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1. %% getDiffOpenAlGaAs: function description
2. function [Ec, meff, Alx] = getDiffOpenAlGaAs(x_Al, checkTime, dx, T)
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.     D_Al = 0.2*exp(-3.5/(kT*JtoEv))*1e-4; % m^2/s
18.
19.     C_Al = x_Al*n_Al;
20.     len = length(x_Al);
21.
22.     d1 = [D_Al*dtdx2*ones(1, len-2), 0];
23.     d2 = [ 1, 1 - 2*D_Al*dtdx2*ones(1, len-2), 1 ];
24.     d3 = [0, D_Al*dtdx2*ones(1, len-2)];
25.
26.     Matrix_Al = diag(d1, -1) + diag(d2) + diag(d3, +1);
27.
28.     if (find(0 == checkTime))
29.         [Ec(1, :), ~, meff(1, :), ~] = getBandPropAlGaAs(C_Al);
30.         Alx(1, :) = C_Al./n_Al;
31.     end
32.
33.     C_Al = C_Al';
34.     for j = 0 : dt : Time
35.         % clc; disp(j/Time*100);
36.         C_Al = Matrix_Al*C_Al;
37.         ind = find(j == checkTime*12*30*24);
38.         if (ind & j ~= 0)
39.             [Ec(ind, :), ~, meff(ind, :), ~] = getBandPropAlGaAs(C_Al');
40.             Alx(ind, :) = C_Al'./n_Al;
41.         end
42.     end
43. end

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