Computational Microelectronics

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1. Simulation explanation

저는 자성체를 연구하고 있기 때문에, Ferrimagnetic insulator 인 YIG(Yittrum Iron Garnet) 과 Topological insulator 인 Bi2Se3 의 Heterostructure 구조에 대해서, 두께 방향의 위치에 따른 Potential energy 변화를 Generalized Poisson equation 을 통해, Numerical computation을 진행했다. 그리고 이를 Analytical solution 과 비교한다.

물질	YIG	Bi2Se3
두께	10 nm	10 nm
Relative permittivity	15.3	18

2. Result and discussion

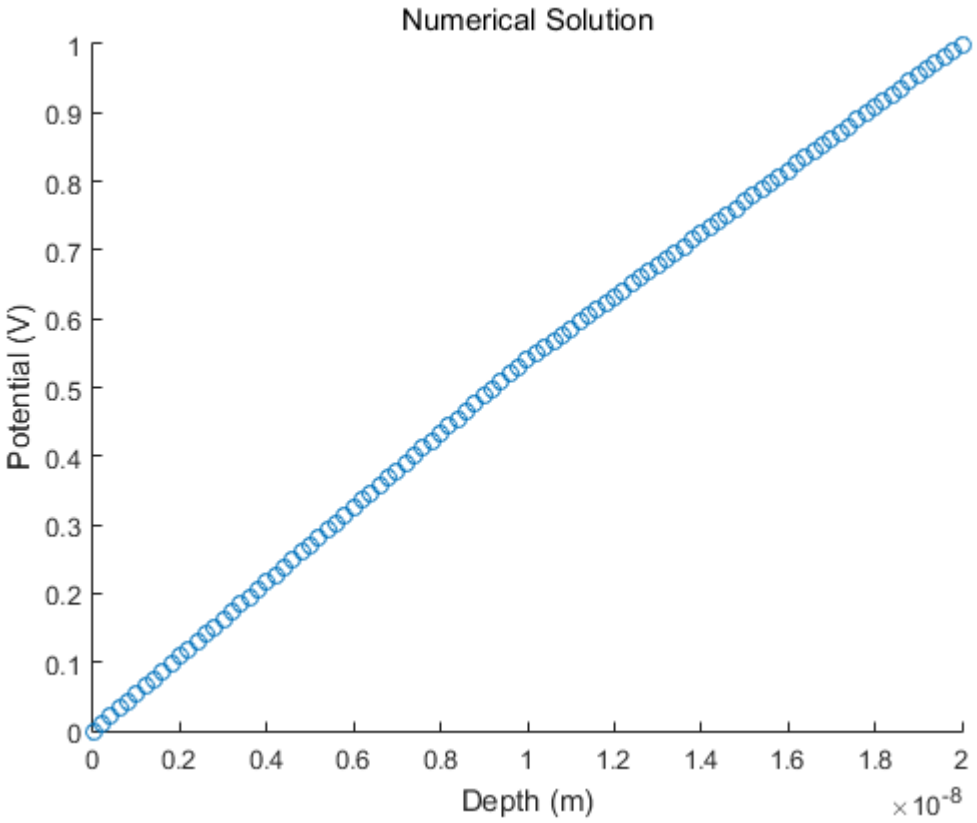

Figure 1 Potential vs Depth_position

Numerical 방법과 Analytic 방법, 각각을 통해 얻은 Capacitance, Potential Data 들의 차이가 Grid points 를 증가시킬수록 줄어드는 것을 확인했다.

	$\Delta interface\ /_{interface}$	$\Delta C\_YIG\ /_{C\_YIG}$	$\Delta C\_Total\ /_{C\_Total}$	$\Delta V\_interface\ /_{V\_interface}$
N = 11	20 %	20 %	1.6216 %	18.6813 %
101	2	2	0.16	1.8408 %
1001	0.2	0.2	0.0162	0.1838
10001	0.02	0.02	0.0016	0.0184

< Matlab Code >

```
clear all;
clc;

%% Material constants

eps0 = 8.854187817e-12; % Vacuum permittivity, F/m

n = 11; % Grid number (odd number)
eps_rel_1 = 15.3; % 15.3 YIG
eps_rel_2 = 18 ; % 18 Bi2Se3

eps_1 = eps_rel_1*eps0;
eps_2 = eps_rel_2*eps0;

width_1 = 10e-9; % [m] YIG
width_2 = 10e-9; % [m] Bi2Se3

T = width_1 + width_2; % [nm] Total thickness
delta_x = T/(n-1); % [nm] the spacing btw the grids

interface_1 = floor((n-1)- (width_1)/delta_x); % Grid point for the
interface

Pot_ini = 0; % [V] Potential for initial contact
Pot_fin = 1; % [V] Potential for final contact

pot_diff = Pot_fin - Pot_ini ; % [V] poential difference


dist_x = zeros(n,1);
for i = 2:(n-1)
    dist_x(i,1) = (i-1)*delta_x;
end
dist_x(1,1) = 0;
dist_x(n,1) = T;

%% Numerical solution

% Matrix to calculate the potentials

A = zeros(n,n);
A(1,1) = 1.0;
A(n,n) = 1.0;

for i = 2:n-1
    if (i < interface_1); A(i,i-1) = eps_1; A(i,i) = -2*eps_1; A(i,i+1) =
eps_1;
    elseif (i == interface_1); A(i,i-1) = eps_1; A(i,i) = -eps_1 - eps_2;
A(i,i+1) = eps_2;
    elseif (i > interface_1); A(i,i-1) = eps_2; A(i,i) = -2*eps_2; A(i,i+1)
= eps_2;
    end
end
```

```
b = zeros(n,1);
b(n,1) = pot_diff; % Potential difference on the final grid
Pot = zeros(n,2);


Pot(:,1) = dist_x;
Pot(:,2) = A\b; % Potential difference
V_1_num = Pot(interface_1,2); % potential at the boundary of Numerical sol
V_2_num = Pot(n,2) - Pot(interface_1,2);
C_1_num = eps_1/(dist_x(interface_1)); % capacitance for YIG
C_2_num = eps_2/(T-dist_x(interface_1)); % capacitance for YIG
C_num_tot = (C_1_num*C_2_num)/(C_1_num + C_2_num); % Total Capacitance
Diff_interface_1 = 100*(width_1 - dist_x(interface_1))/width_1

scatter(Pot(:,1),Pot(:,2))
xlabel('Depth (m)')
ylabel('Potential (V)')
title('Numerical Solution');


%% Analytic solution

C_1_anal = eps_1/(width_1); % capacitance for YIG
C_2_anal = eps_2/(width_2); % capacitance for Be2Se3
V_anal = C_2_anal/(C_1_anal+C_2_anal); % potential at the boundary of
Analytic sol
C_anal_tot = (C_1_anal*C_2_anal)/(C_1_anal + C_2_anal); % Total Capacitance

Diff_C_1 = 100*(C_1_num - C_1_anal)/C_1_num
Diff_C_2_tot = 100*(C_num_tot - C_anal_tot)/C_num_tot

Diff_V_1 = 100*(V_anal-V_1_num)/V_anal
```