLevelToDOS.m
GetFullDOS		
Obtain electron density (occupation)		
GetDensityInBand.m	GetDensityInGauss.m	GetDensityInLevel.m
FIntegrationForBands.m	FDIntegrantGauss.m	
FermiDirac.m		

Evaluate charge neutrality		
chargeNeutrality.m		
chargeNeutralityIntrinsic.m		

Additionally required functions, service functions		
GaussDOS.m	DensityOfBandStates.m	SetPlotProperties.m
AddContributionsToDOS.m	FindRootNestedIntervals.m	

Appendix C: Overview of textbook expressions on charge carrier statistics in thermal equilibrium

Table 2.4 Carrier Modeling Equation Summary.

Density of States and Fermi Function

$$g_c(E) = \frac{m_n^* \sqrt{2m_n^*(E - E_c)}}{\pi^2 \hbar^3}, \quad E \geq E_c$$

$$g_v(E) = \frac{m_p^* \sqrt{2m_p^*(E_v - E)}}{\pi^2 \hbar^3}, \quad E \leq E_v$$

$$f(E) = \frac{1}{1 + e^{(E - E_F)/kT}}$$

n, p, and Fermi Level Computational Relationships

$$n = \frac{N_D - N_A}{2} + \left[\left(\frac{N_D - N_A}{2} \right)^2 + n_i^2 \right]^{1/2}$$

$$E_i = \frac{E_c + E_v}{2} + \frac{3}{4} kT \ln\left(\frac{m_p^*}{m_n^*} \right)$$

$$n \simeq N_D \qquad N_D \gg N_A, N_D \gg n_i$$

$$p \simeq n_i^2 / N_D$$

$$E_F - E_i = kT \ln(n/n_i) = -kT \ln(p/n_i)$$

$$p \simeq N_A \qquad N_A \gg N_D, N_A \gg n_i$$

$$n \simeq n_i^2 / N_A$$

$$E_F - E_i = kT \ln(N_D/n_i) \quad N_D \gg N_A, N_D \gg n_i$$

$$E_i - E_F = kT \ln(N_A/n_i) \quad N_A \gg N_D, N_A \gg n_i$$

Carrier Concentration Relationships

$$n = N_C \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_c)$$

$$p = N_V \frac{2}{\sqrt{\pi}} F_{1/2}(\eta_v)$$

$$N_C = 2 \left[\frac{m_n^* kT}{2\pi\hbar^2} \right]^{3/2}$$

$$N_V = 2 \left[\frac{m_p^* kT}{2\pi\hbar^2} \right]^{3/2}$$

$$n = N_C e^{(E_F - E_c)/kT}$$

$$p = N_V e^{(E_v - E_F)/kT}$$

$$n = n_i e^{(E_F - E_i)/kT}$$

$$p = n_i e^{(E_i - E_F)/kT}$$

n_i, np-Product, and Charge Neutrality

$$n_i = \sqrt{N_C N_V} e^{-E_G/2kT}$$

$$np = n_i^2$$

$$p - n + N_D - N_A = 0$$

Taken from R. F. Pierret, Semiconductor Device Fundamentals, Addison Wesley, 1996.

Appendix D: Reference of functions

Function	description	input	output
AssignSemiconductor	choose effective masses and bandgap according to a semiconductor	string with semiconductor composition	effective electron m^*_e and hole masses m^*_h, energies of conduction band minimum E_C and valence band maximum E_V (in eV)
InitializeEnergyAndDOS	creates an energy interval with desired resolution	E_C and E_V (in eV); maximal and minimal energy to be considered (in eV); number of bins in the energy interval	vector with discretized energy interval, empty vectors capable of storing DOS and occupation info with respect to energy interval
InitializeDOSAdministration	creates a data structure DOS_admin capable of holding information necessary to describe the nature of the states participating in the overall DOS	energy interval	DOS_admin
AddConductionBandToDOS	adds a conduction band to the DOS	DOS_admin, energy interval, m^*_e, E_C	DOS_admin
AddValenceBandToDOS	adds a valence band to the DOS	DOS_admin, energy interval, effective hole mass, energy of valence band maximum	DOS_admin
AddGaussToDOS	adds Gaussian-shaped DOS the DOS	DOS_admin, energy interval, total density, energy, width of Gaussian	DOS_admin
AddLevelToDOS	adds sharply defined level to the DOS	DOS_admin, energy interval, total density, energy	DOS_admin
AddContributionToDOS	service routine required by the former 4 routines to add DOS contributions to DOS_admin	DOS_admin, vector with size of energy interval, label (internal), type, position in energy interval (in eV), parameter, e.g., Gaussian width, density of states (in m^{-3})	DOS_admin
GetFullDOS	retrieves complete DOS information from DOS_admin and stores it a vector DOS of the size of the energy interval	DOS_admin	filled vector DOS
GetDensityInBand	provides electron density in a band	data set in DOS_admin, chemical potential, E_C, m^*_e, temperature	electron density
GetDensityInLevel	provides electron density in a sharply-defined level	chemical potential, E_v, m^*_h, temperature	electron density
GetDensityInGauss	provides electron density in a Gaussian-shaped DOS	chemical potential, temperature	electron density
FIntegrationForBands	performs an integration of the DOS*FermiDirac distribution in a band	chemical potential, temperature	occupation probability in the band
FDIntegrantGauss	performs an integration of the DOS*FermiDirac distribution in a Gauss-DOS	chemical potential, temperature	occupation probability in the Gauss DOS
GaussDOS	Gauss function	energy *E* (in eV) mean energy (in eV) width of Gaussian (in eV)	value of the Gauss function at energy *E*
FermiDirac	Fermi Dirac distribution function	chemical potential temperature	occupation probability
DensityOfBandStates	provides effective density of states for a band	effective mass temperature	density of states in m^{-3}
chargeNeutrality	yields the difference between negative and positive charges considering the properties of the total DOS	variable storing desired chemical potential, DOS_admin, E_v, E_c, m^*_h, m^*_e temperature	difference n-p of negative and positive charges
chargeNeutralityIntrinsic	yields the difference between negative and positive charges assuming an intrinsic	variable storing desired chemical potential, E_v, E_c, m^*_h, m^*_e temperature	difference n-p of negative and positive charges

	semiconductor with CB and VB	chemical potential temperature	
FindRootNestedIntervals	Finds at which argument x a function F(x) becomes zero	function handle referring to function F, energy interval, initial value for x, threshold for relative error below which search stops, number of maximum iterations	argument x fulfilling |F(x)| < threshold, relative error, number of iterations
SetPlotProperties	sets parameters for a unified and convenient appearance of plot figures	--	--

Appendix E: Sample script

Note: The printout of the sample script was created with the publish function of MATLAB. This function might be helpful to document a task completed in MATLAB.

In the MATLAB console: >> myfile = publish('my_MATLAB_script.m','pdf')