Analysis of the sub-wavelength grating in OptiFDTD simulator

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ACKNOWLEDGEMENT

I express my cordial and humble gratitude to Prof. Dr. Dietmar Knipp for giving me an opportunity to carry out profound research in sub wavelength gratings. I would also like to thank him for his continuous support. I thank Mr. Vladislav Jovan Jovanov for his constant guidance, without him the research wouldn’t have completed in time.

I would also like to thank Mr. Ujwol Palanchoke for the support for the research activity.

Dileep Dhakal

ABSTRACT

Standard sub-wavelength grating array is designed and 2D simulation is carried out, on OptiFDTD 8.0 simulation software. Implementation of different types of sub-wavelength grating are discussed and analyzed with simulation results.

The power transmittance at different wavelength under the variation of different grating parameters is demonstrated on the simulation. Grating periods, grating spacing, grating material and the presence and absence of substrate are the parameters varied for the transmittance analysis and also effects of the parameters on power transmittance are studied. Finally, profound analysis of the results is done to have better understanding of sub-wavelength gratings.

MOTIVATION

The main purpose behind profound analysis of sub-wavelength gratings is to understand the effect of grating parameters on the measured transmittance at different wavelength of visible spectrum. Grating spacing, grating period, substrates and materials are basic properties which may have profound effect on the measured power transmittance, which must be individually explored. Also, studying such individual effects might help us in designing high efficiency sub-wavelength gratings. We can also extract any individual property of sub-wavelength grating and realize the novel system which cannot be thought of in micro-sized world.

For e.g. if grating which produces maximum transmittance (~100%) at particular wavelength (say, 620-750nm) then, this grating can be applied for filtering red light. This approach will help in designing ultra low cost color filters.

TABLE OF CONTENTS

Chapter 1: Introduction

Sub-wavelength grating

Gratings where grating period is very small and less than the wavelength (λ) of incident light are termed as sub-wavelength gratings (SWG). For sufficiently small period higher order diffraction are suppressed and only remains is the zero order diffraction. Thus, SWG can be represented as the homogeneous medium with optical properties determined by the grating geometry. There are lots of applications of sub-wavelength grating like anti-reflecting filters [1], phase plates [2], plasmonic lens [3] and negative refractive index [4].

FDTD (Finite difference Time Domain)

FDTD was first developed by Kane S. Yee in 1966. FDTD is the modeling technique to solve the Maxwell equation applying finite difference mathematics. FDTD directly calculates the value of E (Electric field intensity) and H (magnetic field intensity) at different points of the computational domain (i, j, k). Yee proposed the mesh (Fig. 1), where magnetic and electrical field wave vector are distributed such that magnetic field lies exactly half points of the electrical field.

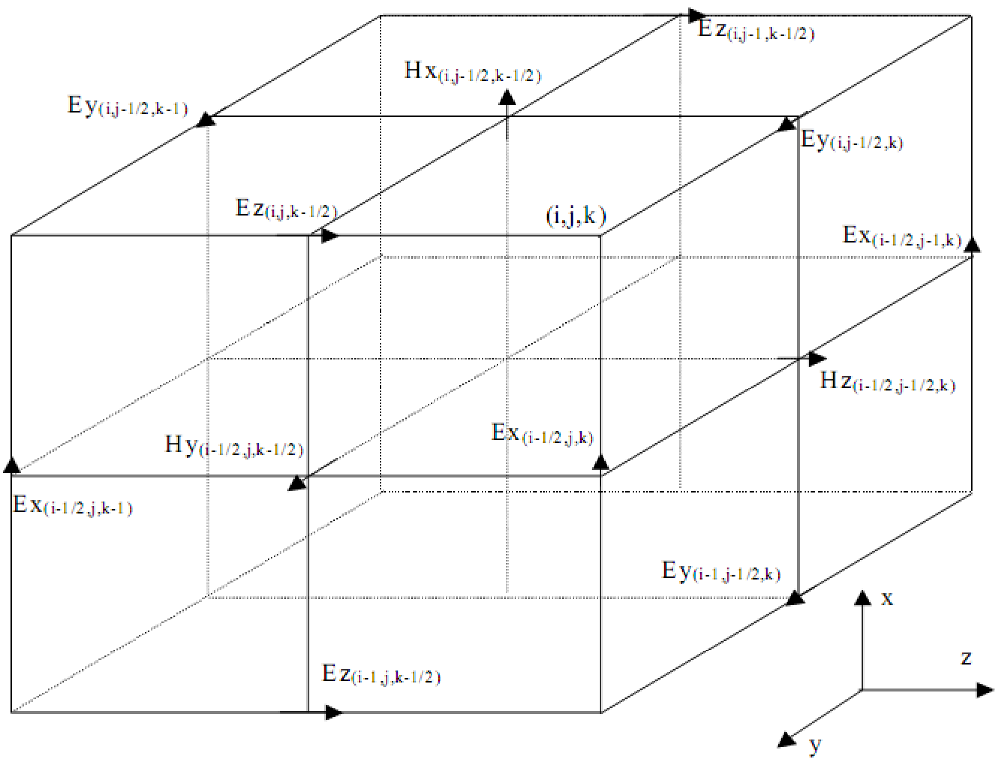


Fig. 1: Yee's mesh in 3D. In the mesh, electrical field points are exactly half grid offset from the magnetic field points [6].

In the 2D TE case (Hx, Ey and Hz are nonzero components, for wave propagating along z-direction and xz-plane is the point of observation) in lossless media, Maxwell's equations take the following form [6]:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0}\left(\frac{\partial E_y}{\partial z}\right), \quad \frac{\partial H_z}{\partial t} = -\frac{1}{\mu_0}\left(\frac{\partial E_y}{\partial x}\right), \quad \frac{\partial E_y}{\partial t} = -\frac{1}{\varepsilon}\left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right) \text{.............} (1)$$

Where, $\varepsilon = \varepsilon_0 \varepsilon_r$ is the dielectric permittivity and μ_0 is the magnetic permeability of the vacuum. The refractive index is $n = \sqrt{\varepsilon_r}$ [6].

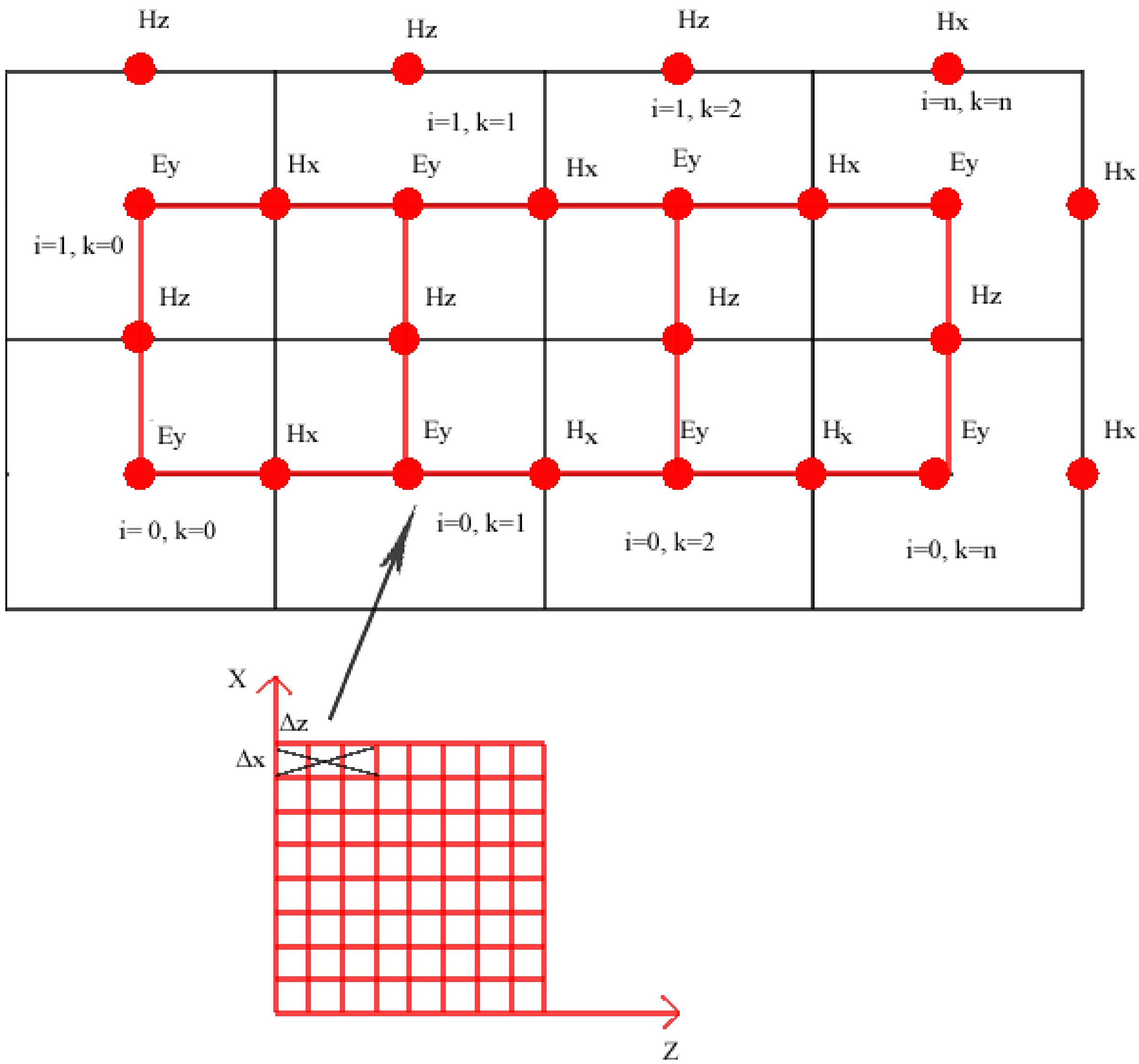


Fig. 2: Mesh for FDTD in TE mode, when z axis is the direction of propagation of wave and y-axis is the point of observation. Hx, Ey and Hz are correspondingly nonzero values of electrical field along x-direction, electric field along y-direction and magnetic field along z-direction. Δx and Δz are the unit mesh size along the x and z-direction.

Relation of stability with the mesh size:

For high degree of accuracy, the grid spacing (Δx, Δy and Δz) in the simulation must be less than the wavelength, usually less than λ/10. The stability condition which must be satisfied and termed as Courant limit [5] is given as:

$$v_{\max}\Delta t = \left[\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}\right]^{-\frac{1}{2}} \text{............ (2)}$$

Where, $v_{\max}$ is the maximum velocity of the input wave. When the step size Δ same in all directions, the stability condition is: [5]

$$\frac{v_{\max}\Delta t}{\Delta} = \frac{1}{\sqrt{N}} \text{............ (3)}$$

Where, N is the number of spatial dimensions in the problem.

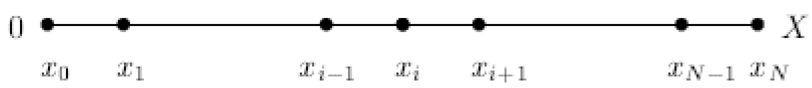
To model the scattering produced by cells at optical wavelengths, the grid size (Δ) must be small. If a wavelength of λ = 0.5nm is applied, the maximum step size is:

$$\Delta = \frac{\lambda}{10} = 0.05nm$$

Finite difference method:

Derivative in the partial differential equation are approximated by linear combinations of functions at the grid point. If we have a 1-D grid, for grid point from 0 to X, functional value $F_i = F(x_i)$, i = 0, 1,…, N, then,

Mesh size is $\Delta x = \frac{X}{N}$ and $x_i = i\Delta x$.



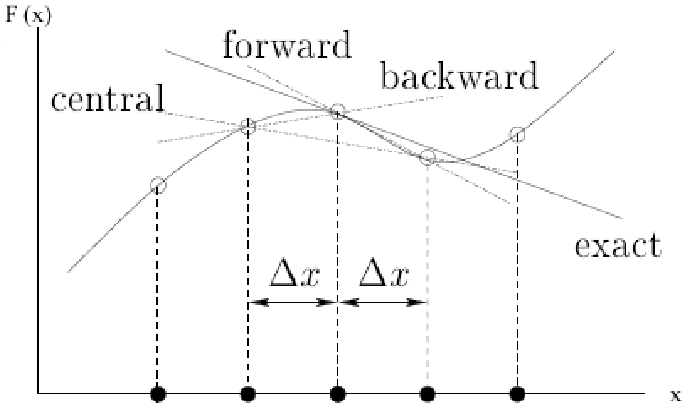


Fig. 3: Finite difference approximation plot for the function F(x) [7].

For the finite difference method we can write the following types of equation as [7]:

Forward difference equation:

$$\frac{\partial F(\bar{x})}{\partial x} = \lim_{\Delta x \to 0} \frac{F(\bar{x} + \Delta x) - F(\bar{x})}{\Delta x}$$

Equals, $\left(\frac{\partial F}{\partial x}\right)_i = \frac{F_{i+1} - F}{\Delta x}$ …………(4)

Backward difference equation:

$$\frac{\partial F(\bar{x})}{\partial x} = \lim_{\Delta x \to 0} \frac{F(\bar{x}) - F(\bar{x} - \Delta x)}{\Delta x}$$

Equals, $\left(\frac{\partial F}{\partial x}\right)_i = \frac{F - F_{i+1}}{\Delta x}$ …………(5)

Central difference equation:

$$\frac{\partial F(\bar{x})}{\partial x} = \lim_{\Delta x \to 0} \frac{F(\bar{x} + \Delta x) - F(\bar{x} - \Delta x)}{2\Delta x}$$

Equals, $\left(\frac{\partial F}{\partial x}\right)_i = \frac{F_{i+1} - F_{i-1}}{2\Delta x}$ …………(6)

The central difference equation yield more accurate results [7].

Applying finite difference method on the equation (1), where we can directly calculate the values of Ey, Hx and Hz at different points (i, k) [6].

$$\frac{E_y^n(i,k) - E_y^{n-1}(i,k)}{\Delta t} = +\frac{1}{\varepsilon}\frac{H_x^{n-1/2}(i,k+1/2) - H_x^{n-1/2}(i,k+1/2)}{\Delta z} - \frac{1}{\varepsilon}\frac{H_z^{n-1/2}(i+1/2,k) - H_z^{n-1/2}(i-1/2,k)}{\Delta x}$$

The total set of numerical values from equation takes the form,

$$E_y^n(i,k) = E_y^{n-1}(i,k) + \frac{\Delta t}{\varepsilon \Delta z}[H_x^{n-1/2}(i,k+1/2) - H_x^{n-1/2}(i,k-1/2)] - \frac{\Delta t}{\varepsilon \Delta x}[H_z^{n-1/2}(i+1/2,k) - H_z^{n-1/2}(i-1/2,k)] \quad \text{........(7)}$$

$$H_x^{n+1/2}(i,k+1/2) = H_x^{n-1/2}(i,k+1/2) + \frac{\Delta t}{\mu_0 \Delta z}[E_y^n(i,k+1) - E_y^n(i,k)] \quad \text{...........(8)}$$

$$H_z^{n+1/2}(i+1/2,k) = H_x^{n-1/2}(i+1/2,k) - \frac{\Delta t}{\mu_0 \Delta x}[E_y^n(i+1,k) - E_y^n(i,k)] \quad \text{...........(9)}$$

Applying above equations, we can directly calculate the values of Ey, Hx and Hz at different points (i, k).

Power Transmittance

Power Transmittance (T_λ) measured at certain wavelength (λ) is the ratio of power transmitted to the power incident by the certain material having width (w).

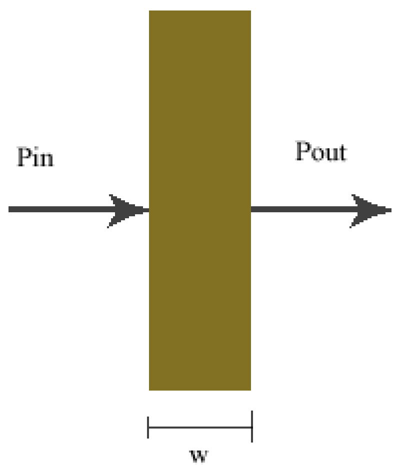


Fig. 4: Power transmission calculation

$$T_\lambda = \frac{P_{out}}{P_{in}} \quad \text{........(10)}$$

$$T = e^{-\alpha w}$$

Where, α is the absorption coefficient and w is the path length.

Chapter 2: Activities and Results

Transmittance for different conditions of sub-wavelength grating (size: 100nm) has been studied on OptiFDTD simulator. Power transmittance for different grating periods (K), grating spacing (d), different grating materials, grating placed in air, grating placed on the glass and grating placed inside the glass, is calculated. Grating period (K) and grating spacing (d) is varied and power transmittance (T) is analyzed at different wavelength. Optical source applied is Gaussian modulated continuous wave with wavelength of 0.5nm.

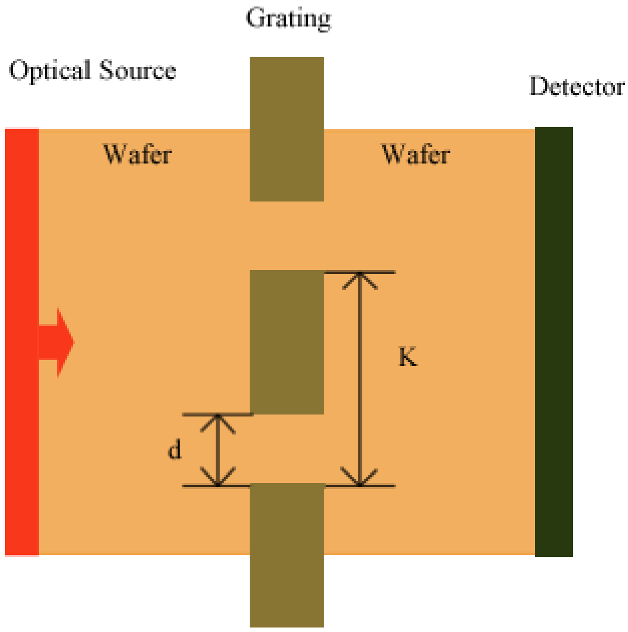


Fig. 5: Array of gratings placed in wafer (air).

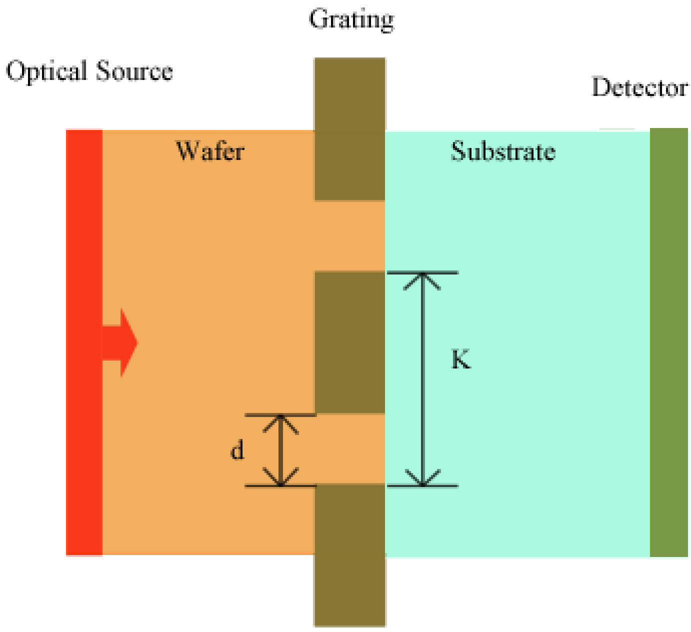


Fig. 6: Array of gratings placed on the substrate (glass). Detector is inside the substrate.

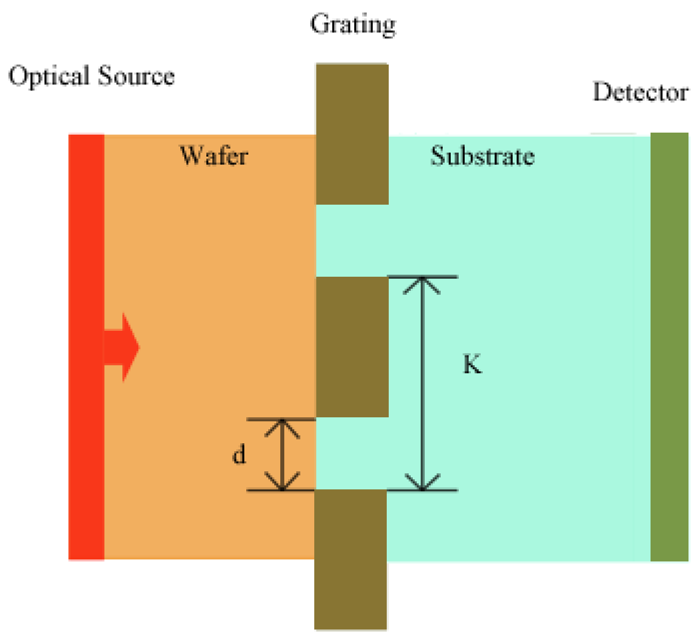


Fig. 7: Array of gratings placed inside the glass substrate. Detector is also inside the substrate.

Variation of transmittance with grating spacing (d):

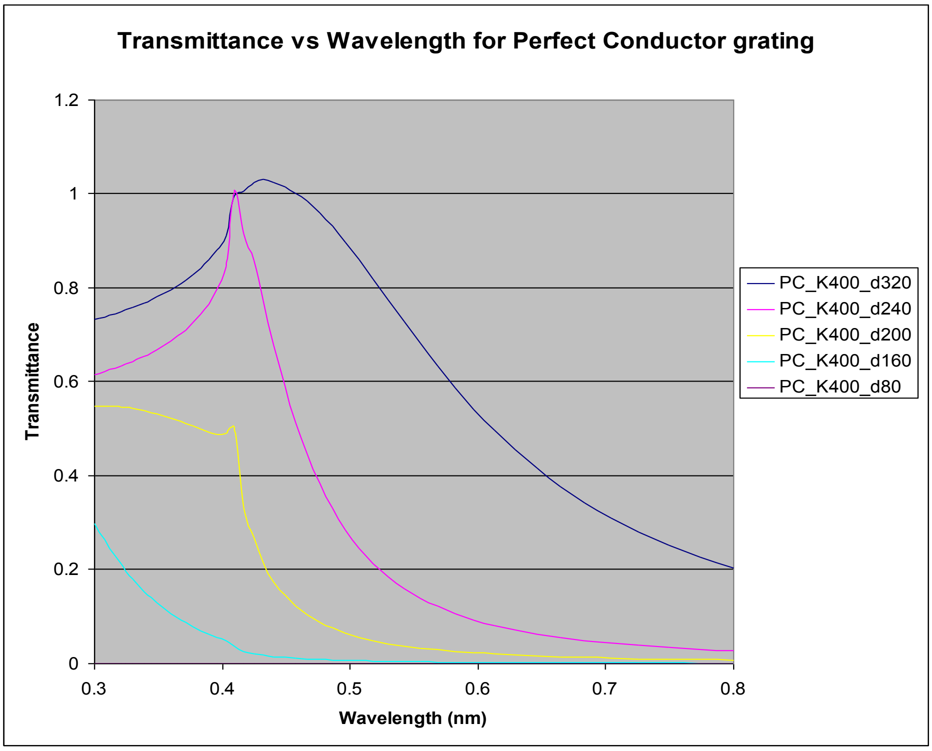


Fig. 8: Plots depicting the variation of transmittance with variation of grating spacing (d), for grating period (K = 400nm).

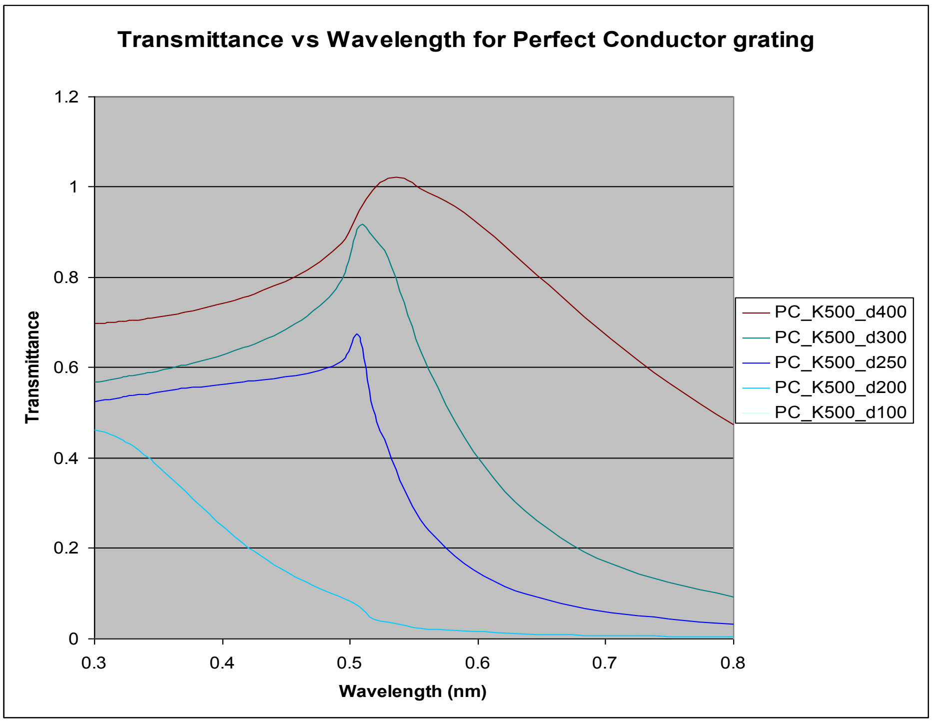


Fig. 9: Plots depicting the variation of transmittance with variation of grating spacing (d), for grating period (K = 500nm).

In fig. 8, when spacing (d) is 320nm for period (K) as 400nm i.e. spacing is 80% of the period, then very high transmittance is found, compared with those cases having slightly low spacing size. Lowest transmittance is seen for very small spacing (80nm) i.e. spacing is 20% of the grating period. The same result is seen in the case for K = 500nm and d-varied from 20% to 80% (fig. 9). Both cases showed some exciting results, (a) maximum transmittance is found at the wavelength equal to the period and (b) for 50% spacing there is uniform transmittance before the wavelength equal to grating period and later decreases rapidly. For e.g. in fig. 8, constant transmittance is seen upto wavelength 400nm (same as period), and later decreased rapidly. Similar result is seen in fig. 9 happening at 500nm (which is equal to the period).

Variation of transmittance with grating period (d):

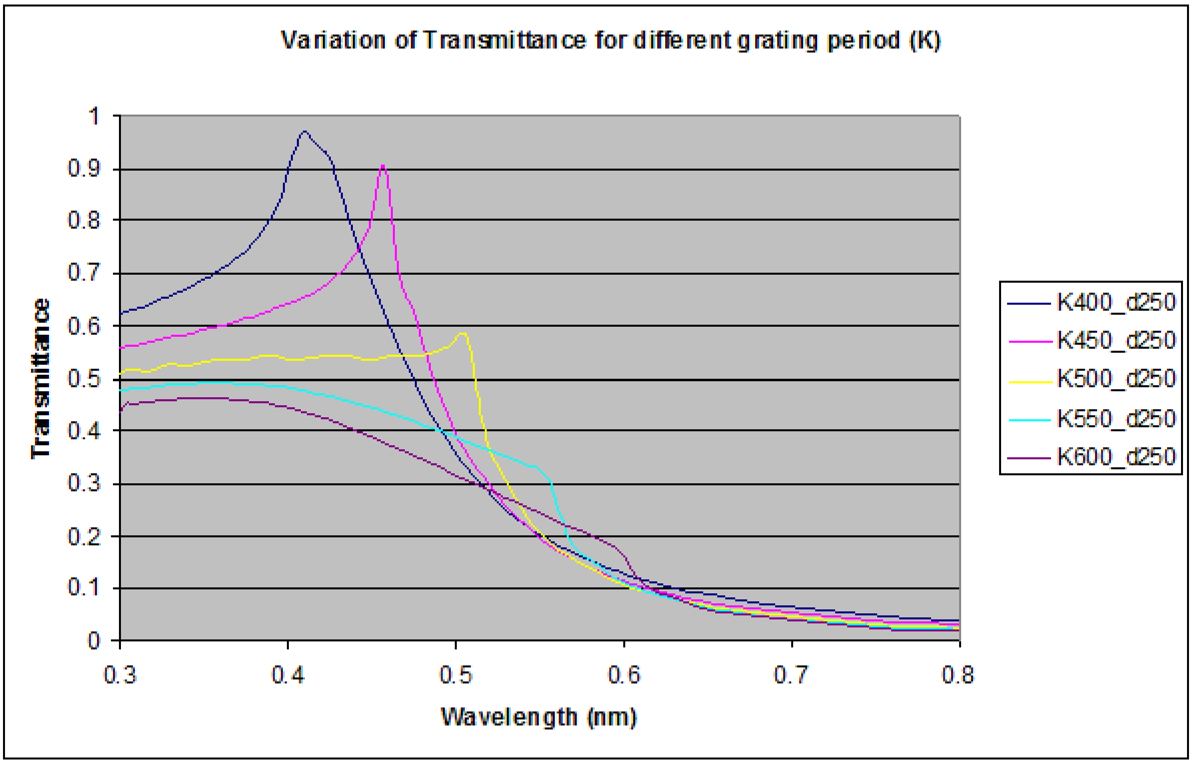


Fig. 10: Above plot depicts the variation of transmittance with grating spacing (d= 250nm) for different grating period (K) for Perfect conductor grating, grating in the air.

When grating period is varied, keeping grating spacing constant (250nm), maximum transmittance is seen for the wavelength at corresponding grating period (K). Maximum transmittance is shifted by the value equal to grating period (Fig. 10). Here also, when K=500nm and d=250nm i.e. spacing is 50% of the period, constant transmittance is observed before the wavelength equal to period and later rapid decrement of transmittance is observed.

Variation of transmittance, when grating is placed inside substrate (glass) and outside the substrate:

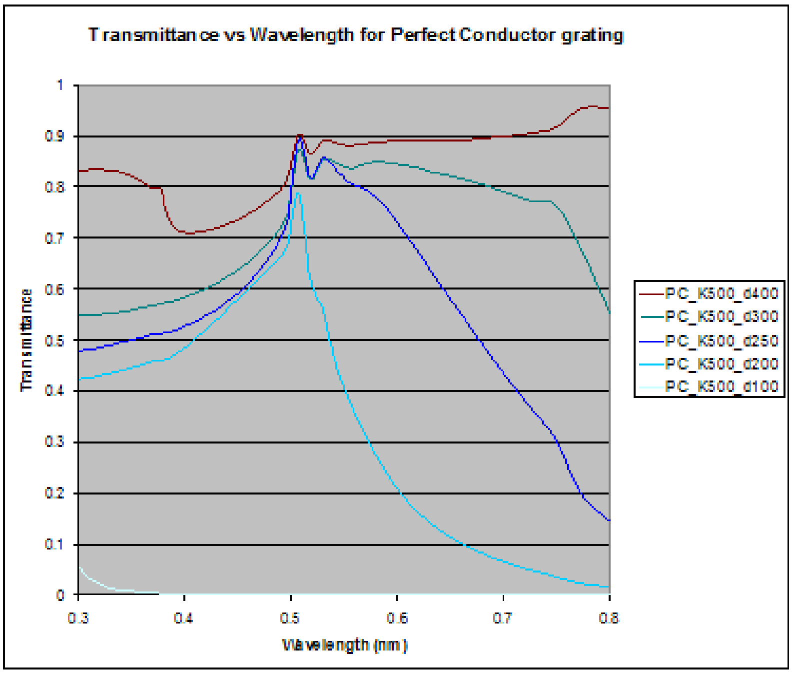


Fig. 11: Grating within the glass (Fig. 3). Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies inside the glass substrate for Perfect Conducting material as grating.

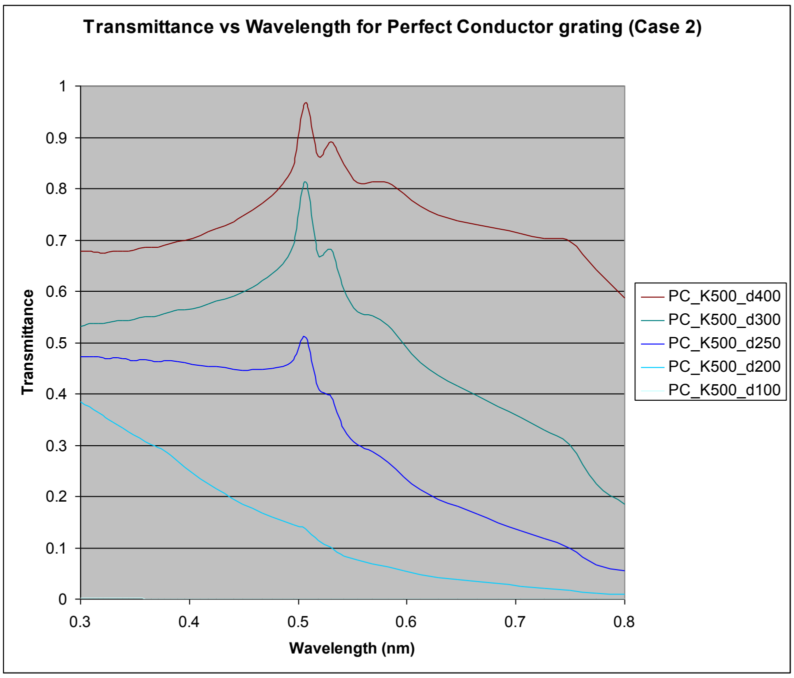


Fig. 12: Grating on the glass (Fig. 2). Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies on the glass substrate for Perfect Conducting material as grating.

When grating is placed on the glass (μ=1.5) (Fig. 12), transmittance at different spacing had different maximum transmittance, but when grating is placed inside the glass substrate then maximum transmittance for different spacing are pretty similar in values. It is seen as the coinciding of different peaks of the transmittance vs. wavelength curve (Fig. 11). Studying the case, where, d is 50% of the period, grating placed on the glass substrate showed similar result as constant transmittance before the wavelength equal to period, and later decreases rapidly.

But, when grating is placed inside the glass substrate, we can observer filter like property where, transmittance increases rapidly upto maximum transmittance and decreases rapidly after attaining maximum value (fig. 13).

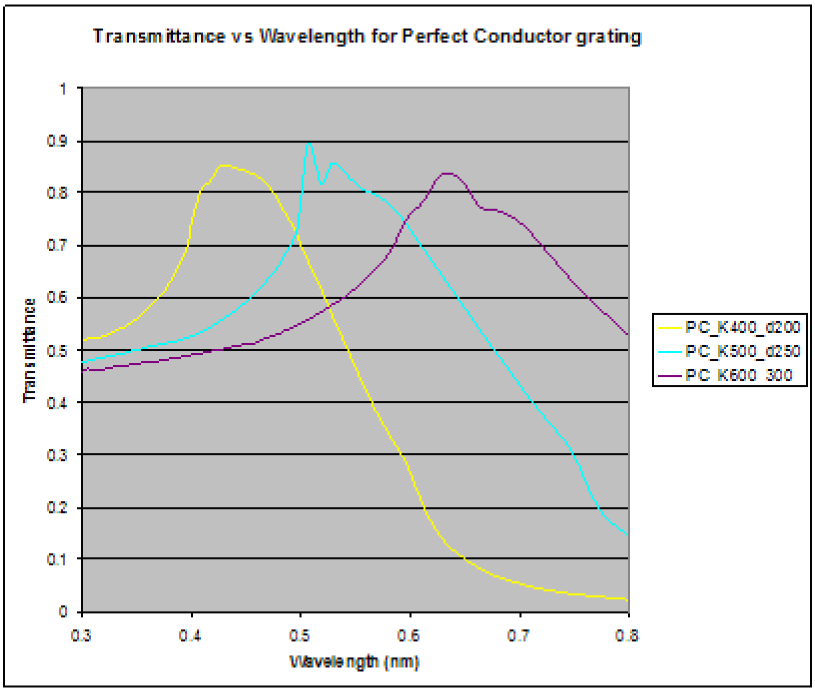


Fig. 13: Grating in the glass (Fig. 2). Above plot depicts the variation of transmittance with grating period (K= 500nm) for 50% grating spacing (d), for grating lies inside the glass substrate for Perfect Conducting material as grating.

Variation of transmittance with grating material:

Aluminium showed maximum transmittance when compared with other materials like: perfect conductor and copper (fig. 14), for spacing (d) kept 50% of period (K).

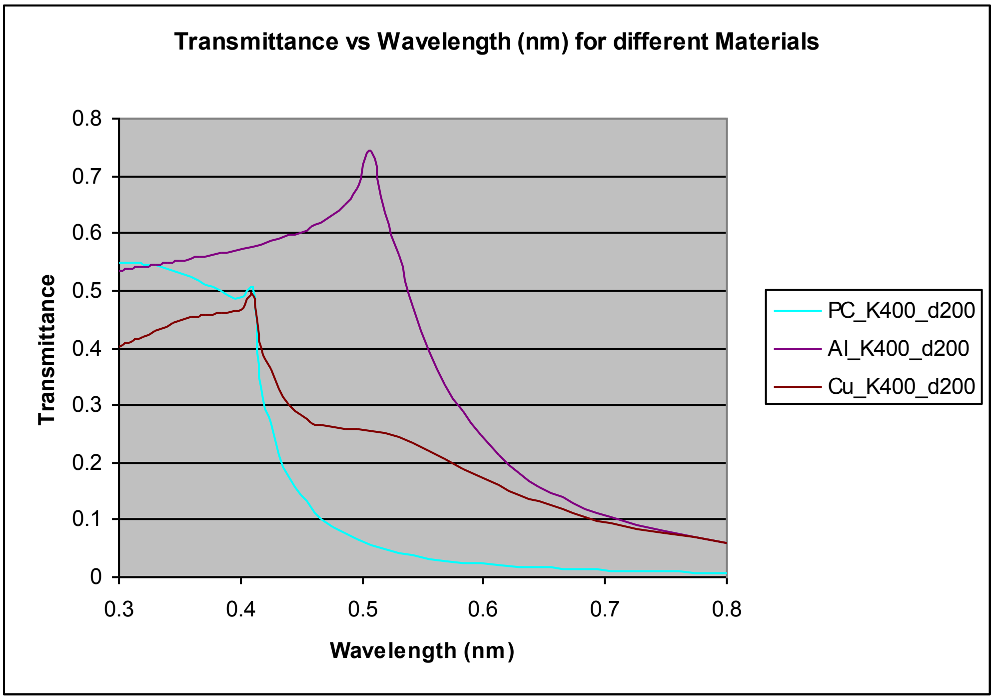


Fig. 14: Transmittance for different materials for grating in the air. Above plot depicts the variation of transmittance for different grating material at 400nm grating period (K) with grating spacing (d) of 200nm.

Summary of Results

Studying the simulation results, it's very clear that, variation of sub-wavelength grating parameter has strong effect on the measured power transmittance at different wavelength.

Effect is notable for spacing (d) is 50% of period (K). Results depicted that sub-wavelength gratings with spacing (d) with period (K), have maximum transmittance at particular wavelength equal to period (exponentially rises and after attaining maximum value, decays exponentially) for d is 50% of the K, only when grating is placed inside the glass. Also, when grating is outside the substrate or without the substrate and d is 50% of the K, transmittance is constant before wavelength equals grating period but exponentially decays later.

Additionally, aluminium is found to be better material compared to perfect conductor and copper, for obtaining high transmittance, after analyzing the results.

References

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Appendix: Simulation Results

Variation of transmittance with variation of grating period (K-nm) and grating spacing (d-nm):

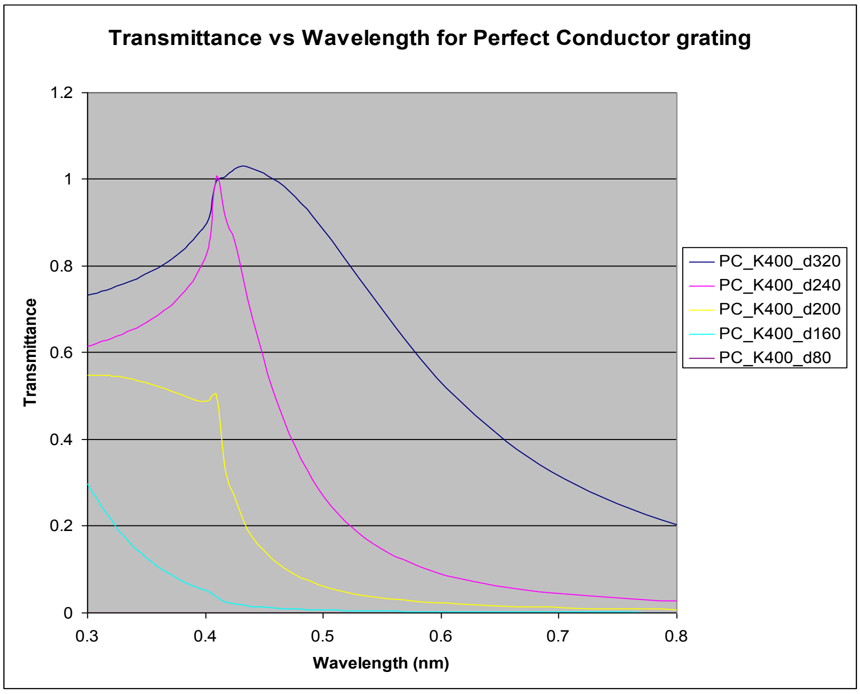

Fig. I: Grating within air for Perfect conductor. Above plot depicts the variation of transmittance with grating period (K=400nm) for different grating spacing (d) for Perfect conductor grating.

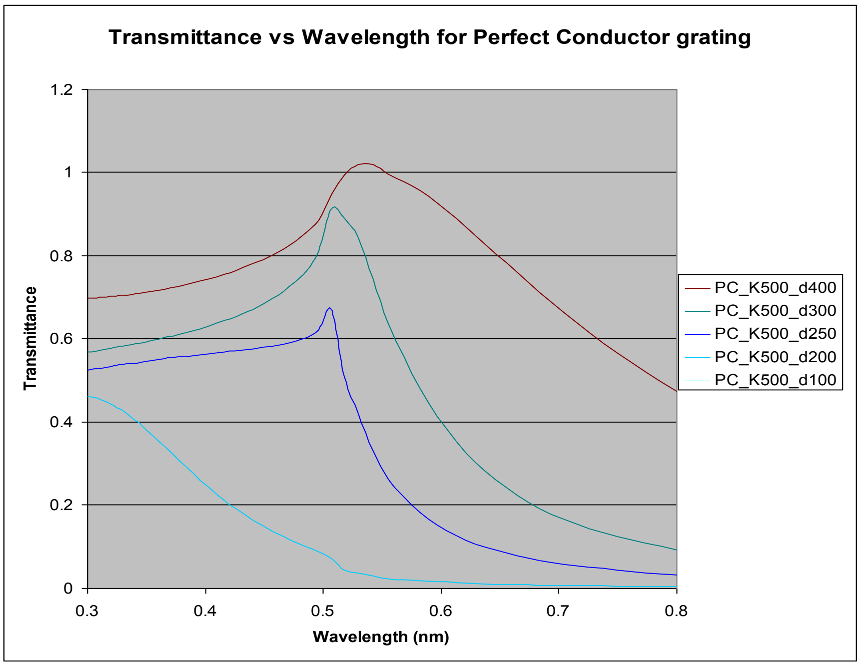

Fig. II: Grating within air for Perfect conductor. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d) for Perfect conductor grating.

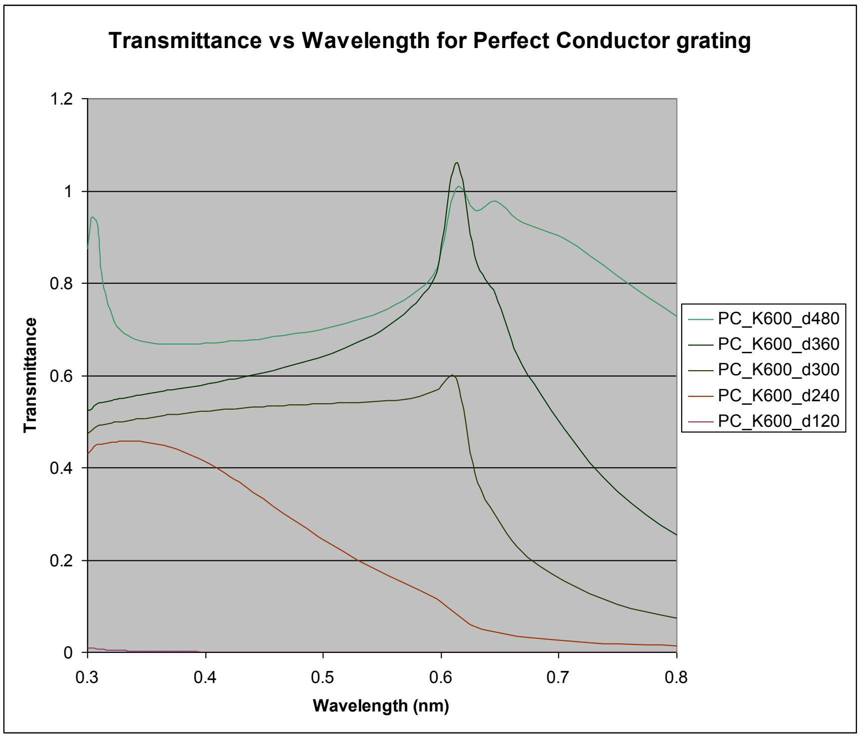

Fig. III: Grating within air for Perfect conductor. Above plot depicts the variation of transmittance with grating period (K= 600nm) for different grating spacing (d) for Perfect conductor grating.

Variation of Transmittance with grating period (K-nm)

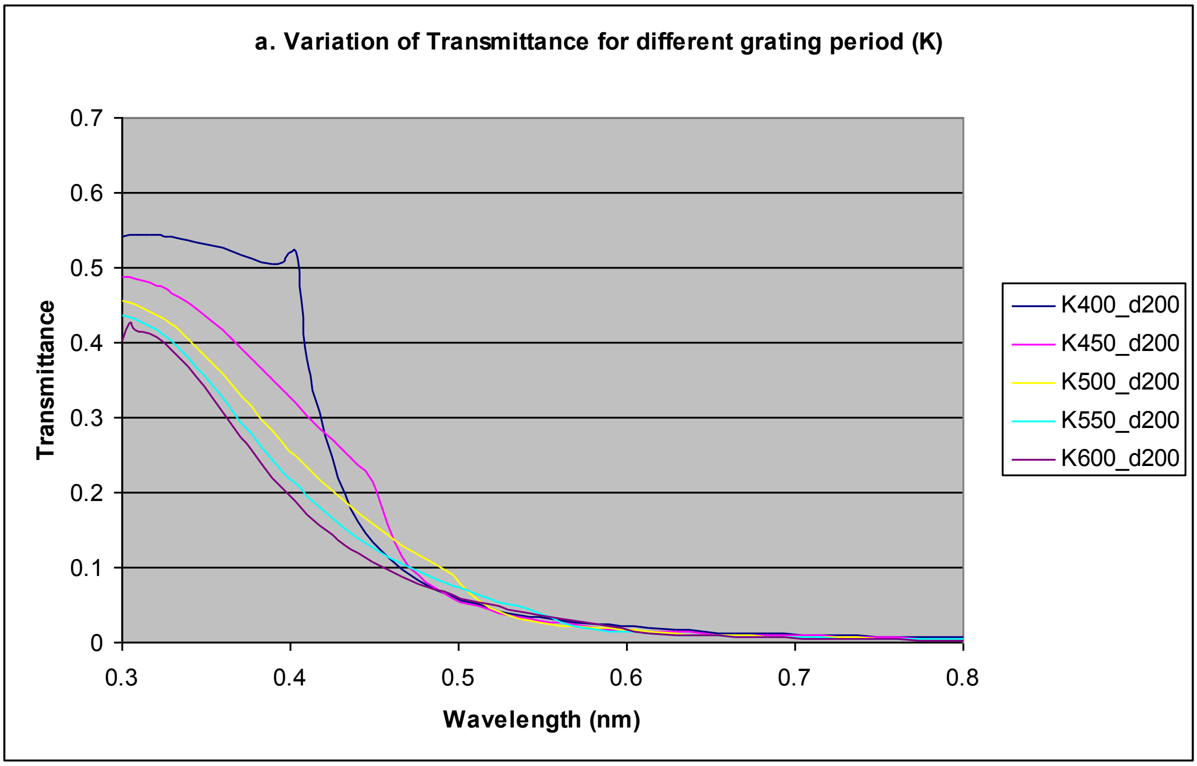

Fig. IV: Above plot depicts the variation of transmittance with grating spacing (d= 200nm) for different grating period (K) for Perfect conductor grating, grating in the air.

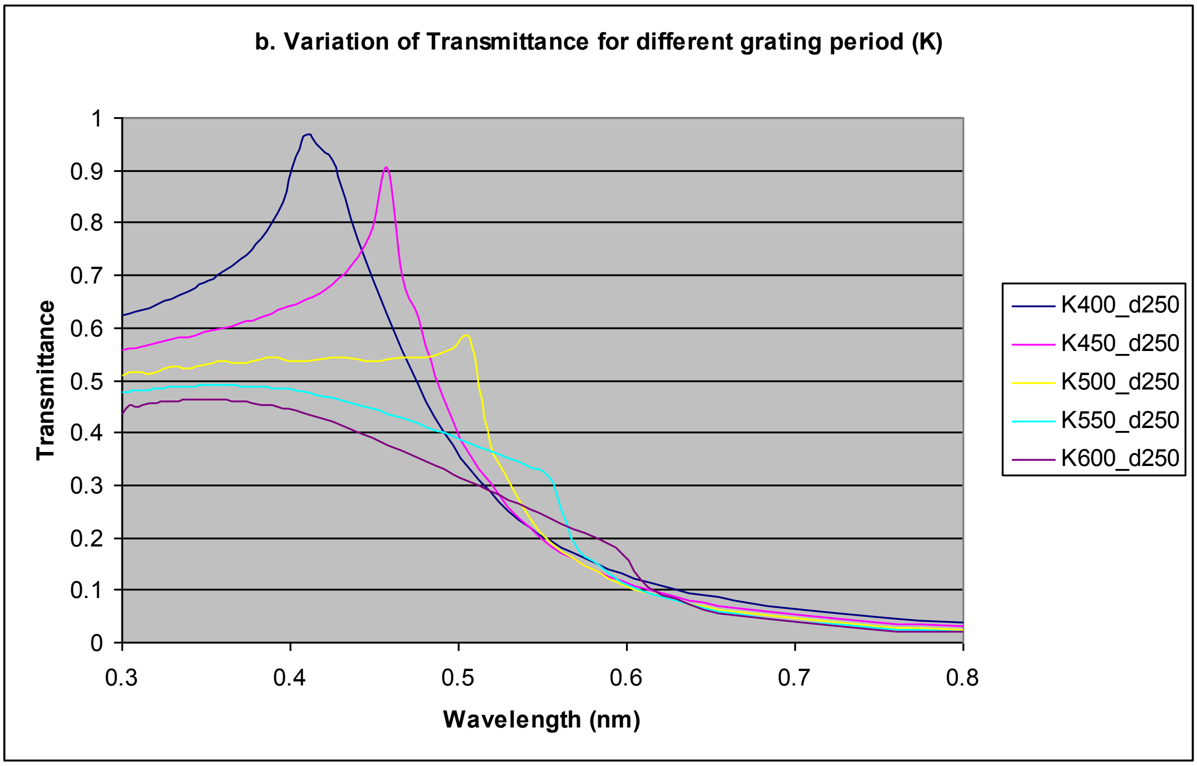

Fig. V: Above plot depicts the variation of transmittance with grating spacing (d= 250nm) for different grating period (K) for Perfect conductor grating, grating in the air.

Variation of Transmittance For different Materials (Perfect conductor-PC, Copper-Cu and Aluminium-Al)

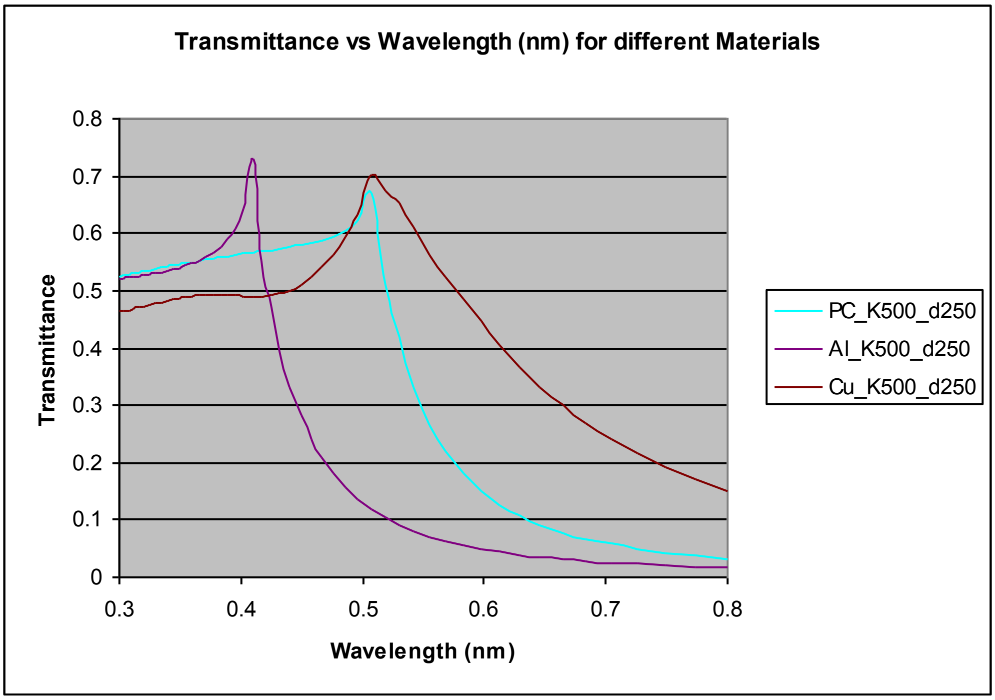

Fig. VI: Transmittance for different materials. Above plot depicts the variation of transmittance for different grating material at 500nm grating period (K) with grating spacing (d) of 250nm, grating in the air.

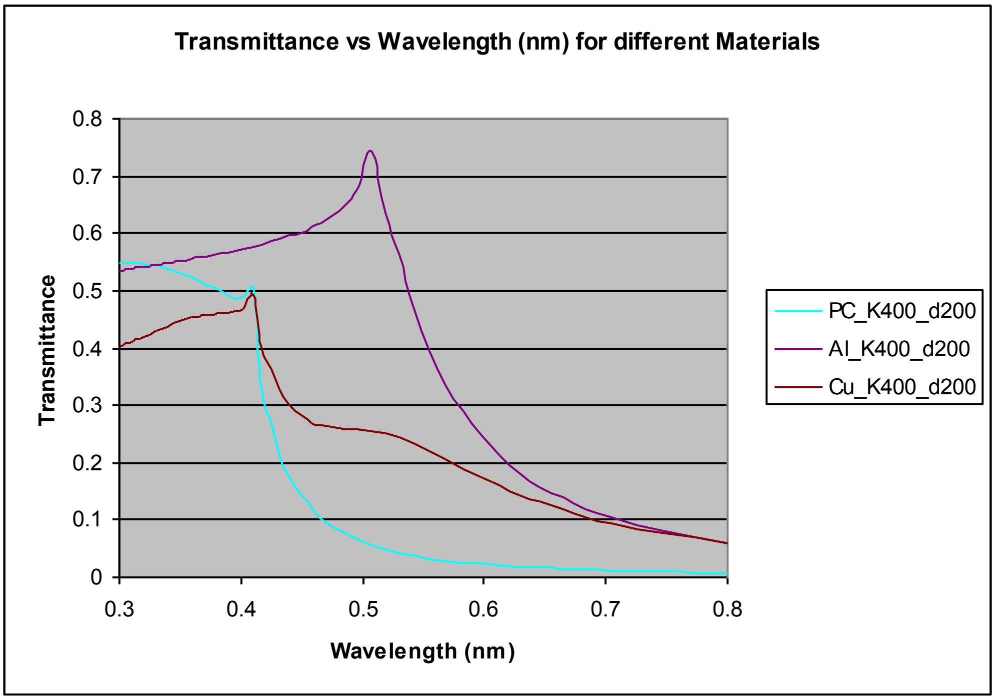

Fig. VII: Transmittance for different materials for grating in the air. Above plot depicts the variation of transmittance for different grating material at 400nm grating period (K) with grating spacing (d) of 200nm.

Transmittance analysis for grating on the glass substrate and in the air:

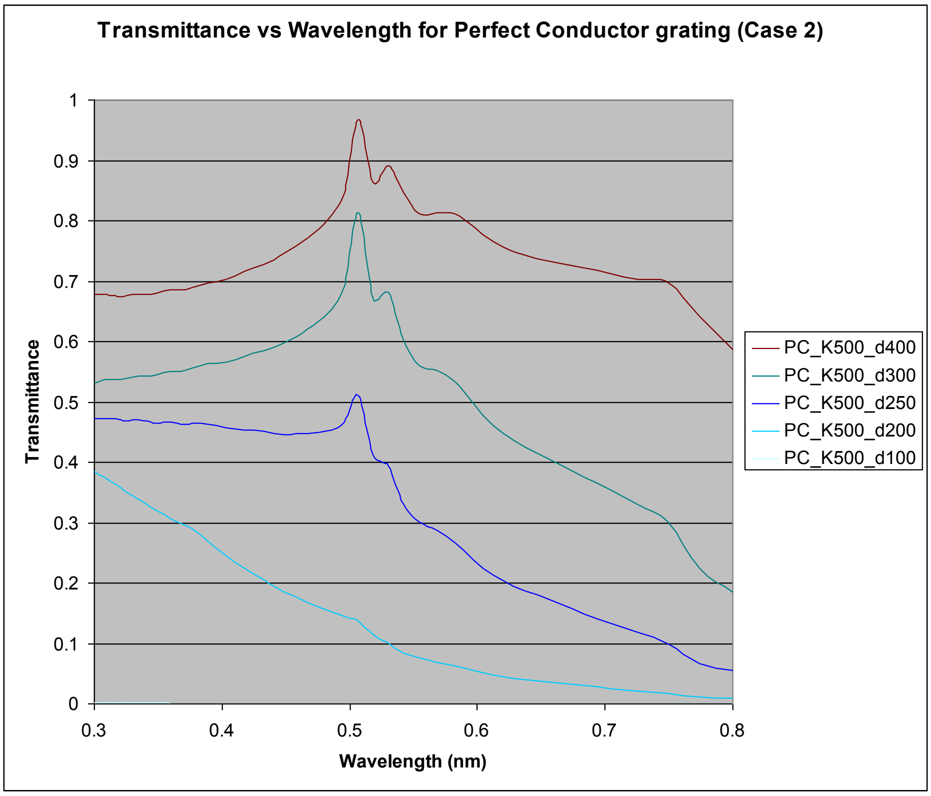

Fig. VIII: Grating on glass substrate. Above plot depicts the variation of transmittance for grating on the glass substrate with grating period (K= 500nm) for different grating spacing (d).

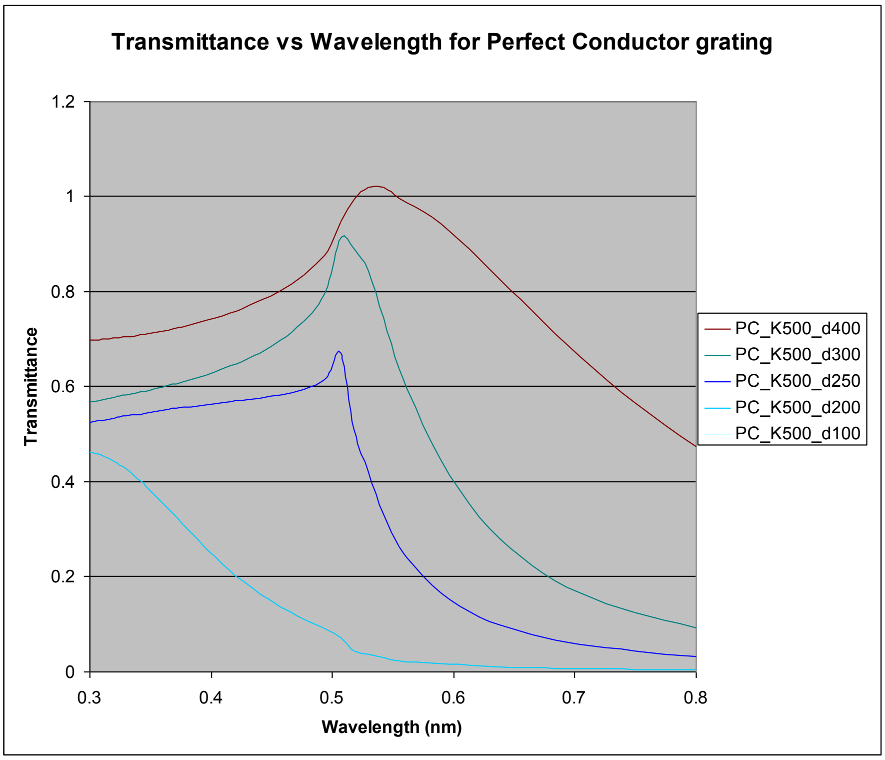

Fig. IX: Grating in Air. Above plot depicts the variation of transmittance for grating in the air with grating period (K= 500nm) for different grating spacing (d).

Transmittance analysis for grating within the glass substrate and on the substrate

A. For Perfect Conductor grating:

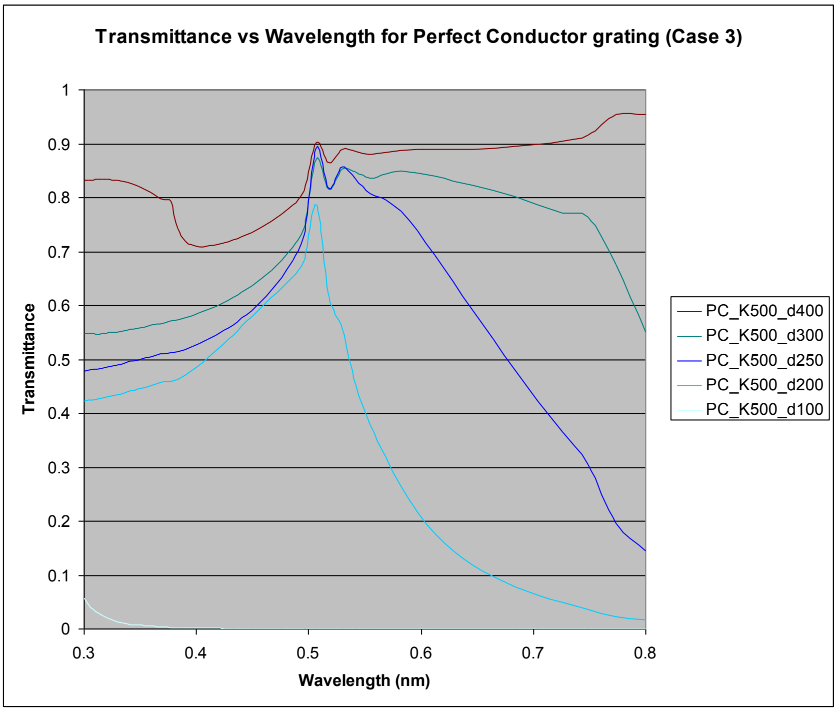

Fig. X: Grating within the Glass Substrate for Perfect Conductor Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies inside the glass substrate for Perfect Conducting material as grating.

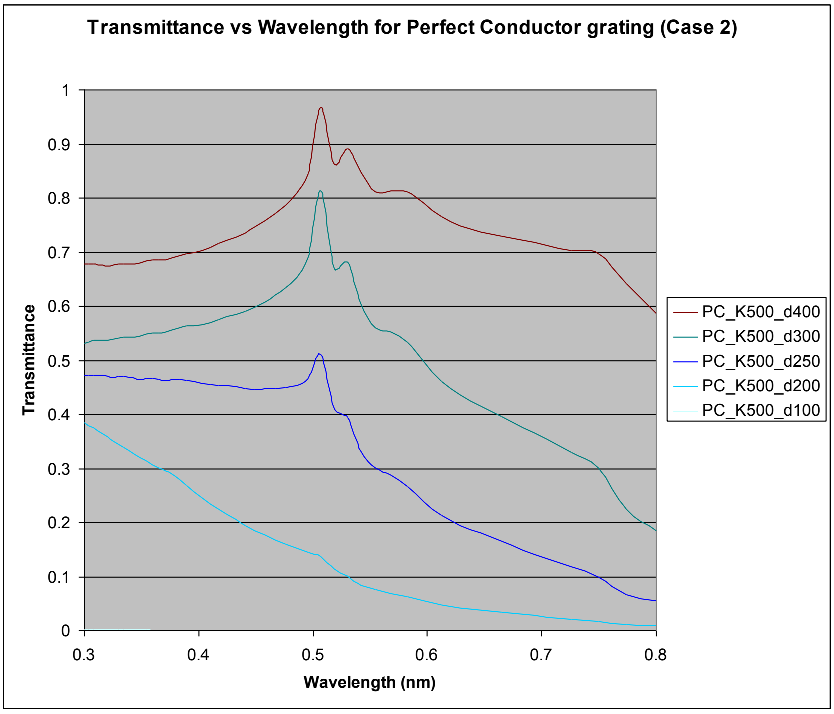

Fig. XI: Grating on the Glass Substrate for Perfect Conductor Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies on the glass substrate for Perfect Conducting material as grating.

B. For Copper Grating

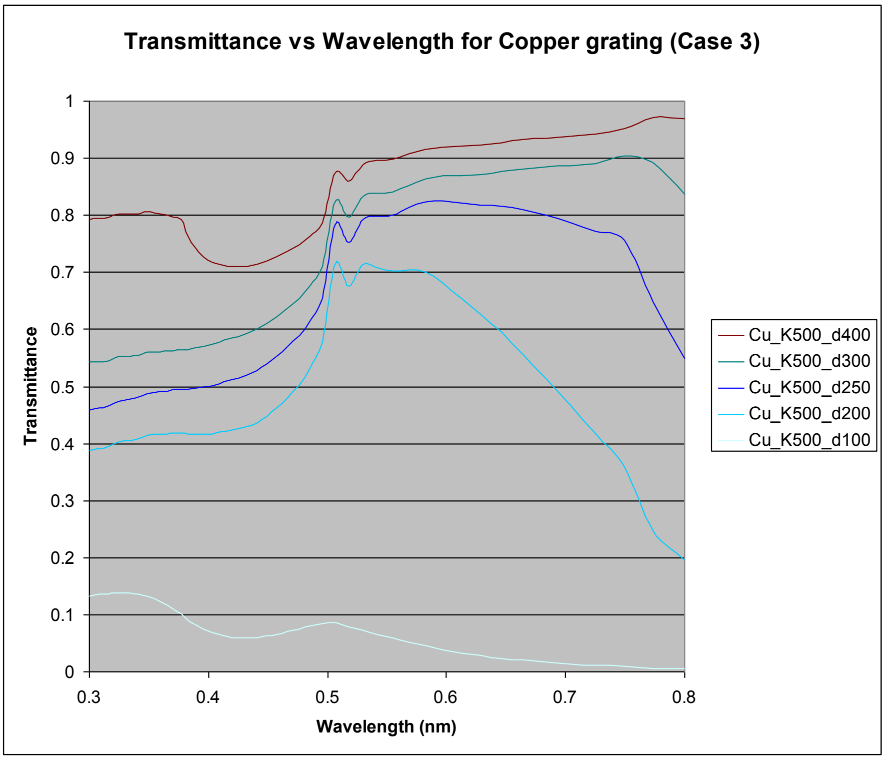

Fig. XII: Grating within the Glass Substrate for Copper Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies inside the glass substrate for Copper as material for grating.

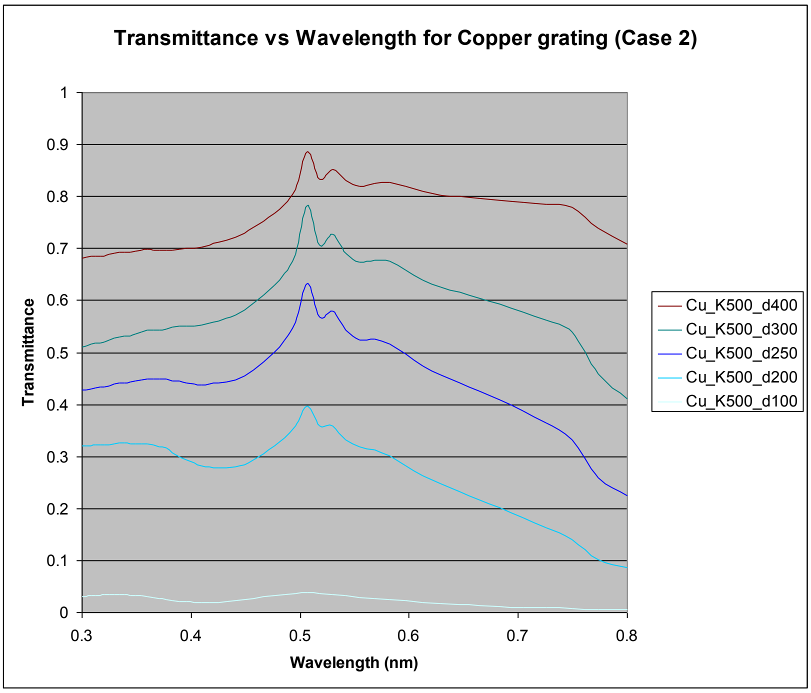

Fig. XIII: Grating on the Glass Substrate for Copper Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies on the glass substrate for Copper as material for grating.

C. For Aluminium grating

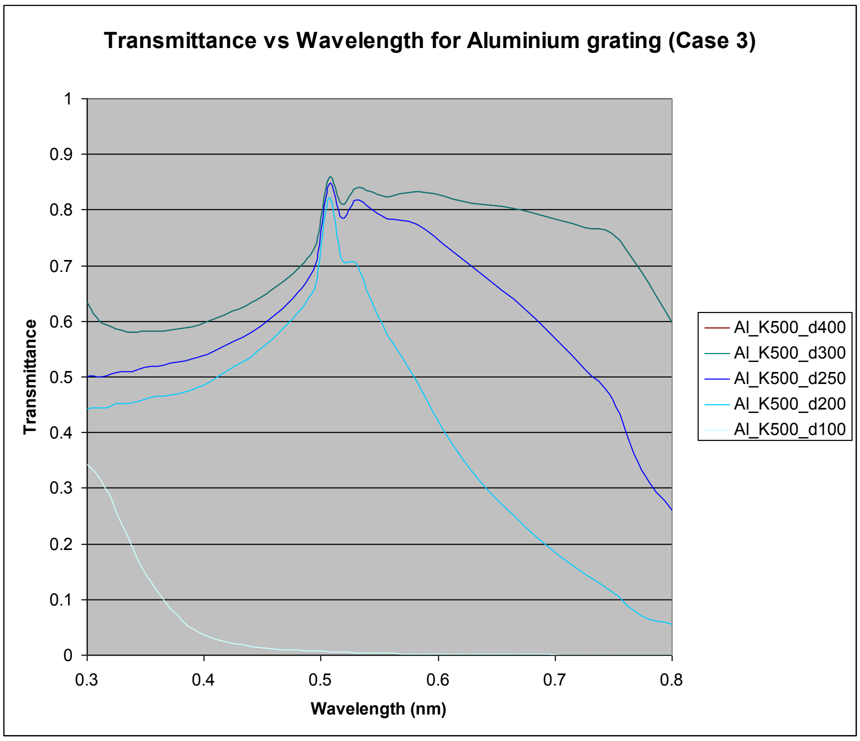

Fig. XIV: Grating within the Glass Substrate for Aluminium Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies inside the glass substrate for Aluminium as material for grating.

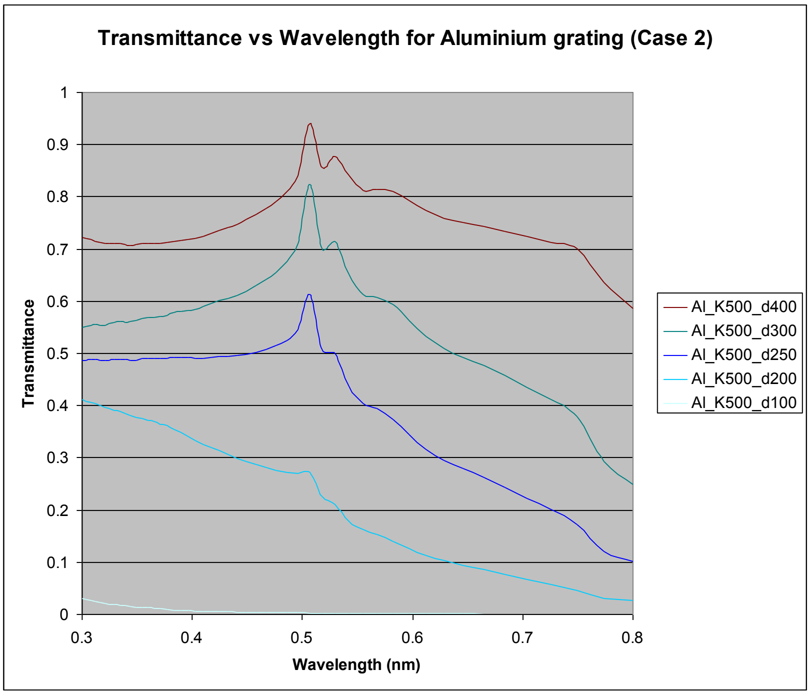

Fig. XV: Grating on the Glass Substrate for Aluminium Grating. Above plot depicts the variation of transmittance with grating period (K= 500nm) for different grating spacing (d), for grating lies on the glass substrate for Aluminium as material for grating.