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1. %% getDiffCloseAlGaAs: function description
2. function [Ec, meff, Alx] = getDiffCloseAlGaAs(x_Al, checkTime, dx, T, Nd)
3.     e = 1.6e-19; eVtoJ = e; JtoEv = e^(-1);
4.     nm = 1e-9; me = 9.1*1e-31;
5.     hbar = 1.054*1e-34; k_B = 1.38e-23;
6.
7.     kT = T*k_B; % J
8.
9.     Time = max(checkTime)*12*30*24; % to hours
10.
11.     n_Atoms = 4.42*1e28; % number Atoms in GaAs ~ AlAs
12.     n_Al = n_Atoms/2; % number atoms of Al in AlAs
13.
14.     dt = 1; % one hour
15.     dtdx2 = dt*60*60/dx^2; % s/m^2
16.
17.     Eg_GaAs = 1.519 - 5.405*1e-4*T^2/(T+204);
18.     Nc = 2*(me*0.067*kT/pi/hbar^2/2)^(3/2);
19.     Nv = 2*(me*0.51*kT/pi/hbar^2/2)^(3/2);
20.     ni = sqrt(Nc*Nv)*exp(-Eg_GaAs/(2*kT*JtoEv));
21.
22.     D_Al = 0.2*exp(-3.5/(kT*JtoEv))*1e-4*(Nd/ni)^3; % m^2/s
23.
24.     C_Al = x_Al*n_Al;
25.     len = length(x_Al);
26.
27.     d1 = D_Al*dtdx2*ones(1, len-1);
28.     d2 = [ 1 - D_Al*dtdx2, 1 - 2*D_Al*dtdx2*ones(1, len-2), 1 - D_Al*dtdx2 ];
29.     d3 = D_Al*dtdx2*ones(1, len-1);
30.
31.     Matrix_Al = diag(d1, -1) + diag(d2) + diag(d3, +1);
32.
33.     if (find(0 == checkTime))
34.         [Ec(1, :), ~, meff(1, :), ~] = getBandPropAlGaAs(C_Al);
35.         Alx(1, :) = C_Al./n_Al;
36.     end
37.
38.     C_Al = C_Al';
39.     for j = 0 : dt : Time
40.         % clc; disp(j/Time*100);
41.         C_Al = Matrix_Al*C_Al;
42.         ind = find(j == checkTime*12*30*24);
43.         if (ind & j ~= 0)
44.             [Ec(ind, :), ~, meff(ind, :), ~] = getBandPropAlGaAs(C_Al');
45.             Alx(ind, :) = C_Al'./n_Al;
46.         end
47.     end
48. end

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