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X-Ray window simulation; the use of COMSOL 3.4 Multiphysics software

By Dikedi P.N.
King's College, London

Abstract - Ways are sought after, to prevent overlying target material on membrane from breaking or melting, by simulating structures (using COMSOL 3.4 Multiphysics software) of various materials. Results of these simulations and graphs (using Origin 7.5 software) are presented. The implications conferred by these graphs on the report are discussed. Power densities, of impinging electrons, thermal conductivities and thickness of membrane are considered as key parameters for optimal performance.

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X-Ray window simulation; the use of COMSOL 3.4 Multiphysics software

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Abstract - Ways are sought after, to prevent overlying target material on membrane from breaking or melting, by simulating structures (using COMSOL 3.4 Multiphysics software) of various materials. Results of these simulations and graphs (using Origin 7.5 software) are presented. The implications conferred by these graphs on the report are discussed. Power densities, of impinging electrons, thermal conductivities and thickness of membrane are considered as key parameters for optimal performance.

I. Introduction

A simulation of the deformed structure (using COMSOL 3.4 multiphysics software) and graphs from results of various simulations (using Origin 7.5 software) are presented.

It is assumed that membrane breakage is caused by both the pressure differential between the top (Ti or Cr) and bottom layer (Si_3N_4) and the maximum temperature at the 1μm spot, (provided that maximum temperature exceeds the melting point of the membrane); hence simulations of Ti or Cr/ Si_3N_4 structures are presented based on temperature and stress/strain distribution within this structure. Using the heat transfer module of COMSOL 3.4 multiphysics software, the present simulations are somewhat modified compared to the previous ones. Simulations of a quarter of the full structure are considered for simplicity; Figure 1 is a 3 d view which showed that the focused electron beam impinged on an area of a quarter of a circle of radius 0.5μm.

II. Simulations of Various Structures

Further modelling of Ti/Si_3N_4 structure was performed (using COMSOL 3.4 multiphysics software) so as to reduce as much as possible the maximum temperature conferred on the hot spot. Although the heat flux/power density is a key parameter upon which the maximum temperature depends, however ways are sought for to avoid reducing the heat flux; a reduction implies that X-ray photon flux would reduce which in turn implies that exposure time of irradiated biological samples would increase.

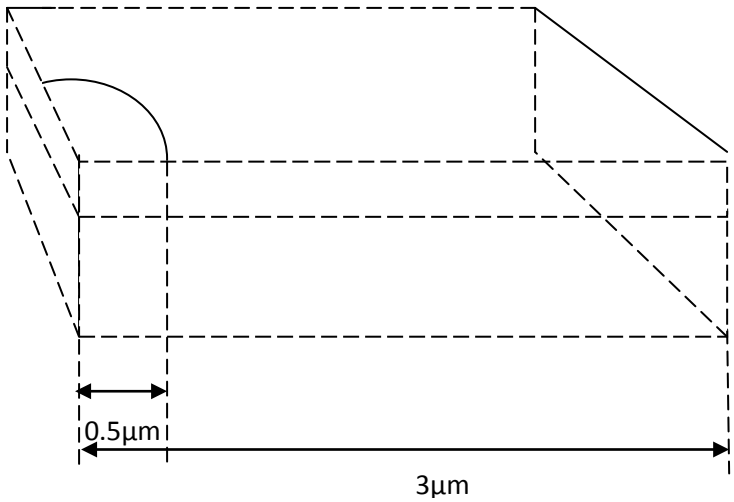

Figure 1 : A 3d view of the Cr/ Si_3N_4 (or Ti/ Si_3N_4) structure showing the hot spot represented by the quarter of a circle of radius 0.5μm.

Figure 2 is a deformed structure of chromium coated silicon nitride membrane whose deformation is due to pressure differential between the top and bottom of the structure describing both temperature and stress distribution within the structure. The deformation occurred the most at the 1 μm hot spot due to heat flux impartation. This region has a maximum temperature and stress of 2122K and 1.109x109 Pa respectively; amazingly, stress has insignificant effect on the maximum temperature of the structure. Figure 3 describes the boundary conditions applied to titanium/silicon nitride structure; boundaries between

Author : Physics Department, King's College, London
E-mail : pdikedi@yahoo.co.uk

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layers are set as 'continuity' meaning that heat flows continuously across layers of dissimilar materials. The outer boundaries are set as 'temperature' meaning that the surrounding is assumed to be have room temperature. The 1μm hot spot is set as 'heat flux' with the description {(s1>0.45)*(s1<0.55)*1e^{10}} meaning that 0.45 to 0.55 describes the hot spot where the maximum temperature must be deposited where 1e^{10} denotes the value of the power density i.e.10^{10}W/m^2. Figure 4(a) is a Simulated structure of 1μm of silicon nitride membrane overlain with 2μm of beryllium and 200nm of titanium.

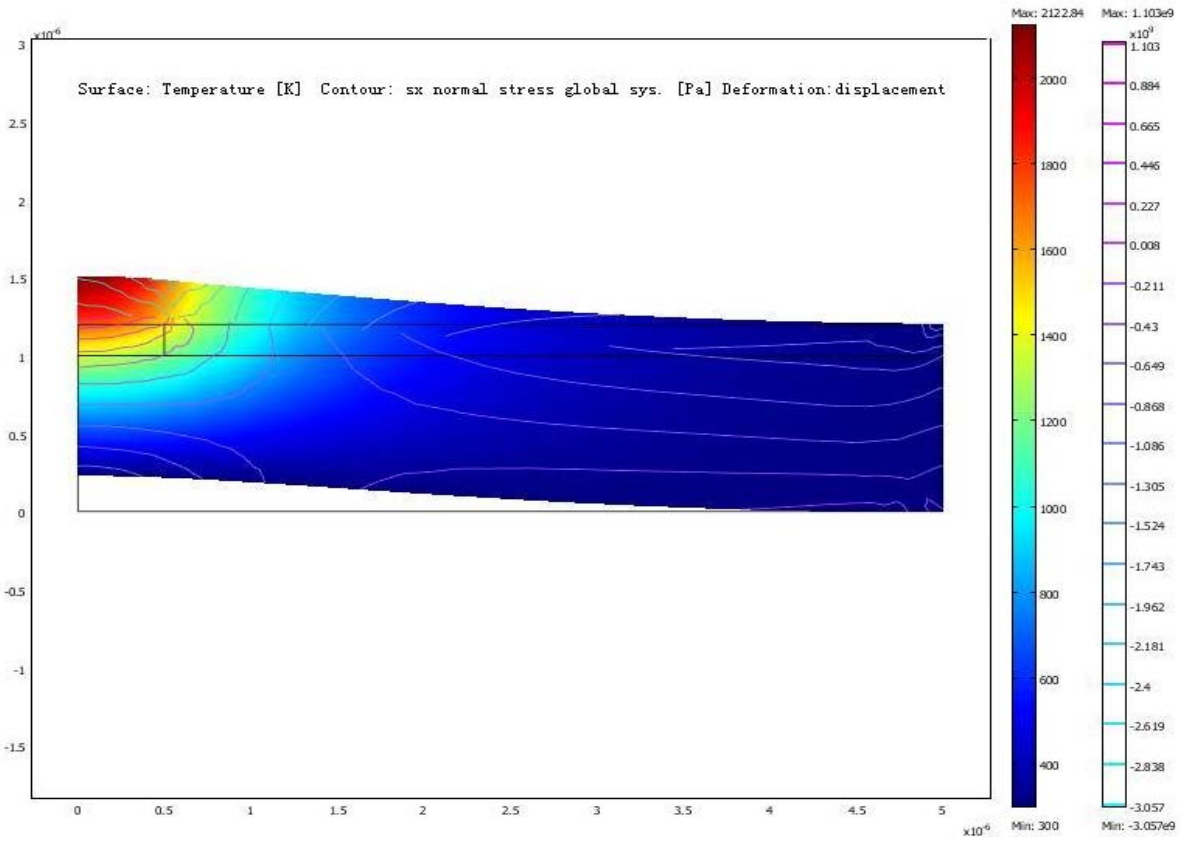

Figure 2 : A deformed structure of Chromium/Silicon nitride showing both temperature and stress distribution.

The maximum temperature achieved at the Titanium surface (upper layer) was 420.926K and the minimum temperature reached at the Silicon nitride surface (lower layer) was 273.15K. The result of the modelling is favourable because the maximum temperature of 420.926K is much less than the melting point of titanium. Maximum temperature at the hot spot varies directly with power density of the focused beam for both chromium and titanium of 100nm thickness. Figure 4(b) is a simulated structure of 1μm silicon nitride membrane overlain with 5μm of beryllium and 200nm of chromium; maximum temperature attained is 2184.549K and minimum is 273.15K. Figure 4(c) is a percentage heat flux distribution across five layers of an arbitrary material describing 40%, 30%, 15 %, 10 % and 5% of the total heat flux distributed through first, second, third, fourth and fifth layer.

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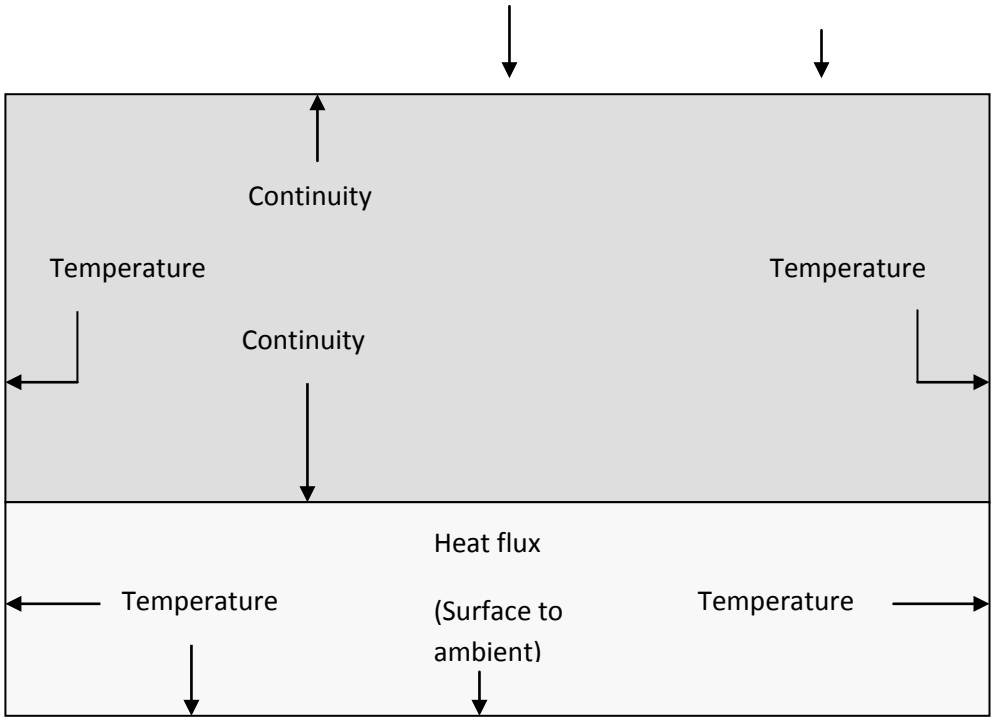
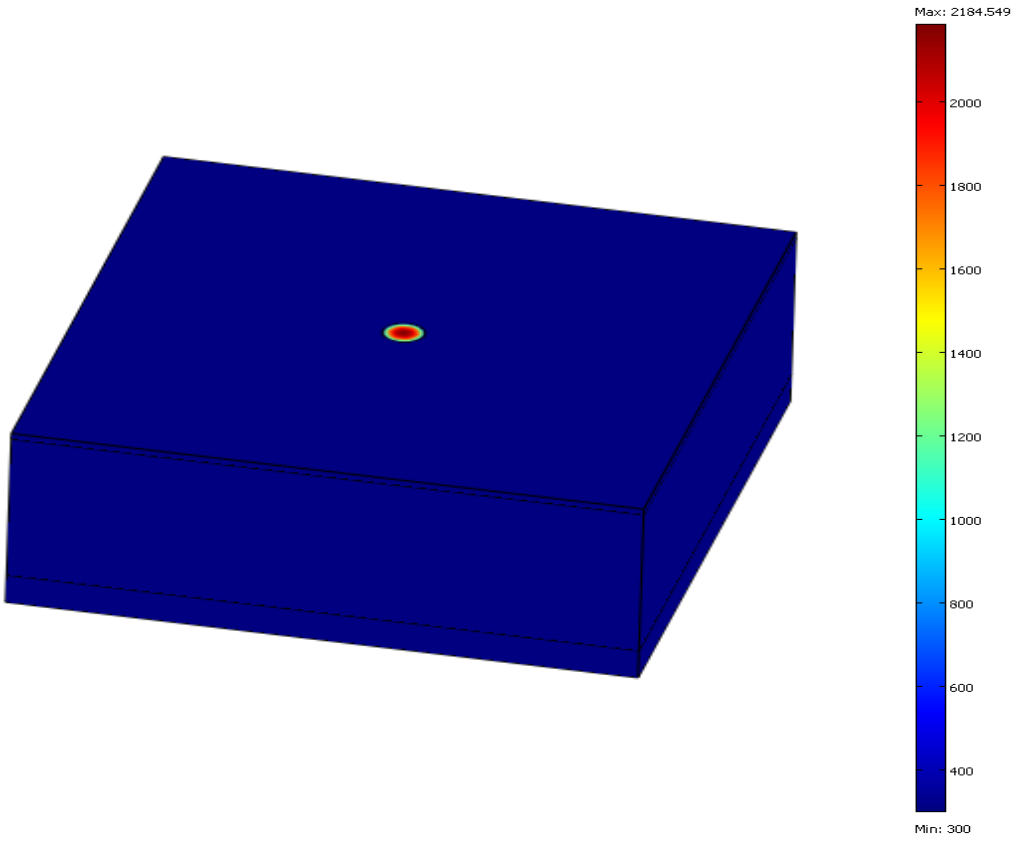


Figure 3.3 : Titanium/Beryllium /Silicon nitride Silicon nitride structure made of $2\mu m$ Beryllium layer overlain with a $200nm$ Titanium layer and underlain with $1\mu m$ Silicon nitride layer



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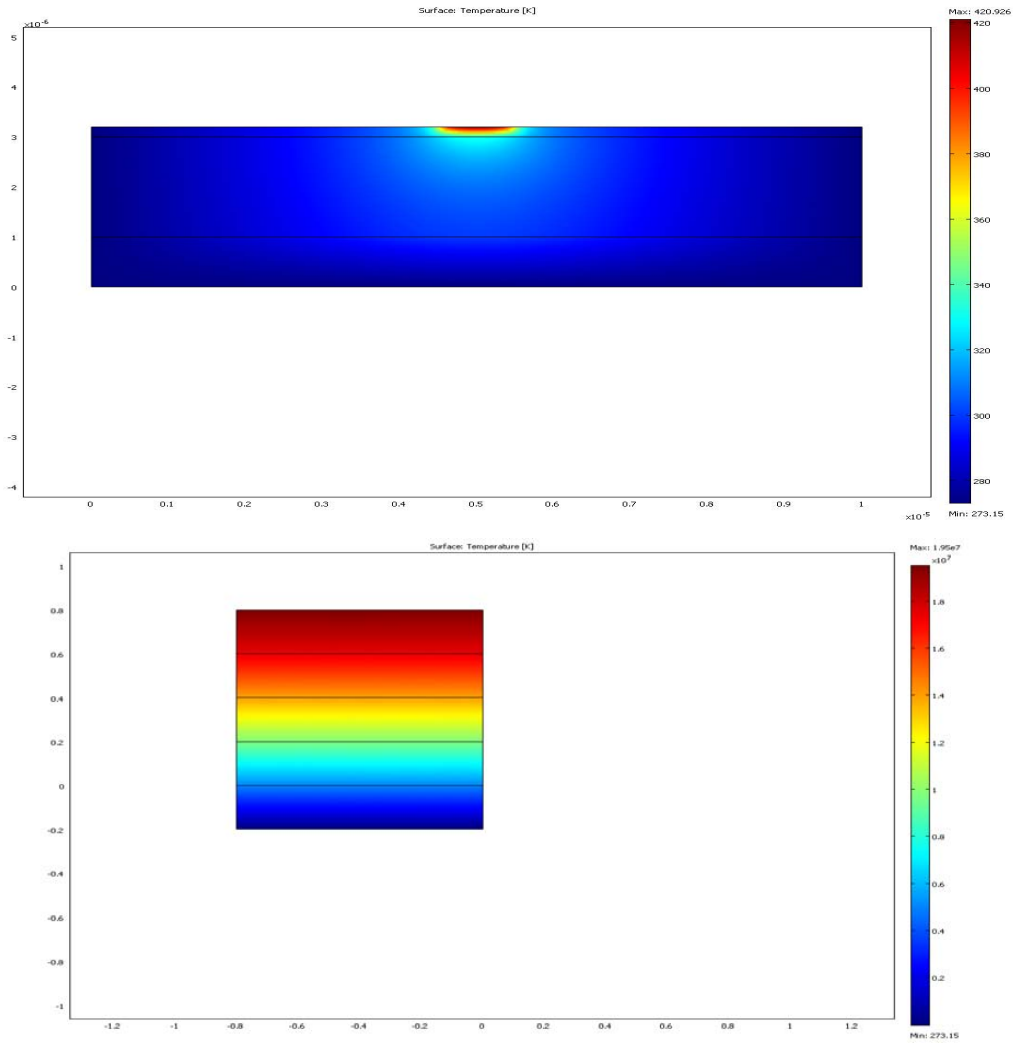

Figure 4(a) simulated structure of 1μm of silicon nitride membrane overlain with 2μm of beryllium and 200nm of titanium. Figure 4(b) Simulated structure of 1μm silicon nitride membrane overlain with 5μm of beryllium and 200nm of chromium. Figure 4(c) Percentage heat flux distribution across five layers of an arbitrary material

The relationship between the maximum temperature and the power density or heat flux is well established by the homogeneous hyperbolic heat equation [1] given by

$$q''(x,t)) + \tau \frac{\partial q''}{\partial t}(x,t) \cong -k\partial \frac{\partial T}{\partial x}(x,t), \qquad (3.1)$$

Where q" is the dissipated heat flux; and T and k are the temperature and thermal conductivity of the medium. Compared to chromium, a higher maximum temperature is achieved in titanium when both samples are exposed to the same power density- Figure 5 shows this with more steepness from chromium

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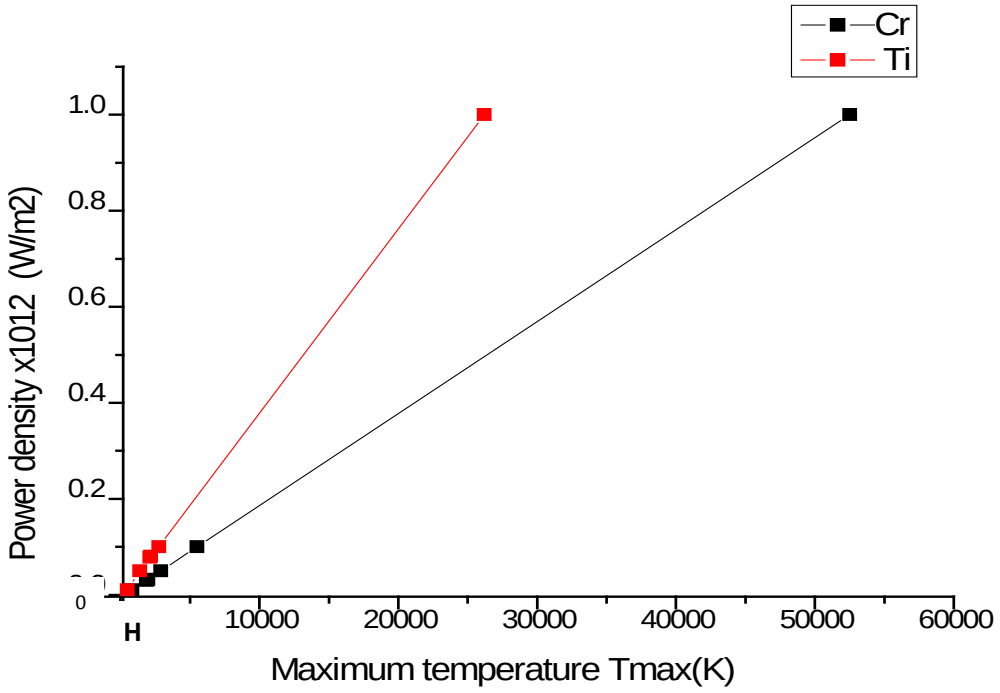

Figure 5 : A graph of power density of focused beam as a function of maximum temperature of the 1 μm spot.

III. Thickness of The Window as a Function of Maximum Temperature

The results from simulations also show that maximum temperature at the hot spot changes with thickness of both chromium and titanium. Maximum temperature increases with increasing thickness of chromium; maximum temperature also increases but with decreasing thickness of titanium. From previous simulations, it is well established that for arbitrary top and bottom layers, provided that the top layer material has a higher thermal conductivity, maximum temperature of the top layer will increase with increasing thickness. However, provided that the top layer has a lower thermal conductivity, maximum temperature of the top layer will increase with decreasing thickness. Figure 6 illustrates that at optimised power density of $\leq 0.078 W/m^2$ and $0.03\ W/m^2$ for chromium and titanium respectively, each of 200nm thickness; the maximum temperature attained are unable to cause breakage.

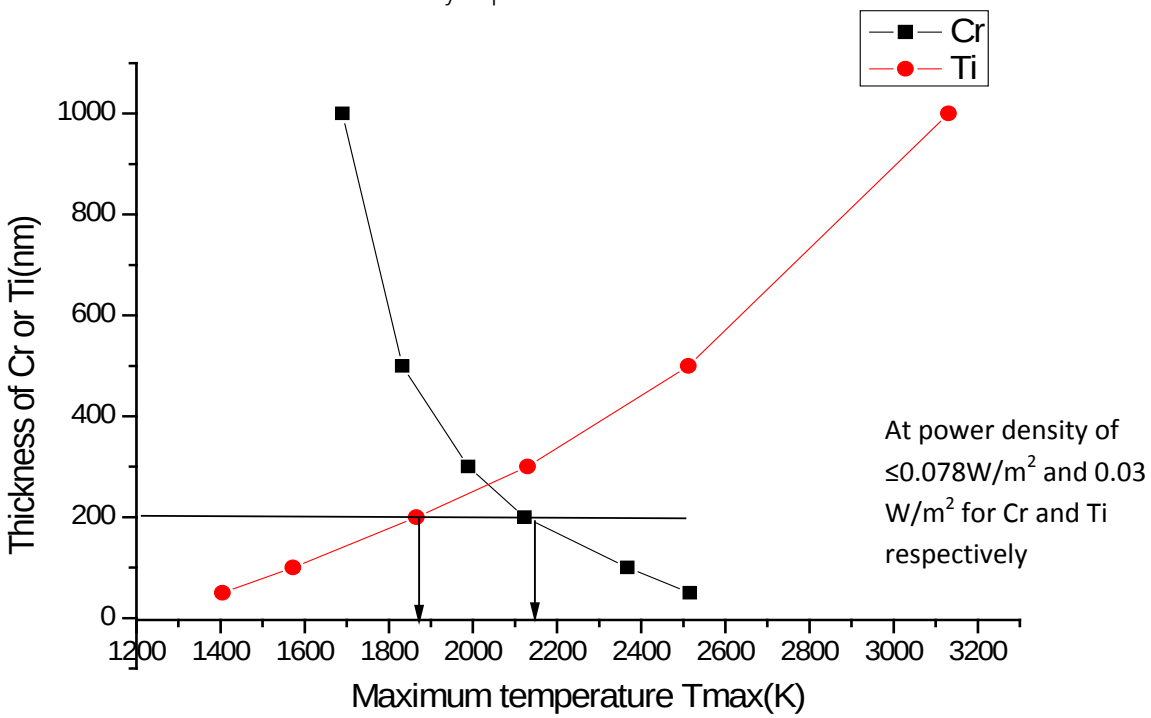

Figure 6 : A graph of thickness of chromium and titanium as a function of maximum temperature.

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IV. Optimised Power Density as a Function of Window Thickness

Results from simulations show how optimised power densities of focused electron beam vary with thickness of titanium and chromium as illustrated in figure 7 Chromium is able to withstand more heat flux than titanium. Increasing the thickness of chromium makes it more able to withstand heat flux; however increasing the thickness of titanium makes it less able to withstand heat flux. 230nm thickness each of chromium and titanium can withstand power density of $0.081 W/m^2$ and $0.029 W/m^2$ respectively. It implies that time spent for irradiation is less if the membrane is made of chromium (more X-ray photon flux). Care must be taken when considering various membrane thicknesses, to ensure optical transparency. The more robust membranes show a decline in optical transparency.

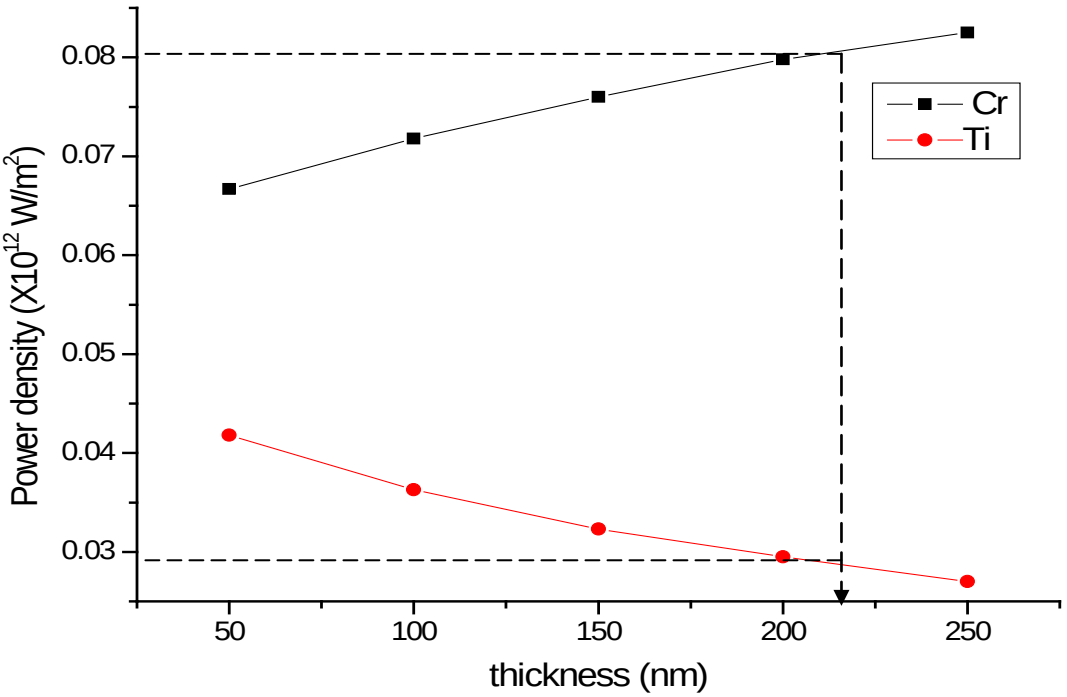

Figure 7 : A graph of power density of focused beam as a function of thickness of chromium and titanium.

V. The Effect of Stress

By varying the pressure at the bottom layer while keeping the pressure at the top layer constant the maximum temperature at the hot spot remained the same, hence work was discontinued on this

VI. Conclusion

Power density is directly related to maximum temperature; maximum temperature increases or decreases with it which agrees perfectly well with the homogenous heat equation. The thickness of membrane material is a function of maximum temperature on it; provided that the top layer material has a higher thermal conductivity, maximum temperature of the top layer will increase with increasing thickness. However, provided that the top layer has a lower thermal conductivity, maximum temperature of the top layer will increase with decreasing thickness.

Though there are some ambiguities in presented results of the simulation, chromium is preferred to titanium as a target material due to its higher thermal conductivity and melting point of 90.3W/mk and 2180K respectively, meaning that it can withstand more heat flux with less maximum temperature passed to it. This implies that chromium will emit more X-ray photon flux, thus reducing the time spent in irradiating cells-more cells can be irradiated. Pressure differential has an insignificant effect on the maximum temperature of the hot spot.

Future work will be directed towards creating more simulations by varying the temperature of helium gas, to check how it affects the maximum temperature of the membrane as well as finding more parameters which may affect the temperature of the hot spot.

References Références Referencias

1. Vladimir VK, Vasily BN (2002). "The relationship between the local temperature and the local heat flux within a one –dimensional semi-infinite domain of heat wave propagation" Mathematical Problems in Engineering **2003** (2003), Issue 4, Pp 173-179
2. Comsol 3.4 multiphysics software kit

Appendix

Basic Thermal Properties of materials considered in the simulation (From CRC handbook)

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Titanium

Thermal conductivity k = 0.219 W/ (cm. K) = 21.9 W/ (m. K) at 300K
Density r = 4500 kg/m3
Heat capacity Cp = 0.125cal/ (g. K) = 523 J/ (kg. K)

Silicon nitride

Thermal conductivity k = 0.072 cal.cm-1.s-1.k-1 = 30.1 W/ (m. K) @300K
Density r = 3180 kg/m3
Heat capacity Cp = 0.17 cal/ (g. K) = 712 J/(kg. K)

Aluminium

Thermal conductivity k = 2.37 W/ (cm. K) = 237 W/ (m. K) at 300K
Density r = 2700 kg/m3
Heat capacity Cp = 0.215 cal/ (g. K) = 900 J/ (kg. K)

Chromium

Thermal conductivity k = 0.903 W/ (cm. K) = 90.3 W/ (m. K) at 300K
Density r = 7190 kg/m3
Heat capacity Cp = 0.107 cal/ (g. K) = 448 J/ (kg. K)

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