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Richard H. White
G. Richard Wirtenson

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**Effects of Oxide Layers on Optical Properties
and X-ray Hardness of Al-Be Mirrors**

Richard H. White and G. Richard Wirtenson

**University of California
Lawrence Livermore National Laboratory
P.O. Box 808, L-298
Livermore, CA 94550**

ABSTRACT

Oxide layers form on the surfaces of many metallic mirrors. The oxidation may occur during fabrication or after the mirror is finished and installed. Some oxide layers may be intentionally added to protect the mirror or to change its optical properties. Computer calculations predict the effect of oxide layers on optical and ultraviolet reflectance as well as the x-ray absorption and concomitant thermal damage to the mirrors.

I. INTRODUCTION

A thin aluminum reflective coating applied to a beryllium substrate produces a mirror that has high reflectivity over a wide spectral range and yet resists damage by soft x-ray's, even at fluences exceeding 1 cal/cm^2 and for pulse durations as short as 5 ns. After manufacture of such mirrors, it is inevitable that at least some thin oxide layers form on the various mirror surfaces. These may grow thicker with the passage of time.

The computer code LXRT is used to explore the effect of oxide layers on the melt fluence of aluminum - beryllium mirrors exposed to soft x rays. (See Section II for a description of LXRT.) The thermal response of mirrors to deposited x rays strongly depends upon the incident x-ray spectrum and the x-ray pulse length. Unless otherwise noted, all calculations reported here are for a 1 keV blackbody

spectrum and a temporal pulse shaped as an isosceles triangle, 10 ns across the base. (The intensity rises linearly with time to a maximum in 5 ns, then falls linearly to zero in another 5 ns.)

The mirror design considered here is an aluminum reflective coating, 10 to 100 nm thick, on a beryllium substrate. The dependence of reflectance and melt fluence upon thickness of the aluminum reflector is explored for "bare" aluminum on beryllium mirrors. Oxide layers in various combinations are added to this configuration (Fig. 1). Reflectances and melt fluences are calculated for these "oxidized" mirrors.

Oxide layers may be intentionally deposited to act as heat sinks, to protect the surface from mechanical or chemical damage, or to alter the optical properties of the mirror. Intentionally deposited oxide layers of various thicknesses are explored. Layers intentionally deposited on the front (irradiated) surface of the mirror are herein called "coatings" or "coats."

Fig. 1 Aluminum-beryllium mirror with various possible oxide layers shown. Some oxide layers may have zero thickness.

II. MODELING USING LXRT

LXRT is a version of the XRTH computer code developed by J.R. Triplett et al. of S-Cubed corporation.¹ It is a one-dimensional calculation. Incident radiation is described by a frequency independent temporal pulse shape and a frequency dependent intensity. X ray deposition is by exponential attenuation. Secondary x rays, produced by scattering and fluorescence, are analyzed by a discrete ordinates method. Electron transport is calculated using a P1 approximation to the Spencer-Lewis equation. A time-dependent energy deposition and heat diffusion calculation follows this determination of energy deposition by x rays and electrons. Melting and vaporization are treated. A succinct summary of the physics embraced by LXRT (and XRTH), including differential equations and boundary conditions is given in the article by Rhoades and Triplett².

The reported calculations do not assess damage due to thermally induced stress. Calculated melt fluences are given. Damage often occurs at a fluence somewhat less than the calculated melt fluence. Nevertheless, the patterns of heat flow are essentially the same whether a mirror is subjected to melt fluence or to a fluence somewhat below melt fluence. The calculated melt fluence is a useful indicator of vulnerability and defines an ideal upper limit on performance.

Though LXRT includes an optional one-dimensional hydrodynamic calculation that couples to the thermal transport, this option was disabled in all reported calculations. Experience shows that a one-dimensional treatment of hydrodynamics cannot credibly calculate the stresses developed at interfaces between thin layers of materials, which expand transversely at markedly different rates.

In all calculations reported here, material properties are taken from the compilation prepared by Childs³. (Note that this compilation is for bulk materials and does not necessarily correspond to the data applicable to thin films. In particular, thin films that exhibit structural disorders introduced during their construction may have thermal conductivities an order of magnitude less than those of the bulk material.⁴)

III. ALUMINUM MIRRORS

The reflectance of bare polished beryllium is about 50% for incident wavelengths ranging from visible light through the near ultra-violet. The reflectance of polished aluminum, in this same spectral region, is over 90%. Aluminum films can be deposited onto beryllium mirrors to enhance reflectance.

Figure 2 shows how reflectance (at 250 nm wavelength) depends upon aluminum film thickness for an aluminum-beryllium mirror.⁵ In general, the reflectance increases as the aluminum film thickness increases and asymptotically approaches an upper limit that is the reflectance of a thick aluminum slab.

Fig. 2 Reflectance of 250 nm wavelength vs. reflector thickness for a mirror with an aluminum reflector on a beryllium substrate.

According to Fig. 2, fifty nanometers of aluminum brings the reflectance of a 250 nm wavelength very near its limiting value. Fifty nanometers of aluminum give nearly the limiting reflectance for wavelengths longer than 250 nm, as well.

The need to make films thick to provide maximum reflectance competes with a need to make them thin to decrease x-ray vulnerability. Figure 3 shows the dependence of melt fluence on reflector thickness for aluminum films on beryllium substrates with no oxide coats present. The incident spectrum is a 1 keV blackbody. The temporal pulse shape is an isosceles triangle. The figure shows results of calculations for pulse durations (triangle base lengths) of 5, 10, and 20 ns.

Fig. 3 Melt fluence vs. thickness of aluminium reflector for an aluminum-beryllium mirror with no oxide layers. The incident spectrum is a 1 keV blackbody. The x-ray pulse is an isosceles triangle, with base 5, 10, or 20 ns (as indicated).

Blackbody spectra with temperatures higher than 1 keV are less stressing on the system than the 1 keV spectrum. For example, a 2 keV blackbody spectrum delivered in a 10 ns triangular pulse melts 50 nm of aluminum on a beryllium substrate with the fluence 7.4 cal/cm^2 . For a 1 keV spectrum in a 10 ns triangular pulse, this same mirror design melts at 1.8 cal/cm^2 .

IV. ALUMINUM OXIDE ON THE FRONT SURFACE

Aluminum Oxide (Al_2O_3) coats may be applied to the front surface of the mirror either to alter the optical properties or as a protective coating for the aluminum reflector. Figure 4 compares the reflectances, as a function of wavelength, for aluminum mirrors with and without oxide coats. Each mirror consists of 50 nm of aluminum on a beryllium substrate. The oxide coated mirror has a 20 nm thick coat of aluminum oxide.

Fig. 4 Reflectance vs. reflected wavelength for mirrors with and without oxide coats. The Al reflector thicknesses are each 50 nm. Substrates are Be. The oxide coated mirror has a 20 nm coat of Al_2O_3 .

The solid curve in Fig. 5 gives the dependence of melt fluence on oxide coat thickness for a mirror consisting of an aluminum oxide coat on a 20 nm aluminum reflecting film on a beryllium substrate. The mirror may be destroyed either because the aluminum reflector melts or because the oxide coat melts. For some coat thicknesses, the aluminum melts at a lower fluence than does the oxide coat; for other coat thicknesses, the coat melts at a lower fluence than the

reflector. The melt fluences for the aluminum reflector and aluminum oxide coat are shown with dashed lines in Fig. 5. The spectrum is a 1 keV blackbody and the pulse is a triangle with a 10 ns base.

Fig. 5: Melt fluence vs. oxide coat thickness for an Al_2O_3 coat on 20 nm of Al on a Be substrate. The spectrum is a 1 keV blackbody. The pulse is a 10 ns isosceles triangle. One dashed curve gives the fluence that melts the Al reflector, the other dashed curve is the melt fluence for the Al_2O_3 coat. The melt fluence for the coated mirror is the lesser of these as indicated by the solid line.

The mirror melt fluence versus oxide thickness indicated by the curves in Fig. 4 shows four distinct features.

- 1) For oxide coats between 0 and 1 nm thick, the melt fluence is essentially the same as for a bare aluminum reflector: 2.6 cal/cm².
- 2) For oxide coats thicker than about 1 nm, the melt fluence drops sharply from the value for bare aluminum. The decline in melt fluence with increasing oxide-coating thickness continues to a minimum of 1.05 cal/cm² for an oxide coat 100 nm thick.

- 3) As the oxide coat thickness increases beyond 100 nm, the melt fluence of the aluminum increases. This is because the thick coat acts as a combined x-ray shield and heat sink. The part of the oxide coat near the irradiated surface absorbs the x rays so they do not reach the aluminum reflector. The coat is thick enough that when the resultant heat is distributed through the coat, the temperature remains too low to melt the adjacent aluminum.
- 4) As the oxide coat thickness increases beyond 200 nm, the oxide itself melts at a fluence of about 1 cal/cm². In general, it then takes a somewhat higher fluence to melt the aluminum but the optical figure of the mirror has already been destroyed due to the melting of the oxide.

Figure 6 compares the melt fluence versus oxide thickness curves for reflectors of 20, 50, and 100 nm. The behaviors of the 50 and 100 nm reflectors are similar to that described for the 20 nm reflector.

Fig. 5: Melt fluence vs. oxide coat thickness for an Al₂O₃ coat on an Al reflector on a Be substrate. Curves are shown for 20, 50 and 100 nm reflectors. The spectrum is a 1 keV blackbody. The pulse is a 10 ns isosceles triangle.

V. BERYLLIUM OXIDE ON THE FRONT SURFACE

Though aluminum oxide forms a naturally occurring coating on aluminum reflectors, aluminium oxide coats thicker than about 1 nm seriously degrade a mirror's hardness to x rays. Beryllium oxide has lower x-ray absorption and larger heat capacity per unit volume than does aluminum oxide. This suggests that it may be a useful coating material.⁶

Melt fluences were calculated for a mirror with a beryllium oxide coat on the front surface. (The optical performance of beryllium oxide is similar to aluminum oxide; therefore, no additional reflectance calculations were done.) Figure 6 shows the melt fluence versus thickness for a 50 nm aluminum reflector coated with various thicknesses of either aluminum oxide or beryllium oxide. The incident spectrum is a 1 keV blackbody. The x-ray pulse is a 10 ns isosceles triangle.

Fig. 6 Melt fluence vs. oxide coat thickness for mirrors with an oxide coat (BeO or Al₂O₃) on 50 nm of Al on a Be substrate. The spectrum is a 1 keV blackbody. The pulse is a 10 ns isosceles triangle.

Beryllium oxide coated mirrors are less susceptible to x-ray thermal effects than mirrors coated with aluminum oxide. This is because beryllium oxide absorbs less x-ray energy and has a higher specific heat than aluminum oxide. Increasing the beryllium oxide coat thickness degrades the hardness of the mirror until a coat thickness of about 200 nm is reached. Beryllium oxide coats thicker than 200 nm provide a heat sink for the energy deposited near the surface of the coat and hence increase the hardness. Even with beryllium oxide coats 1000 nm thick, a larger fluence is required to melt the oxide than to melt the aluminum reflector. This contrasts with the situation for aluminum oxide coats discussed in Section III.

VI. NATURALLY OCCURRING OXIDE LAYERS

Sections IV and V treat oxide coats on the front surface. This section explores the effect of oxides on other surfaces. Here, the oxide layers are viewed as a byproduct of the manufacturing process. It is assumed that there has been no effort to increase the natural oxidation. Therefore, these naturally occurring oxide layers are assumed to be thin: ~4nm thickness.

The aluminum surface that adjoins the beryllium substrate has minimal exposure to oxygen during or after manufacture of the mirror. It is unlikely to be oxidized to the same degree as is the front surface. Nevertheless, for completeness, some calculations include a 4 nm deep oxidation of this "backside" of the aluminum. Calculations for 50 nm aluminum oxide and beryllium oxide coats on the front surface are reported. These are given for mirrors with and without expected naturally occurring oxide layers.

Table I summarizes the calculations that are for a 1 keV blackbody spectrum delivered in an isosceles triangular pulse of duration 10 ns. Calculated melt fluences are quoted to three figures only to display the relative effects of various oxide configurations. Accuracy is probably no better than ten percent and may be worse due to uncertainty in the physical properties of the thin films.

TABLE I. Melt Fluences for Various Oxide Layer Configurations
(See Fig. 1 for schematic diagram of layer configurations)

Layer Thickness (nm)				Melt Fluence	
BeO	Al ₂ O ₃	Al	Al ₂ O ₃	BeO	cal/cm ²
0	0	50	0	0	1.77
0	0	50	0	4	1.76
0	0	50	4	0	1.64
0	0	50	4	4	1.60
0	4	50	0	0	1.67
0	4	50	0	4	1.63
0	4	50	4	0	1.53
0	4	50	4	4	1.49
0	50	50	0	0	1.08
0	50	50	0	4	1.07
50	0	50	0	0	1.38
50	4	50	0	4	1.31

VII. CONCLUSIONS

Aluminum films of thickness of order 50 nm or more, deposited on a beryllium substrate, have substantially higher reflectivity than a bare beryllium mirror.

Ultra thin (< 1 nm) oxide coats do not alter the damage threshold of aluminum-beryllium mirrors. Coats of thickness between 1 and 10 nm moderately increase vulnerability to x rays. Oxide coats of thickness 10 to 100 nm significantly increase x-ray vulnerability. Beryllium oxide coats do not increase vulnerability as much as do aluminum oxide coats.

Coats of beryllium oxide exceeding 100 nm in thickness act as heat sinks for the energy absorbed near the irradiated surface and provide some protection against x-ray induced thermal damage. However, even a 1000 nm thick beryllium oxide coating will not match the performance of a "bare" aluminum-beryllium mirror.

Naturally occurring oxide layers of about 4 nm thickness slightly increase a mirror's vulnerability to x rays. With probable naturally occurring oxidation configurations, the net effect is approximately a 10% decrease in melt fluence.

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REFERENCES

- ¹J.R. Triplett, B. Shkoller, and M. Merker, "XRTH User's Manual and Reference Guide", S-Cubed, La Jolla, CA, Report No. SSS-R-878420 (1986)
- ²C.E. Rhoades Jr. and J.R. Triplett, J Appl. Phys 69, 1909 (1991)
- ³ Childs, W.H. "Thermophysical Properties of Selected Space Related Materials" Aerospace Corp. , El Segundo, CA, Report TOR-0081(6435-02) [1981 (Vol I), 1986 (Vol II)].
- ⁴J.C. Lambropoulos, M.R. Jolly, C.A. Amsden, S.E. Gilman, M.J. Sinicropi, D. Diakomhalis, and S.D. Jacobs, J. Appl Phys. 68, 4230 (1989)
- ⁵All reflectance calculations reported here used the program "Film Calc" available from FTG Software Associates, P.O. Box 579, Princeton NJ, 08542
- ⁶G.R. Wirtenson, Patent Disclosure, LLNL File No.IL-8136 with Department of Energy case No. S-68, 749 (RL-10,572)

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