

On Diamond Windows for High Power Synchrotron X-Ray Beams

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Abstract

Recent advances in chemical vapor deposition (CVD) technology has made available thin, free-standing polycrystalline diamond foils that can be used as the window material on high heat load synchrotron x-ray beamlines. Diamond windows have many advantages that stem from the exceptionally attractive thermal, structural, and physical properties of diamond.

Numerical simulations indicate that diamond windows can offer an attractive and at times the only alternative to beryllium windows for use on the third generation x-ray synchrotron radiation beamlines. Utilization, design, and fabrication aspects of diamond windows for high heat load x-ray beamlines are discussed, and analytical and numerical results are presented to provide a basis for the design and testing of such windows.

Introduction

X-ray windows are often used on the front-ends of synchrotron beamlines to isolate the ultra high vacuum of the storage ring from the downstream environment. The windows are usually made of low atomic number materials, such as beryllium, for maximum x-ray transmission.

The intense x-ray beams generated by the undulators at high energy storage ring can deposit substantial amounts of localized heat in passing through the commonly used beryllium windows. Although these windows are actively cooled, the temperature or stress in a window can become unacceptably high, leading to the failure of the window.

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One solution to this problem is to reduce the thermal load by using thermal filters upstream of the beryllium window. Thermal filters are made of thin foils of low-atomic-number materials which withstand high temperatures. They may also be cooled radiatively. Foils of pyrolytic graphite are often used for this purpose. Thermal filters will absorb primarily low energy photons that would otherwise be absorbed by the beryllium window. Fig. 1 depicts the absorbed power in two successive 10 mil thick beryllium windows as the thickness of the upstream carbon filter is increased. The radiation source is the 5 m-long Undulator A at the Advanced Photon Source (APS), with a total power of about 10 kW (see Table I). Fig. 1 illustrates two important points. First, as the thickness of the thermal filter(s) is increased, the reduction in the absorbed power in a beryllium window becomes less pronounced. Absorption in the beryllium window will then be primarily due to Compton scattered photons as few photons with energies below 4 keV remain after the beam passes through a few hundred microns of carbon filter. The transmittance curves for diamond and carbon are shown in Fig. 2. Secondly, as shown in Figure 1, after a few hundred microns of filter, the x-ray beam deposits almost identical amount of heat in each of the two beryllium windows. Therefore, one of the reasons for using a double beryllium window assembly (where the first window is expected to take the brunt of the heat load leaving the second one with a much smaller thermal load and thus more durable) vanishes. This will have implications in the design of windows for high heat load beamlines.

In the calculations reported here, it is conservatively assumed that all the attenuated photons are absorbed in a medium. As such, the absorption values given here may exceed the actual absorptions by as much as thirty percent.

The total absorbed power (shown in Fig. 1) as well as its spatial distribution in a window are estimated by simulating the insertion device (ID) spectrum by a bending magnet spectrum of an appropriate characteristic energy. The PHOTON¹ program is used for this purpose. PHOTON gives both the absorbed power and its distribution in the vertical direction. In the horizontal direction, it has throughout been assumed that the absorption profile is similar to the source profile; the implicit assumption being that the ID beam is horizontally uniform in energy.² This, of course, is not true, as the x-ray beam softens as

one moves off-axis in the horizontal direction. In fact, it has recently been shown that the peak absorbed heat flux in a beryllium foil subjected to an ID beam may not be in the central region of the beam footprint print, but at a horizontally off-axis location³. This will not significantly affect the present thermal and structural analyses, but will have to be incorporated in refined design analyses. The development of an extension to the PHOTON program, named PHOTON3D, to properly account for the vertical as well as the horizontal energy distribution of a wiggler beam and its absorption in media is being completed.⁴

An Analytical Model of a Cooled Window

In order to estimate the temperature and stress in a thin foil of a window subjected to an incident x-ray beam, a simple one-dimensional model is devised.

As shown in Fig. 3, the foil is represented by an infinitely long thin plate of thickness t and width w (corresponding to the vertical opening size of a window). The absorbed heat in the foil is approximated by an infinitely long line-source which is uniformly distributed throughout the thickness of the foil. The window is convectively edge-cooled along its length, as illustrated in Fig. 3.

Assuming a linear heat flux of q' [W/cm] for the absorbed radiation in the thin foil, one can write (see Fig. 3):

$$\frac{d^2T}{dx^2} = 0 \quad (1)$$

$$-k \frac{dT}{dx} = \frac{q'}{2t} \quad \text{at } x = 0 \quad (1a)$$

$$-k \frac{dT}{dx} = h(T - T_\infty) \quad \text{at } x = w/2 \quad (1b)$$

where k [W/cm-K] is the thermal conductivity of the foil, T [°C] is the temperature, x [cm] is the lateral distance measured from the center of the foil, t is the thickness of the foil [cm], h [W/cm²-K] is the heat transfer coefficient, and T_{∞} [°C] is the temperature of the coolant.

The solution to Eq. 1 with boundary conditions given by Eqs. 1a and 1b is

$$T(x) - T_{\infty} = \frac{q'}{2t} \left[\frac{(w - 2x)}{2k} + \frac{1}{h} \right] \quad (2)$$

and in particular, the overall maximum temperature rise is

$$\Delta T_{\max} = T(0) - T_{\infty} = \frac{q'}{2t} \left[\frac{w}{2k} + \frac{1}{h} \right] \quad (2a)$$

while the maximum temperature rise in the foil is given by

$$\Delta T_{\text{foil}} = T(0) - T(w/2) = \frac{q'}{2t} \left[\frac{w}{2k} \right] \quad (2b)$$

The initial temperature of the foil is the same as the coolant bulk temperature, T_{∞} . The displacement $u(x)$ [cm] in the heated foil (assuming it is simply supported) is

$$u(x) = 2 \int_0^{w/2} \alpha f(T) dx \quad (3)$$

Where α [K⁻¹] is the thermal expansion coefficient and $f(T)$ specifies the temperature variation in the foil given by Eq. 2. Assuming a temperature independent α and an initial temperature, T_{∞} , one obtains

$$u(x) = \frac{q' w \alpha}{2t} \left[\frac{w}{4k} + \frac{1}{h} \right] \quad (4)$$

The strain ϵ is then

$$\varepsilon = \frac{u(x)}{w} = \frac{q'\alpha}{2t} \left\{ \frac{w}{4k} + \frac{1}{h} \right\} \quad (5)$$

while the stress σ [N/cm²] that would result in the foil, if it were laterally constrained, is

$$\sigma = -\varepsilon E = -\frac{q'}{2t} \left[\frac{w}{4k} + \frac{1}{h} \right] \alpha E \quad (6)$$

The negative sign emphasizes that the stress is compressive.

The width of a beryllium foil which is mounted on a cooled, conductive platform is somewhat larger than the opening size of the window, by about 1 cm or so. Thus, from a cooling point of view, there is a fin effect that the above analytical model ignores. In fact, cooling is substantially better than the assumed convective edge cooling. A better approximation in this case may be obtained by assuming that the window edge is maintained at the coolant temperature. Then Eqs. 2a and 2b become identical, and the temperature variation (Eq 2) and the stress in the window are, respectively, given by

$$T(x) - T_{\infty} = \frac{q'}{2t} \left[\frac{(w-2x)}{2k} \right] \quad (7)$$

$$\sigma = -\frac{q'w}{8tk} \alpha E \quad (8)$$

As an example, Eqs. 7 and 8 can be used to estimate the maximum allowable temperature and stress in a diamond and a beryllium foil. For beryllium, the absorbed power is limited by the allowable stress. Assuming a stress level equivalent to the yield strength of beryllium (~350 MPa), and using data in Table II, the maximum allowable linear flux q' in a 250 μ m thick, 1.05 cm wide beryllium window is

$$q' = -\frac{8tk\sigma}{w\alpha E} = 35 \text{ W / cm} \quad (9)$$

and the maximum temperature rise in the window will be

$$\Delta T_{\max} = \frac{q' w}{4tk} = 182^{\circ}\text{C} \quad (10)$$

so that for a coolant temperature of 32°C , the maximum temperature in the beryllium window will be about 214°C .

For diamond, on the other hand, the absorbed power is limited by its oxidation temperature of about 600°C (it is understood, however, that the window will be in a high vacuum environment). Then from Eqs. 2b and 8, the maximum allowable linear heat flux and stress in a $50\text{ }\mu\text{m}$ thick, 1.05 cm wide diamond window will be 92 W/cm and 715 MPa , respectively. Diamond properties at an average temperature of 350°C are evaluated and used in these calculations.

Detailed finite element analyses discussed next show a maximum temperature of about 180°C (cf. analytic models 214°C) in the beryllium window and a compressive stress of about 1100 MPa (cf. analytic models 715 MPa) for the diamond window.

The simple analytical expressions derived here must be used with caution in estimating the temperature and stress levels in the windows.

These results can be used, however, to establish thermal and structural figures of merits for various window foil materials. The absorption of the x-ray beam in diamond and beryllium is assumed to be roughly proportional to the square of their atomic numbers (Z) of 6 and 4, respectively. This gives 2.25 times more absorption in diamond than in beryllium. More detailed calculations (shown in Fig. 7) indicate that for the APS undulator A beam, this figure is between 5 and 2. Defining a thermal figure of merit as proportional the inverse of the maximum temperature rise ΔT_{\max} (Eq. 10), and replacing q' by Z^2 results in $(\Delta T_{\max})^{-1} \sim k/Z^2$. Similarly, a structural figure of merit can be defined as being proportional to the inverse of the thermal stress in the foil. From Eq. 8 one obtains the relationship $\sigma^{-1} \sim k/(Z^2 \alpha E)$. Using the material properties given in

Table II, the relative figures of merits for beryllium and diamond are obtained and listed in Table III.

Computational Analyses of Beryllium and Diamond Windows

In order to provide a more reliable simulation of the window performance under realistic heating condition of the undulator beam, a finite element model is setup and used for analyses. The model allows an accurate description of the window configuration, the spatial variation of the absorbed heat flux, the thermal and structural boundary conditions, and temperature dependency of the physical properties of the window material. The window configuration used for the analysis is sketched in Fig. 4. Due to symmetry, one quadrant of the window is shown and modeled. The diamond or beryllium foil is mounted on a back-cooled copper block. The window opening is 1.05 cm which corresponds to a $6/\gamma$ opening angle at 24 m from the source ($1/\gamma$ is the intrinsic opening angle of the x-ray beam, and for the APS it has a value of 73 μ rad). The horizontal extent of the APS Undulator A beam at the window is about 1 cm. The much larger horizontal dimension of the window is to allow it to be used on the wiggler beamlines as well.

The main objective here is to determine the minimum amount of upstream thermal filter necessary to reduce the absorbed power in a window to an acceptable level. One way to do this is to assume a certain amount of filter(s) upstream of the window, obtain the maximum temperature and stress in the window, compare these with the applicable limits, and repeat this process until the minimum amount of filter necessary is obtained. Alternatively, maps of the absorbed power, absorbed power profile, temperature, and stress can be developed from which the filter requirement can be determined.²

For the purpose of the present study, a typical absorbed power profile in the window is assumed: it has gaussian profile in the vertical direction (along the width of the window) with a full width at half maximum (FWHM) of 0.6 cm, and a parabolic profile in the horizontal direction (along the length of the window) similar to the incident beam on-axis horizontal power profile. It must be noted that the vertical FWHM of the absorbed power varies with the thickness of the upstream thermal filters, and the 0.6 cm value used here is only a representative.

Figures 5 and 6 show, respectively, the maximum temperature and the maximum (equivalent) stress as a function of the total absorbed power in one beryllium window and in two diamond windows. The beryllium window is 250 μm thick while the diamond windows are 50 μm and 100 μm thick. As stated earlier, for the beryllium window, the stress is limited to some 350 MP while for the diamond window, the maximum temperature must not exceed 600°C. These conditions, as shown in Figs. 5 and 6, limit the absorbed power in the beryllium window to about 40 W, and in the 50 and 100 μm diamond windows to about 150 and 300 W respectively.

From Fig. 1, it can be seen that several millimeters of carbon filter is needed to reduced the absorbed power in the beryllium window to about 40 W. This much filter, as Fig. 2 indicates, will attenuate the 8 keV photons by about three orders of magnitude, and 12 keV photons by about one. Thus, this window/filter arrangement is not acceptable.

Turning now to the diamond alternative, and considering the 50 μm thick window (which can accept about 150 W of power), it is noted that if exposed directly to the undulator A beam, it will absorb some 900 W of heat (Fig. 7). Thus, thermal filters are necessary even in this case. The amount of *carbon* filter needed can be estimated by considering the absorption equation for *diamond* obtained by a curve fit through the computed data points shown in Fig. 7, i.e.,

$$P_{abs,D}[W] \approx 190t^{0.4}[\mu m] \quad (11)$$

Differentiating Eq. 11 and using the 150 W allowable absorbed power in the 50 μm -thick diamond window, one obtains

$$\frac{dP_{abs,D}}{dt} \equiv \frac{150W}{50\mu} \approx 76t^{-0.6} \quad (12)$$

which gives the total thickness of *diamond* filter upstream as

$$t \approx 215 \mu m \quad (13)$$

This corresponds to about 360 μm of carbon ($\rho=2.1 \text{ g/cm}^3$). From Fig. 2, it is now seen that the transmission of the 8 keV photons through this much carbon filter is over 30%, and still higher for the 12 keV photons. This clearly demonstrates the advantage of diamond windows.

A moderate increase or decrease in the thickness of the diamond window will not have a significant impact on its temperature or stress, since the absorbed power is similarly increased or decreased. Using thinner, yet vacuum tight, diamond windows, however, remains a possibility since they would allow a somewhat higher transmission. With beryllium, the windows have to be at least 5 mil (127 μm) thick to ensure their vacuum integrity.

Finally, it should be noted that in the the present analyses, an important parameter, namely, the window opening was fixed at a value of 1.05 cm ($=6/\gamma$ at 24 m from the source). As seen from the analytic solution (e.g., Eqs. 8 and 10) and verified with more accurate analyses, reducing the window opening will correspondingly reduce the temperature and stress levels in the windows. The conservative window opening of $6/\gamma$ used here is consistent with the present designs at various synchrotron facilities and with the overriding concerns with beam mis-steering and stability. The high heat load of the APS undulator beamlines, however, has provided a compelling reason to carefully examine the window size requirements imposed by the stability of the beam. It has been shown⁵, for example, that for the 2.5m-long APS undulator A beamline it is possible to use a beryllium window with an opening size of 0.7 cm (corresponding to an opening angle of $4/\gamma$ at the source) with only a moderate amount of upstream carbon filter. And with an opening size of 0.35 cm (corresponding to an opening angle of $2/\gamma$ at the source), a beryllium window can be used on the 5m-long APS undulaor beamline. But even for smaller window openings, diamond windows remain superior since they can be used with lower amount of thermal filters upstream resulting in higher photon transmission through the filer-window assemblies.

Concluding Remarks

Although the superior thermo-physical properties of diamond make a diamond window an attractive and at times the only option for high heat flux synchrotron x-ray beamlines, a number of issues remain unresolved. First is the question of radiation damage and stability of diamond foils, and possible degradation of its mechanical properties. On this score, limited tests⁶⁻⁸ on CVD

diamond membranes for use in x-ray lithography diamond show no noticeable degradation for x-ray exposures of several MW/cm³. Nevertheless, this issue, and particularly long-term exposure effects must be further investigated. A 50μm diamond window on the APS undulator beamline, for example, must survive several hundred MW/cm³ of radiation exposure. Secondly, since CVD diamond is polycrystalline, as a window it may scatter an appreciable amount of radiation. However, with the established process controls, it is possible to develop CVD diamonds (for example, with very small grain sizes) more suitable for this purpose. This also requires further study. Finally, a number of fabrication and testing related issues remain, for example, with regard to mounting of the diamond foil on a cooled copper platform and the appropriate thermal mechanical and vacuum leak testing of such windows.

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Table I: Parameters* for the APS Undulator A. The ring energy is 7GeV and the current 100 mA.

Period length [cm]	3.1
Device length [m]	5.00
Number of periods	160
Max. magnetic field B_0 [T]	0.80
Characteristic energy E_c [keV]	26.0
$1/\gamma$ [mrad]	0.073
Max. deflection parameter, K	2.51
K/γ [mrad]	0.183
Total power [kW]	10.0
Peak power density [kW/mrad ²]	333
Peak heat flux @24 m [kW/mm ²]	0.58

* Current Undulator A parameters are slightly different from those given here.

Table II Properties of Diamond and Beryllium at Room Temperature.

Property	Diamond	Beryllium
Atomic Number, Z	6	4
Density (g/cm ³)	3.5	1.85
Thermal Conductivity (W/cm-K)	<21	2.0
Thermal Expansion Coeff. (K ⁻¹ x 10 ⁻³)	0.8	12
Specific Heat (J/Kg-K)	520	190
Thermal Diffusivity (cm ² /s)	<11.5	5.7
Young's Modules (GPa)	1,050	320
Poisons Ratio	0.1-0.29	0.02-0.08
Melting Point (°C)	NA	1280
Tensile Strength (GPa)	>3	0.080-0.550
Yield Strength (MPa)	NA	70-480

Table III Figures of Merit for Diamond and Beryllium

Figures of Merit	Relationship	Beryllium	Diamond
Thermal, (ΔT^{-1})	k/Z^2	1	4
Structural, (σ^{-1})	$k/(Z^2\alpha E)$	1	20

Figure Captions

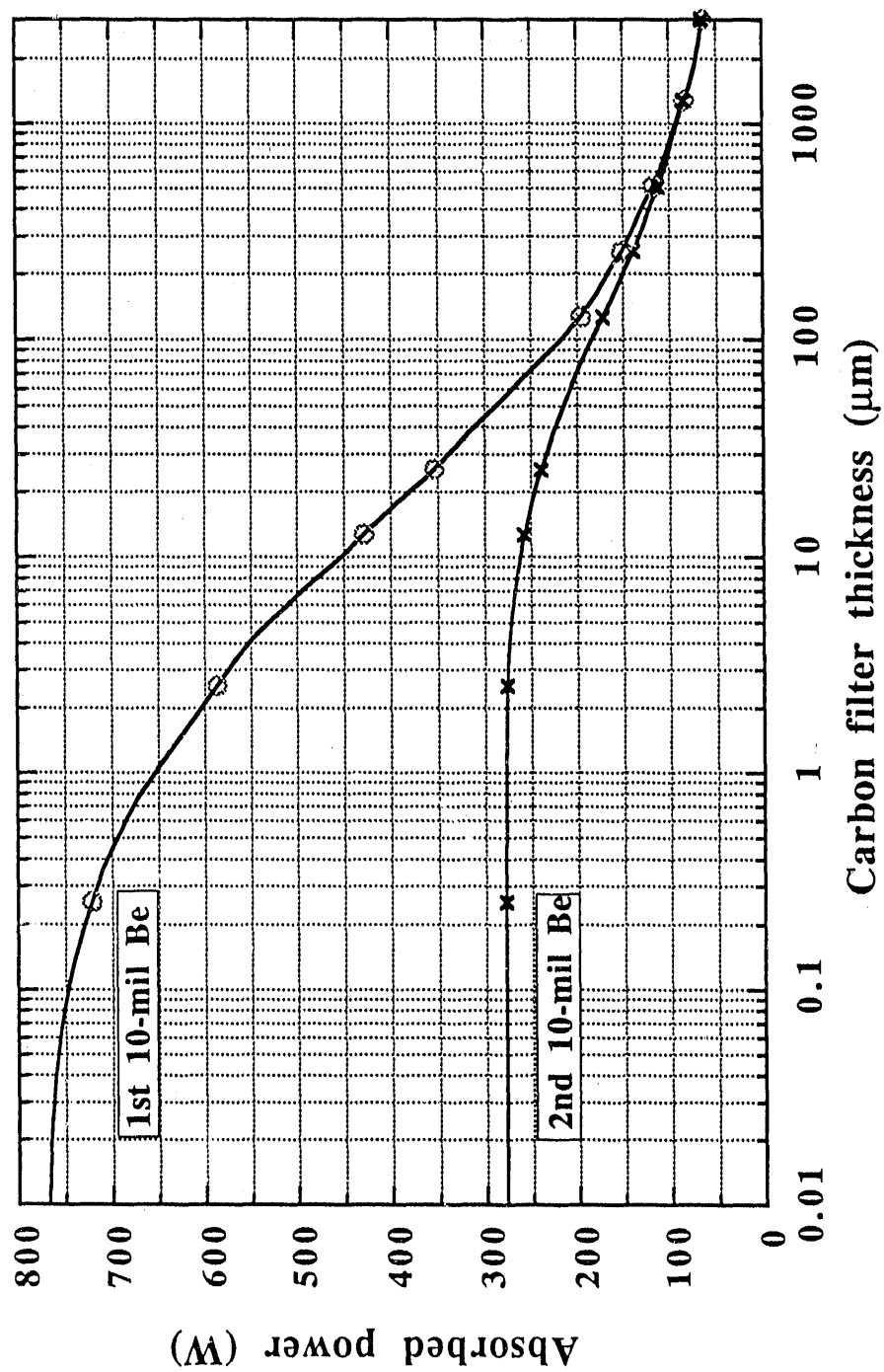
- Fig. 1. The absorbed power of the 5m-long APS Undulator A beam in two successive beryllium foils as a function of the total thickness of the upstream carbon filter(s). The thickness of each beryllium foil is 10 mils (254 μm).
- Fig. 2. Transmittance of photons of various energy through diamond ($\rho=3.5\text{g/cm}^3$) and carbon ($\rho=2.1\text{g/cm}^3$) foils.
- Fig. 3. A sketch of the model foil used to develop a simple analytical solution for temperature and stress in a window. The thin, infinitely long plate of width w (equal to the opening size of the window) is subjected to a line heat source of strength q' [W/cm] deposited uniformly throughout its thickness. The plate is convectively edge-cooled along its length. The shaded region is a sketch of a typical beam power footprint.
- Fig. 4. A typical model used in the finite element analysis of the windows. Due to symmetry, only one quarter of the window is shown here and modeled. The window opening is shown in heavy lines. Also shown are typical temperature contours.
- Fig. 5. Maximum temperature in one beryllium and two diamond window as a function of the absorbed power. The absorbed power has a vertical gaussian profile (FWHM = 0.6 cm) and a horizontal parabolic profile (about 1 cm in extent) similar to that of APS Undulator A beam. Window opening is 1.05 cm ($=6/\gamma$).
- Fig. 6. Same as Fig. 5, but instead of the maximum temperature, the maximum stress is shown here.
- Fig. 7. Absorption of the x-ray beam from the 5 m long APS Undulator A in beryllium and diamond foils. Shown are also curve fits through the data points.

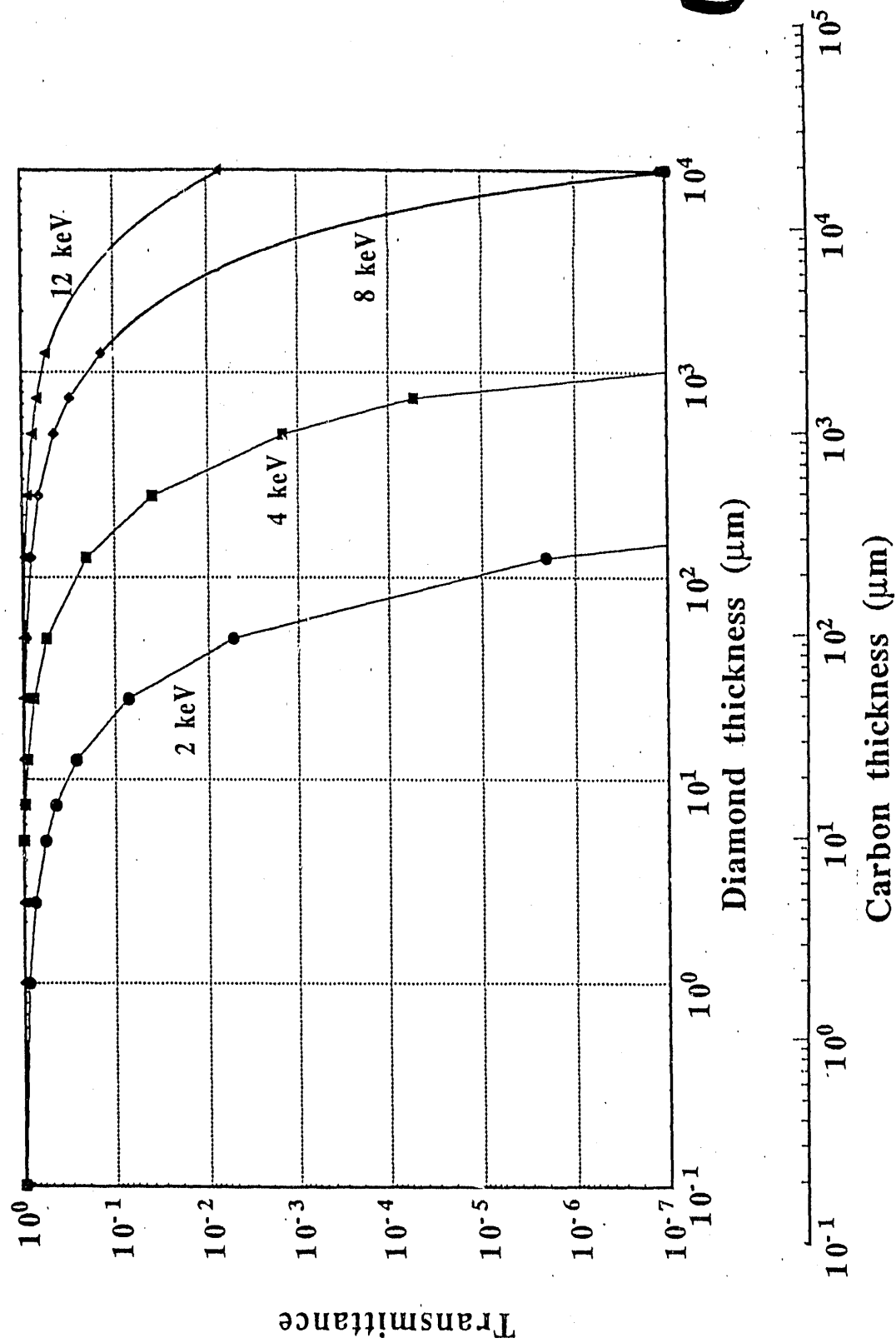
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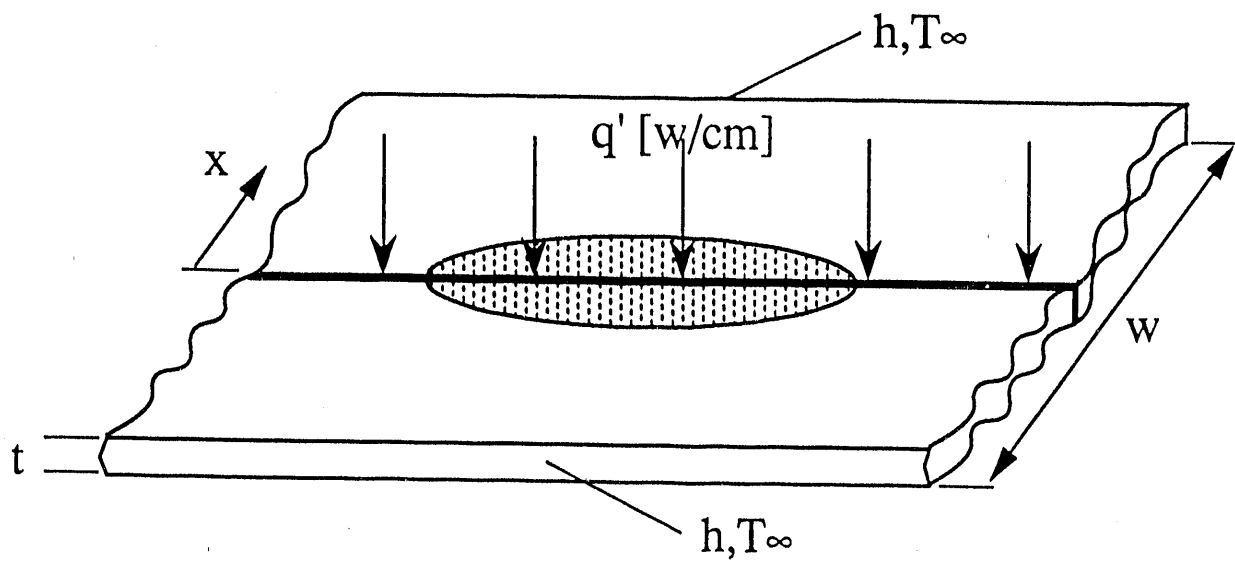
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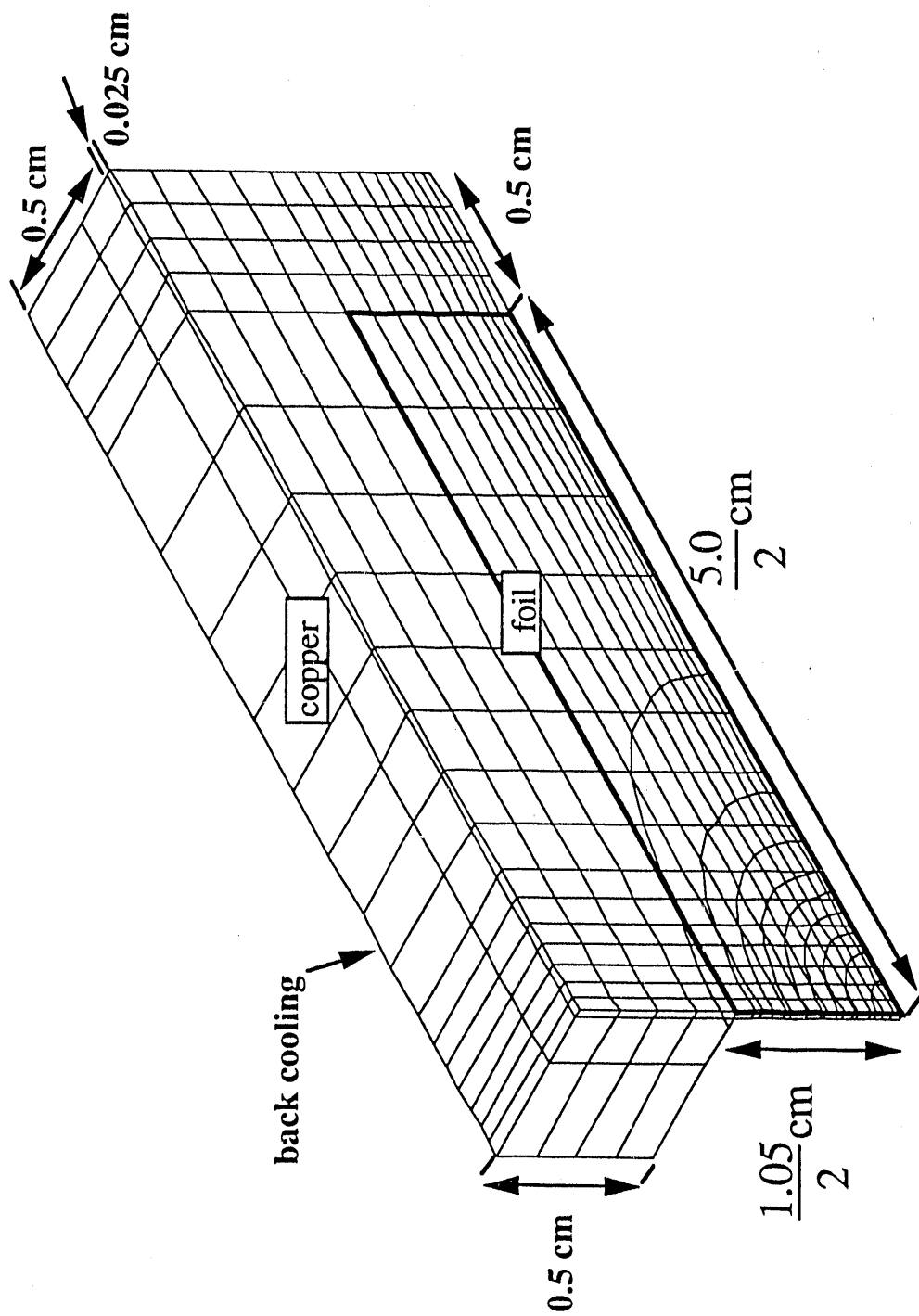




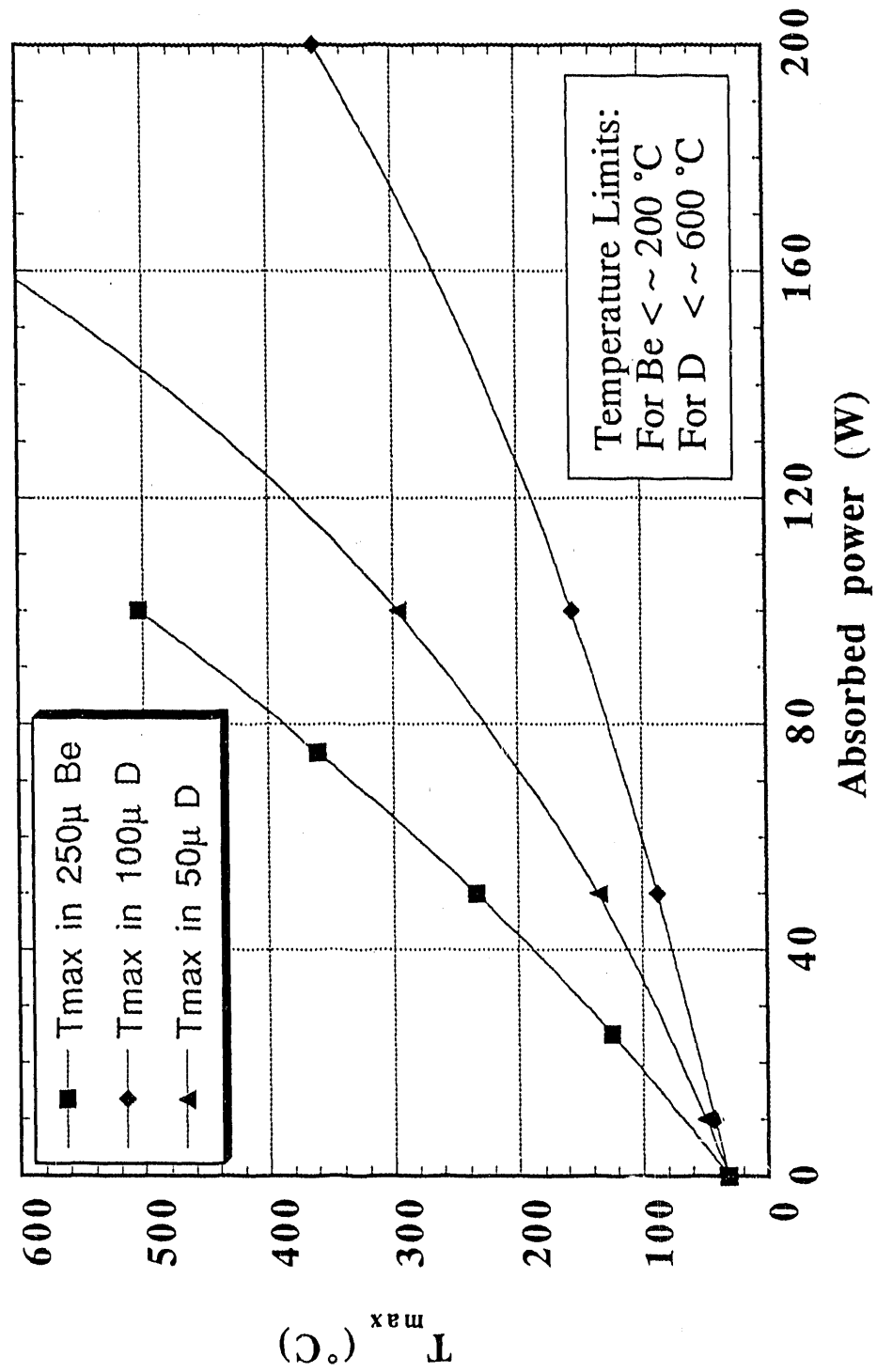
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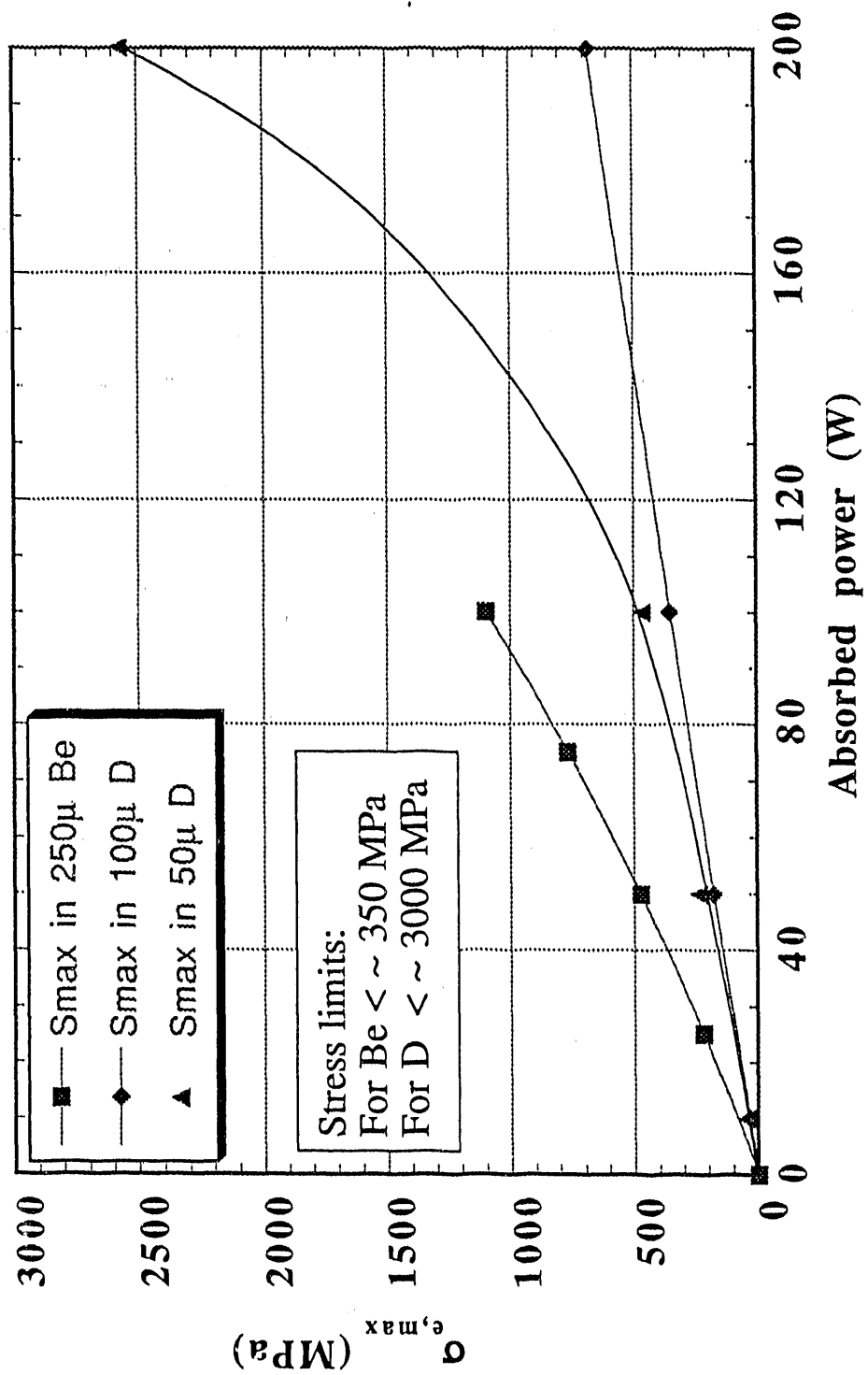
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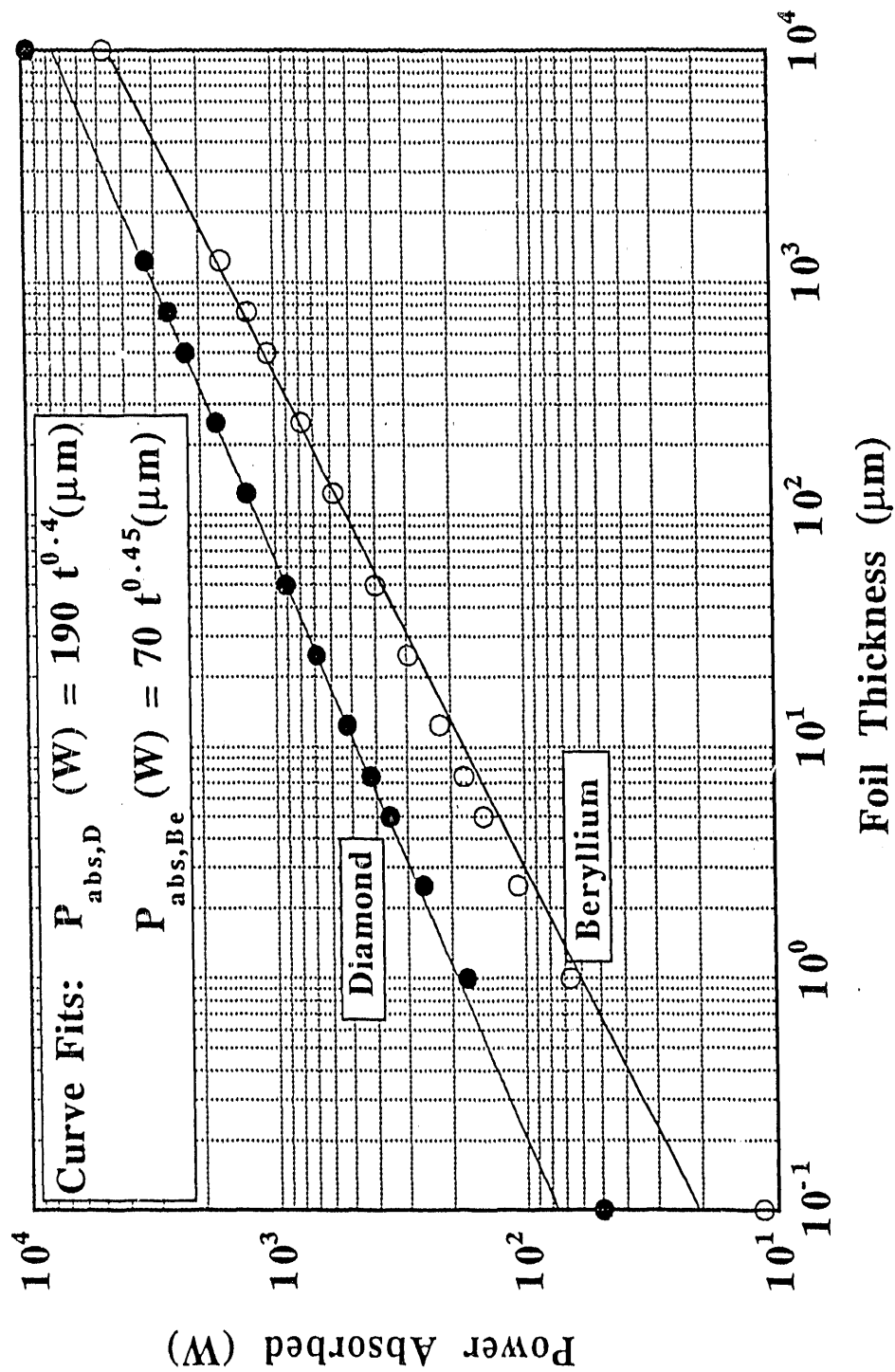
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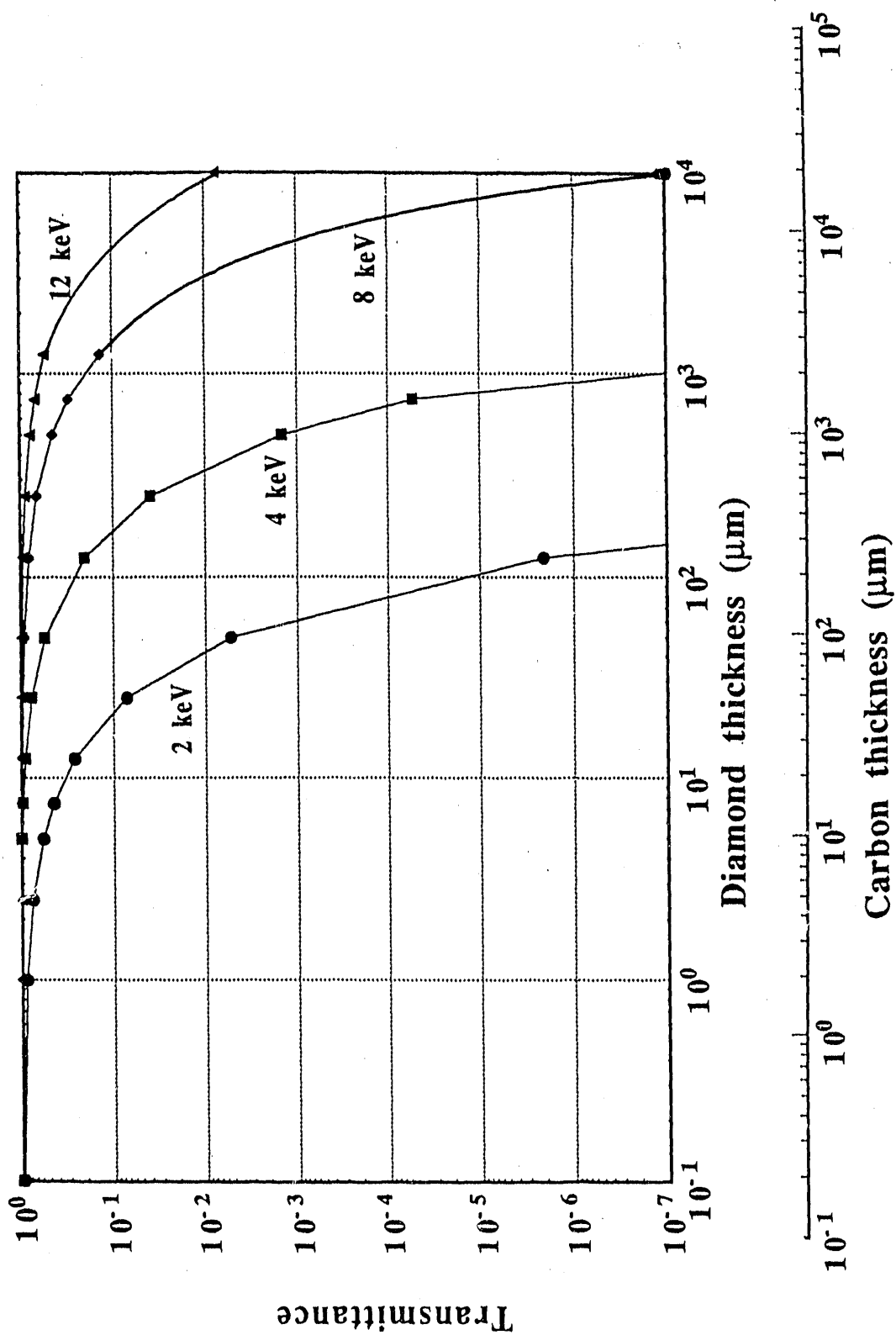
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