SIMULATION OF X-RAY RESIST LINE EDGE PROFILES

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ABSTRACT

X-ray resist line edge profiles are explored as a function of exposure, mask and resist properties. The study is based on an exposure-scission and development-etching model of positive resists. Development rate curves for two actual and three hypothetical resists are used. The simulation is implemented by using a string of points to follow the contour of the developer-resist interface as a function of development time. Control of the resist profile suitable for liftoff of .4μ lines is explored in the context of low flux levels for a high throughput production environment. High aspect ratio lines (3:1) and profile degradation due to mask edge effects for $A\ell_{k_\alpha}$ and Cu_L exposures are considered.

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As resolution in microlithography improves the shape of the resist line edge profiles is becoming more and more important. Profiles for optical e-beam and x-ray exposure have been studied using computer simulation of the exposure and development process based on a surface etching assumption. To date simulation has mostly been used as a diagnostic and exploratory tool. It is being used increasingly to study process operating point tradeoffs and process parameter sensitivity. It is likely that for positive type resists simulation will eventually be able to predict line width openings to an absolute accuracy of 20% for all types of lithography.

The present paper is a theoretical study which uses simulation to explore x-ray line edge profiles in positive type resists. The study is based on a family of five development rate vs. dose models for measured and hypothetically modified resists at 8.34Å. The tradeoff in sidewall angle vs. dose for these models illustrates the usual operating dose levels for x-ray lithography. Simulation of layered resist structures using these models illustrates lift-off and high aspect ratio profiles at relatively low doses and shows profile changes due to finite mask edge angles.

The validity of a surface etch rate vs. exposure model for e-beam and x-ray resists is an open question both on physical and practical reproducibility grounds. However, to illustrate the kinds of effects resist properties could have on line edge profiles a rather simple algebraic surface etching model has been chosen. The development surface etching rate R in Å/sec as a function of the local flux F in mJ/cm^2 is assumed to be

$$R(F) = R_1\left(C_m + \frac{\mu F}{D_0}\right)^{\alpha}$$

This form stems from the solubility work of Ueberreiter[1] and is similar to the characterization used by Hatzakis, et al[2] and Greeneich[3] which show the molecular weight change with exposure. From their work it follows that in the present form the only effect of the molecular weight is through the constant C_m. This constant is inversely proportional to the number average molecular weight and is normalized to 1.0 for PMMA with $\bar{M}_w = 50{,}000$. The constant R_1 is the unexposed etch rate in Å/sec for C_m=1. On a log-log plot of development rate vs. flux the slope of a line asymptotic to the rate curve at high dose is the power law coefficient α. For $C_m = 1.0$ the intersection of this asymptote with the unexposed etch rate gives the reference dose D_0 in J/cm^3 when multiplied by the resist absorption μ in cm^{-1}. Note that the isolation of the molecular weight effect in C_m comes at the expense of the introduction of an additional constant.

Table I gives specific parameter values for five different models of resists at $\lambda = 8.34$Å($A\ell_{k_\alpha}$). The first model corresponds to that given by Hatzakis[2] for PMMA with a $\bar{M}_w$ of 50,000. Model 2 is a hypothetical extension of model 1 with $\bar{M}_w$ increased to 200,000. Model 3 is also hypothetical in that the absorption of model 1 has been increased four fold without changing the other resist parameters. Model 4 is a curve fit (using $c_m = 1.0$) to the experimental resut of Spiller, et al[4] for x-ray exposure of P(MMA-MAA) with synchrotion radiation. The final model is a hypothetical extension of model 4 having four fold increased absorption with no other change.

The development rate vs. exposure flux for these models is shown in Figure 1. The change in development rate with exposure begins to be usable around flux levels of $D_0 C_m \mu^{-1}$. The unexposed etch rate is lowered by a factor of C_m^α for resist 2. (This apparently does not always hold for high molecular weights.[5]) Curves 3 and 5 for modified absorption are simply horizontal translations of 1 and 4 by a factor of 4. The additional straight lines are from Greeneich[3] for PMMA with developers diluted with IPA.

To illustrate how the resist properties effect the line edge profile consider the simple case of 4000Å of resist 1 exposed at 500mJ/cm^2 with a 4:1 contrast mask. The fast etch rate in the exposed area is 40Å/sec while that under the mask is 15Å/sec. The line edge profile contours as a function of development time are shown in Figure 2. In both exposed and masked areas planar facets advance at the appropriate etch rates. The transition between the two is almost a planar facet which occurs in the slow etch rate area. This transition is created by the opening up of the masked region by the more rapidly moving front in the exposed area. For a uniform etch rate with depth (no decay due to absorption) the sidewall would be truely planar at angle from vertical of

$$\theta_v = \sin^{-1}\left(\frac{R_s}{R_f}\right)$$

The contours shown in Figure 2 were produced by a FORTRAN program which models the developer as a string of line segments which advance at a local rate in time[5]. The segments are about 100Å in length. As the string advances new line segments are added and deleted. This gives rise to the slight ripple in the sidewall which is a simulation artifact. A typical simulation requires about 5 seconds on a CDC 6400 (about 5 MIPS) and costs less than one dollar.

The important physical parameter of the profile is the sidewall angle measured from the horizontal ($\theta_H = 90-\theta_v$). It is evaluated as a function of dose and mask contrast in Figure 3. For at least half of the initial resist to remain in the masked areas (etch ratio $\geq$ 2:1) the minimum sidewall angle is 60°. For liftoff with e-beam exposure etch rate ratios of 5:1 or sidewall angles of 78° are typical. For these models the required dose varies from 1500 to 6 mJ/cm^2 depending on the resist, desired etch rate ratio and mask contrast ratio. For a $.1mW/cm^2$ source this corresponds to an exposure time range from 4 hours to 1 min. Roughly a 256 fold improvement is achieved by going from 4:1 to 1:1 mask contrast (2), lowering the etch rate ratio from 5:1 to 2:1 (4), changing from PMMA to P(MMA-MAA) (8) and doping the resist (4). The factor of 8 improvement with change in resist type is probably inflated somewhat by the fact that the PMMA used in comparison has a rather low molecular weight.

Additional line edge profile control is possible with the use of layered resist structures. This control can be exercised at flux levels lower than those generally inferred from Figure 3. This will be illustrated here by simulating profiles in two layer resists using the five resist models. The emperical feasibility of combining two layers of resist and obtaining useable profiles has been beautifully illustrated in SEM's by R. Feder et al.[7] The two layer structure also roughly corresponds to resist chemically treated after exposure and before development.

The concepts and advantages of a two layer resist are illustrated in Figure 4. Here 2000Å of resist 2 has been placed over 2000Å of resist 1 and exposed at 70 mJ/cm^2 with a mask contrast of 4:1. The constant development time contours of the right half of a .4μ linewidth opening are shown. The etch front under the mask is sufficiently delayed that the unmasked front punches through to the lower molecular weight resist which is rapidly removed. There are three important advantages: undercutting is produced, the line width is defined by the more slowly moving top resist edge, and a high effective sidewall angle is obtained at only one fifth the dose of a single layer of resist 2.

Figure 4 also contains an interesting simulation loop artifact. On the 13 minute contour the upward moving front has crossed the horizontally moving edge creating a loop (not darkened). This inside out loop will continue to grow with time and necessitates the repeated calling of a loop deleter to remove these continually generated nonphysical artifacts.

Results for layered P(MMA-MAA) are shown in Figure 5. This case was chosen to approximately correspond to the resist configuration of R. Feder et al.[7] The dose however is minimal (40 mJ/cm^2) and does not produce deep undercutting with a thick upper layer. Profiles with even lower doses have been studied using pre-exposed or modified resist 5 under resist 5. The limiting factor is the ratio masked and unmasked etchrates of the top layer. Generally the fast etch rate must be about twice the masked etch rate to provide sufficiently time for the lower layer to be cleared and yet have a thick top layer remain. (8 mJ/cm^2 for #5)

A new absorbing zipper approach is shown in Figure 6. Here a thin layer of an absorber such as gold is used to convert part (6.72%) of the local x-ray flux to photoelectrons[7,8] which then expose a region on both sides of the absorber. The photoelectrons are assumed to uniformly expose a range of 300Å on both sides of the absorber. By designing etch rates appropriately (the absorption needed depends on mast contrast) an undercut notch has been put in the sidewall of the resist. To reduce the flux to 10 mJ/cm^2 the thickness of the resist has been increased to 8000Å. The profile, while interesting does not appear to be useful for lift-off due to the fact that the bottom sticks out beyond the the overhung edge. The absorbing zipper can be combined with the two layer resist structure for more line edge control. In Figure 7 a 3.6% absorber has been added to the configuration of Figure 5 to produce a more pronounced under etching notch.

A 4:1 mask contrast at 8.34Å requires about 3000Å of gold. For narrow lines such as the .4μ considered here the mask edge taper may extend over a significant portion of the nominal linewidth. The degradation due to this edge has been simulated assuming a linearly tapered edge. In Figure 8 the perfect edge of the mask of Figure 7 has been replaced by a mask with a 45° edge taper to a thickness of 3000Å. To compensate for average linewidth increase the mask edge has been placed at 1000Å instead of 2000Å. The previously useable profile is obviously badly degraded. Using the Cu_L gives a significant improvement as is shown in Figure 9. Here the flux has been reduced to compensate for the (3.78) increase in resist absorption. Although the edge position has been compensated there is a slight increase in overetching sensitivy, due to the edge taper. These comparisons are based on a change in gold absorption from $4.6\mu^{-1}$ to $12.6\mu^{-1}$.

Layer resist structures are also useful for high aspect openings with undercutting. Figure 10 shows 4000Å of resist 4 over 12000Å of resist 5. A higher flux is required to maintain the masked top layer thickness. The opening useable with lift-off is about three times higher than it is wide. Such a high aspect profile might be useful as a FET gate or a cross chip bus where metal resistance is a problem. The effect of a mask edge taper at 45° to a thickness of 3000Å is shown in

Figures 11 and 12 for Aℓ and Cu_L respectively. The Aℓ profile appears more useful. This is due to the fact that with Cu_L less than 20% of the initial flux is available at the bottom to expose the resist due to absorption. This absorption decay is apparent from the fact that the equal development time contours are closer together near the bottom. A much superior Cu_L profile can be obtained by simply doubling the flux (40 mJ/cm^2).

These surface etching simulations have given some indication of how the resist properties and configurations can effect line edge profiles. The modeling approach is contingent upon accurate resist characterizations which is an area where further work is needed. The simulation itself is easily implemented and costs about $1 per profile. The goal undertaken here was profile control in the context of low flux levels for a high throughput production environment. A savings of about a factor of five in exposure of lift-off type profiles appears possible with layered resist structures. The minimum exposure is primarily limited by the need to obtain an exposed etch rate about twice that of the masked etch rate in the top layer. The layered resist approach can be used for high aspect (3:1) ratio line profiles at about twice the dose. For Aℓ a mask edge slope of 45° severely degrades the line edge profile whereas for Cu_L the profile is only slightly changed. Line edge boradening can be compensated by relocating the mask, but the increase in linewidth over-etching sensitivity cannot be reduced. The flux required for Cu_L is about 3.8 times lower than that for Aℓ except in the case of thick resist (1μ) with high absorption ($\mu = 1.5\mu^{-1}$) where the flux must be doubled to adequately expose the bottom of the line. The advantages of layered resist for profile control at lower exposures come at the expense of extra process steps and increased sensitivity to resist properties. However, even with the added sensitivity to resist parameters, well-behaved positive resists will probably still have greater process tolerances than their negative counterparts.

References

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(8) J. R. Maldonado, G. A. Coquin, D. Maydan, and S. Somekh, "Spurious Effects Caused by the Continuous Radiation and Ejected Electrons in X-Ray Lithography," J. Vac. Sci. Tech. 12, 1329-1331 (Nov./Dec. 1975).

LIST OF FIGURES

Figure 9 Improvement in the line edge profile for the same mask and resist of Figure 8 but with Cu_L exposure. The flux has been reduced to 15 mJ/cm^2 to offset the increased resist sensitivity.

Figure 10 Layered P(MMA-MAA) for high aspect ratio lines (4000Å resist 4 over 12000Å resist 5, 70 mJ/cm^2, 4:1 mask contrast, 15 sec contours).

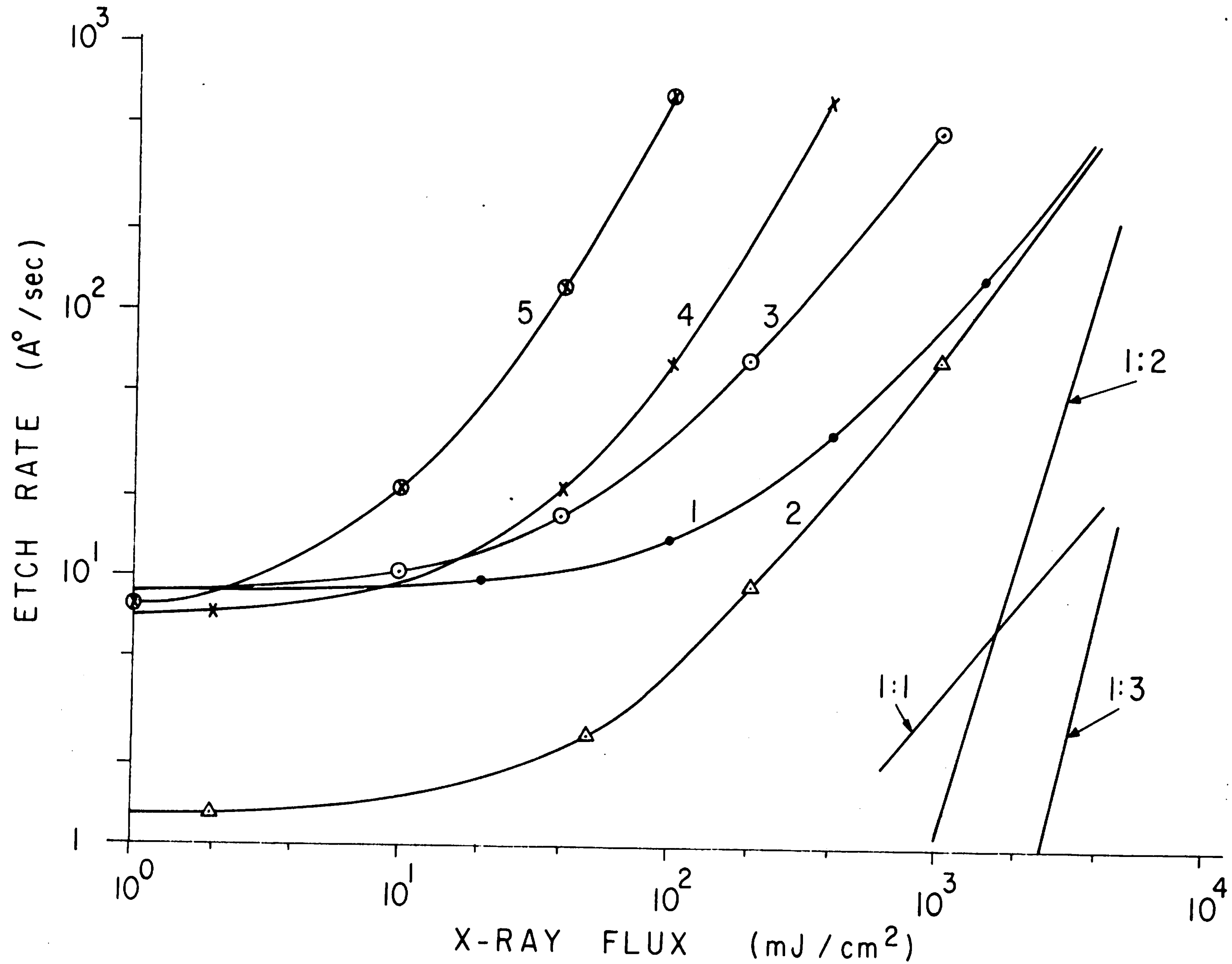
Figure 11 Effect of a 45° mask edge on a 3000Å gold mask for the resist structure and exposure of Figure 10.

Figure 12 Cu_L exposure of the same mask and resist of Figure 11. The dose has been reduced to 20 mJ/cm^2 and resist absorption effects are apparent from the decreased spacing between the contours near the bottom of the opening.

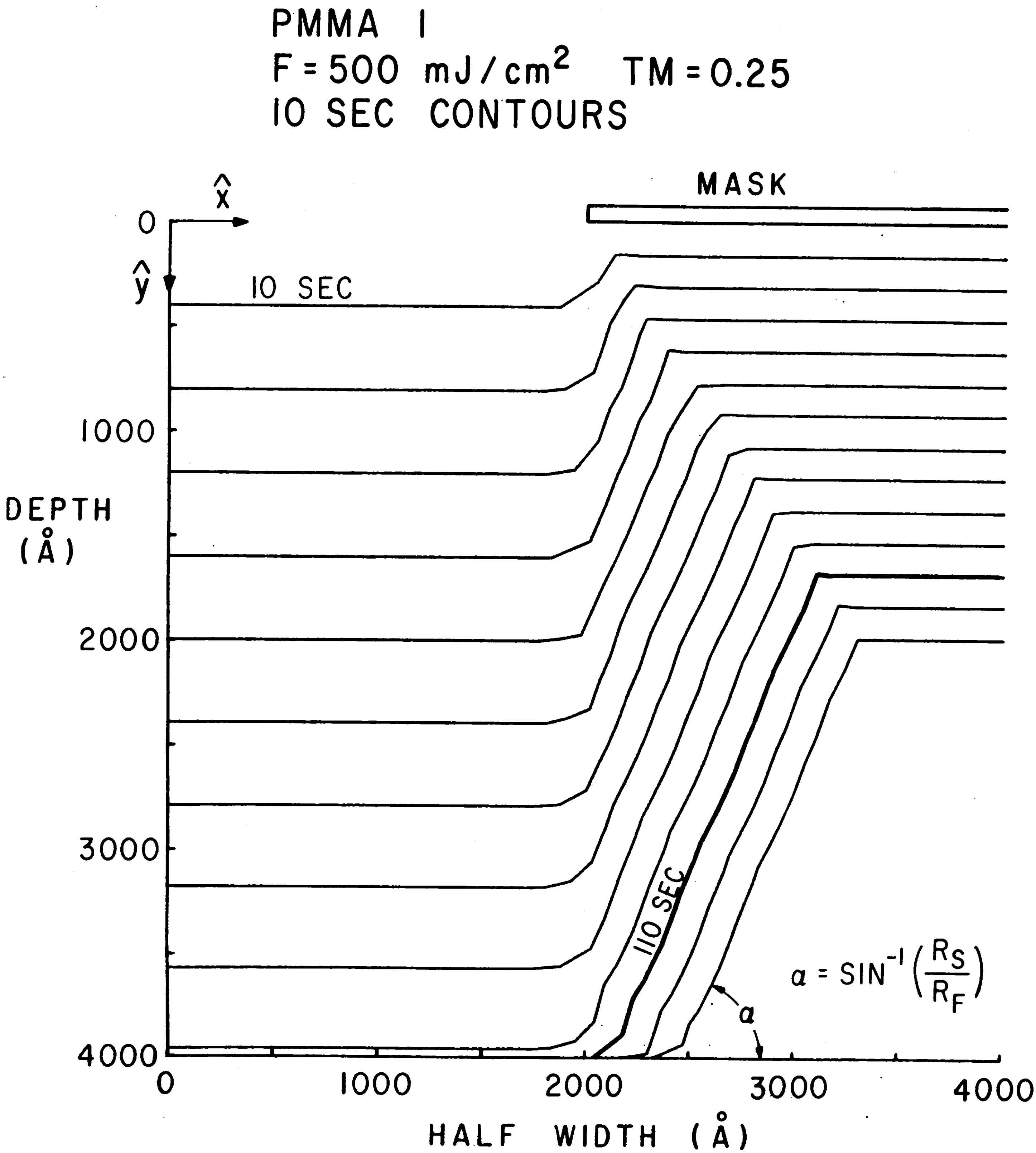
RESIST MODELS

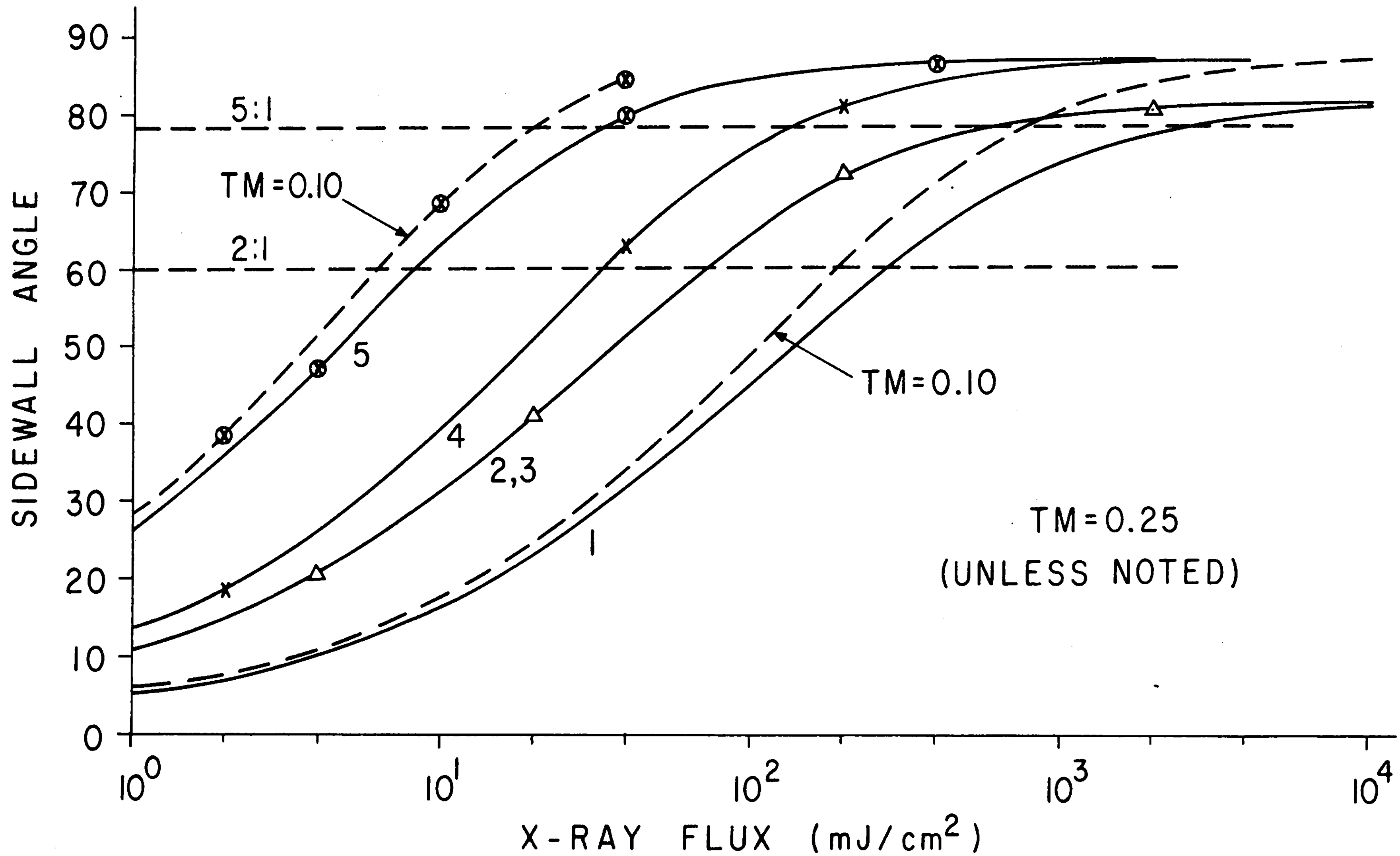
MODEL	R_{1} Å/SEC	C_M	μ CM^{-1}	D_0 J/CM^3	α	COMMENT
PMMA						
1	8.67	1.0	1000	250	1.4	HATZAKIS EXP
2	8.67	0.25	1000	250	1.4	MODIFIED M_N=2x10
3	8.67	1.0	4000	250	1.4	MODIFIED ABSORPTION
P(MMA-MAA)						
4	6.8	1.0	1000	59	2.2	SPILLER EXP
5	6.8	1.0	4000	59	2.2	MODIFIED ABSORPTION

NOTE: DATA FOR $A\ell_{K\alpha}$ AT 8.34 Å



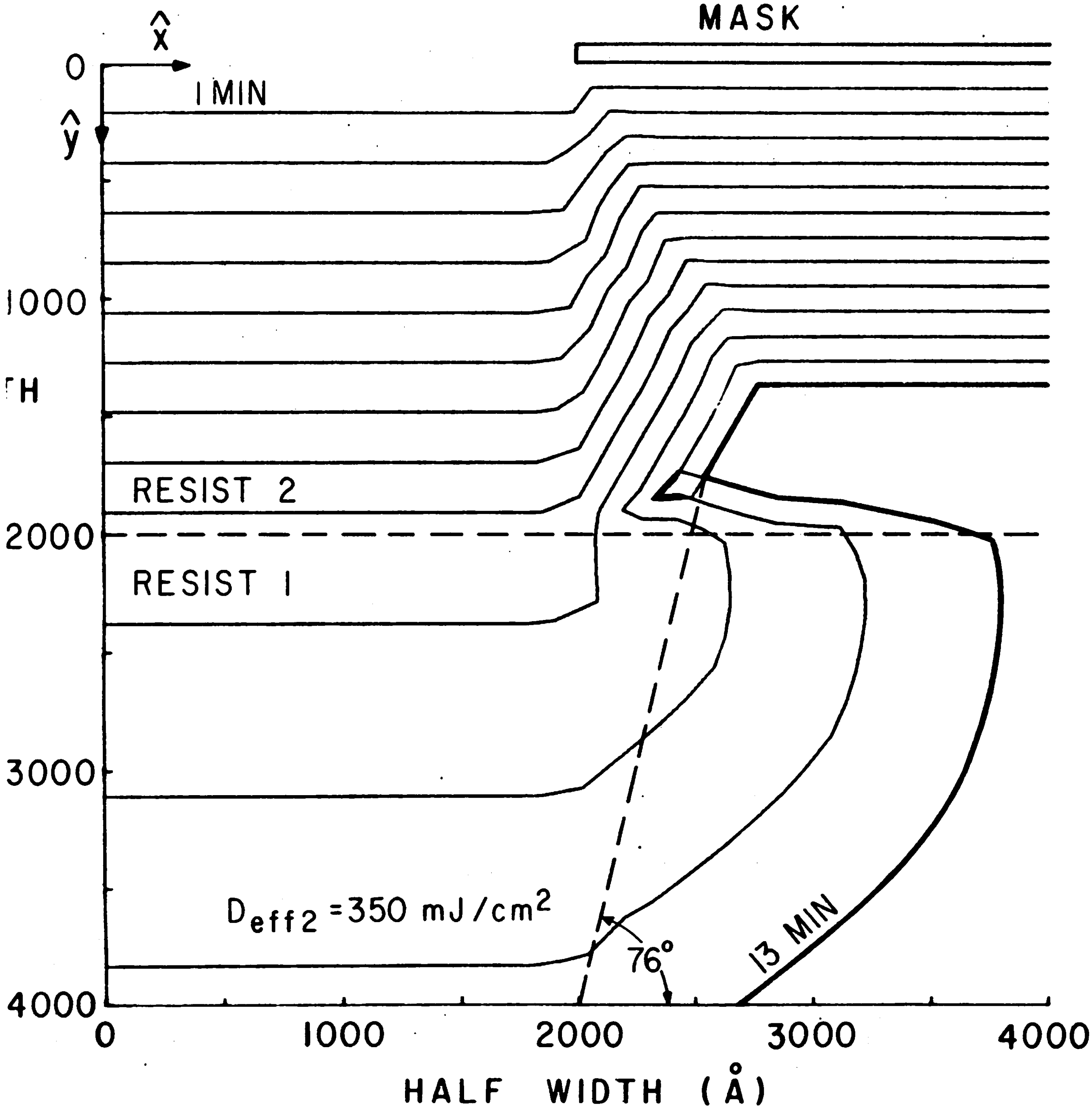
ETCH RATE (A°/sec)
X-RAY FLUX (mJ/cm²)
10³
10²
10¹
1
10⁰
10⁴
1
2
3
4
5
1:1
1:2
1:3

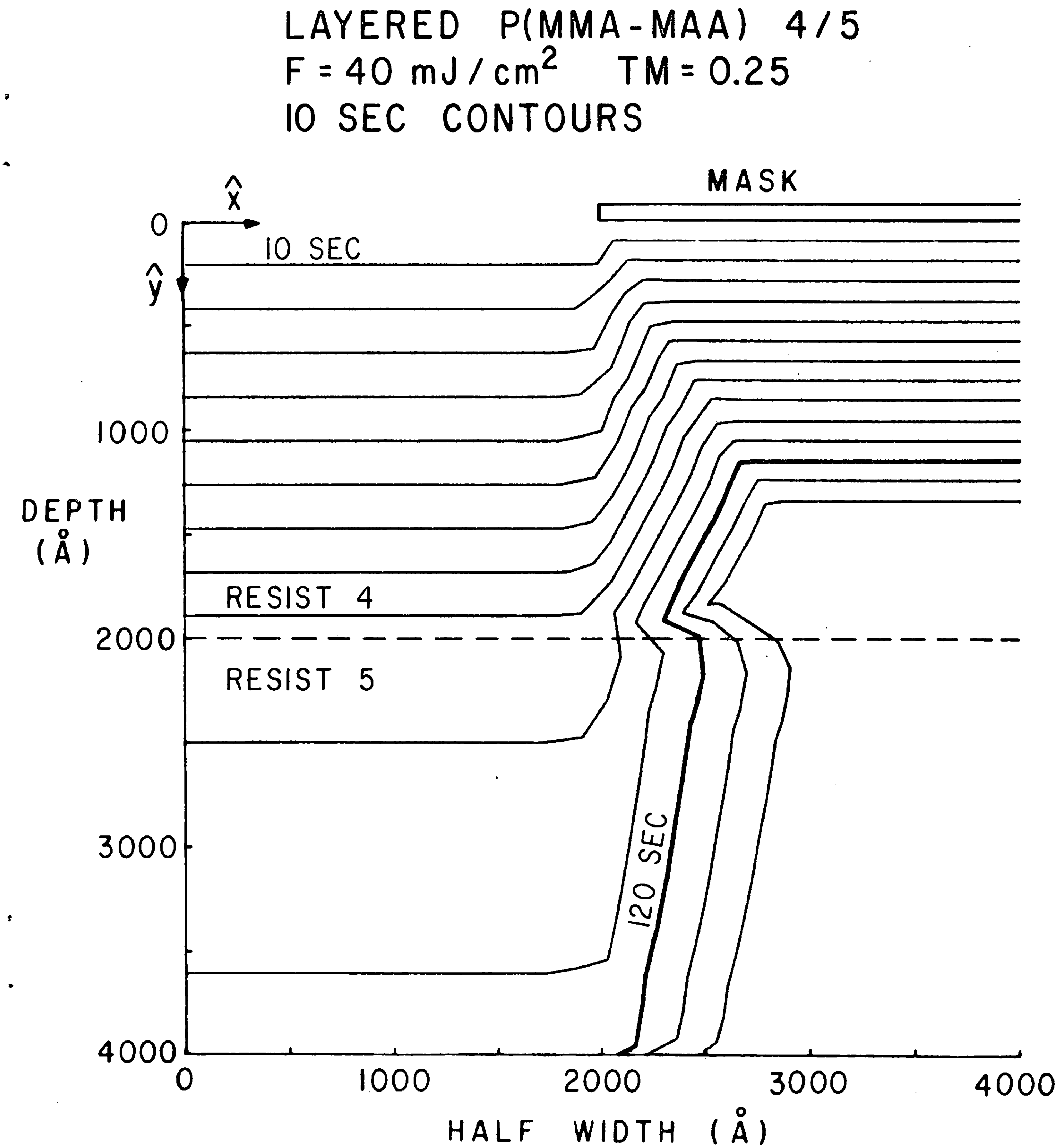

PMMA I
F = 500 mJ/cm2 TM = 0.25
10 SEC CONTOURS
MASK
10 SEC
110 SEC
DEPTH (Å)
0
1000
2000
3000
4000
HALF WIDTH (Å)
0
1000
2000
3000
4000
α = SIN-1 (RS/RF)
α

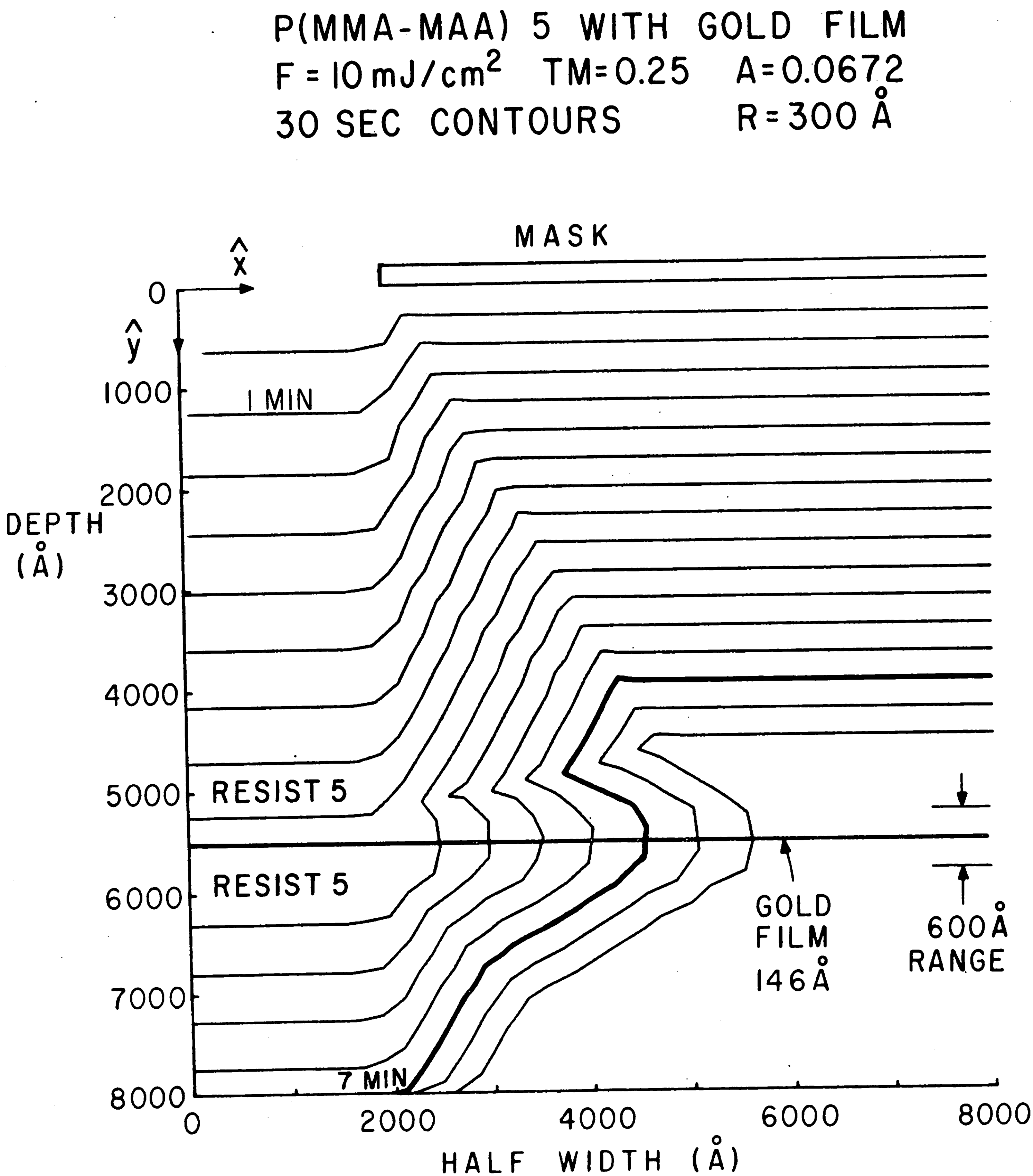

SIDEWALL ANGLE
90
80
70
60
50
40
30
20
10
0
5:1
2:1
TM=0.10
5
4
2,3
1
TM=0.10
TM=0.25
(UNLESS NOTED)
10^0
10^1
10^2
10^3
10^4
X-RAY FLUX (mJ/cm^2)

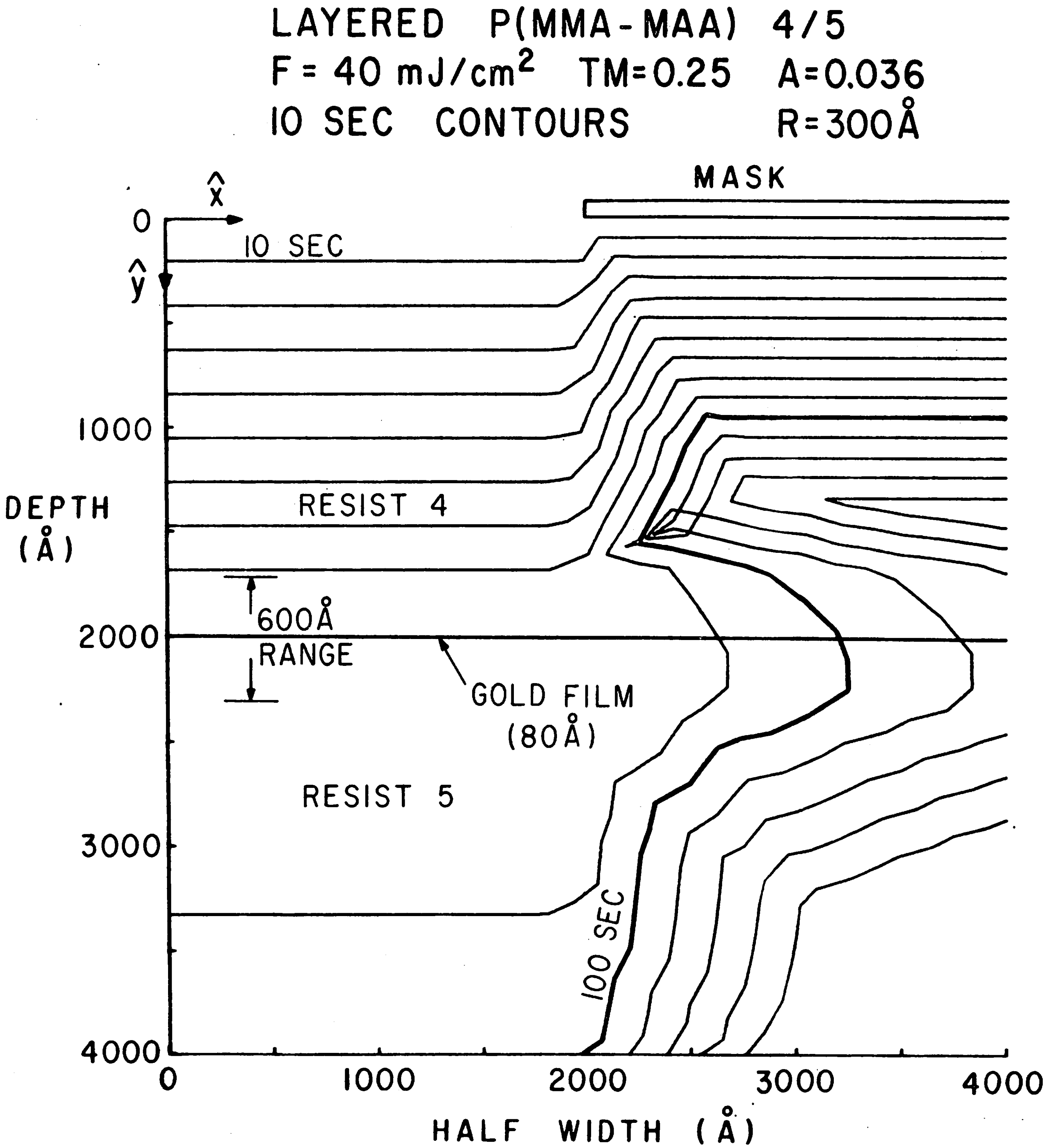
(3)

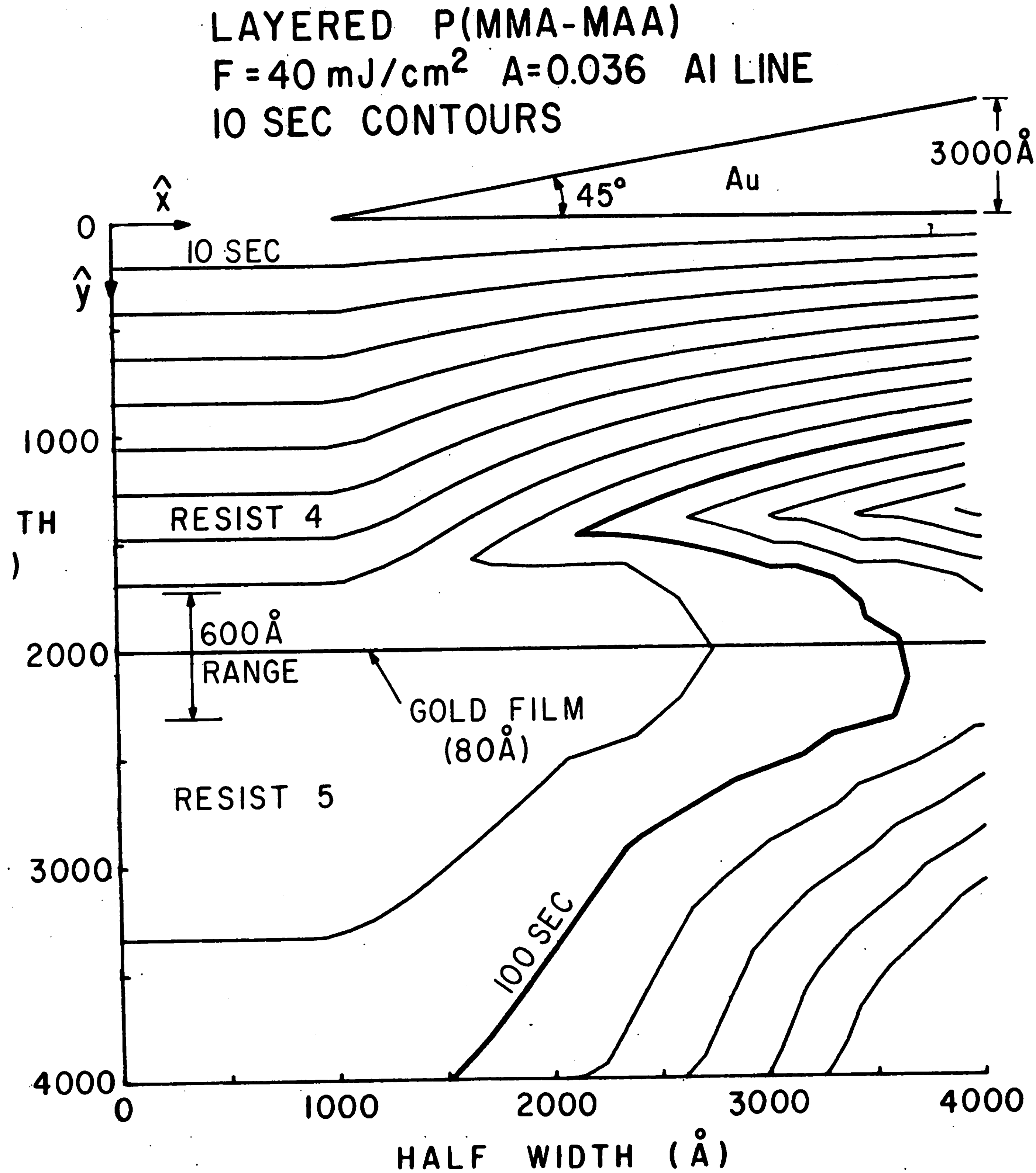
LAYERED PMMA 2/1
F = 70 mJ/cm^2 TM = 0.25
1 MIN CONTOURS




LAYERED P(MMA-MAA) 4/5
F = 40 mJ/cm2 TM = 0.25
10 SEC CONTOURS
MASK
x̂
ŷ
0
10 SEC
1000
DEPTH
(Å)
RESIST 4
2000
RESIST 5
3000
120 SEC
4000
0
1000
2000
3000
4000
HALF WIDTH (Å)

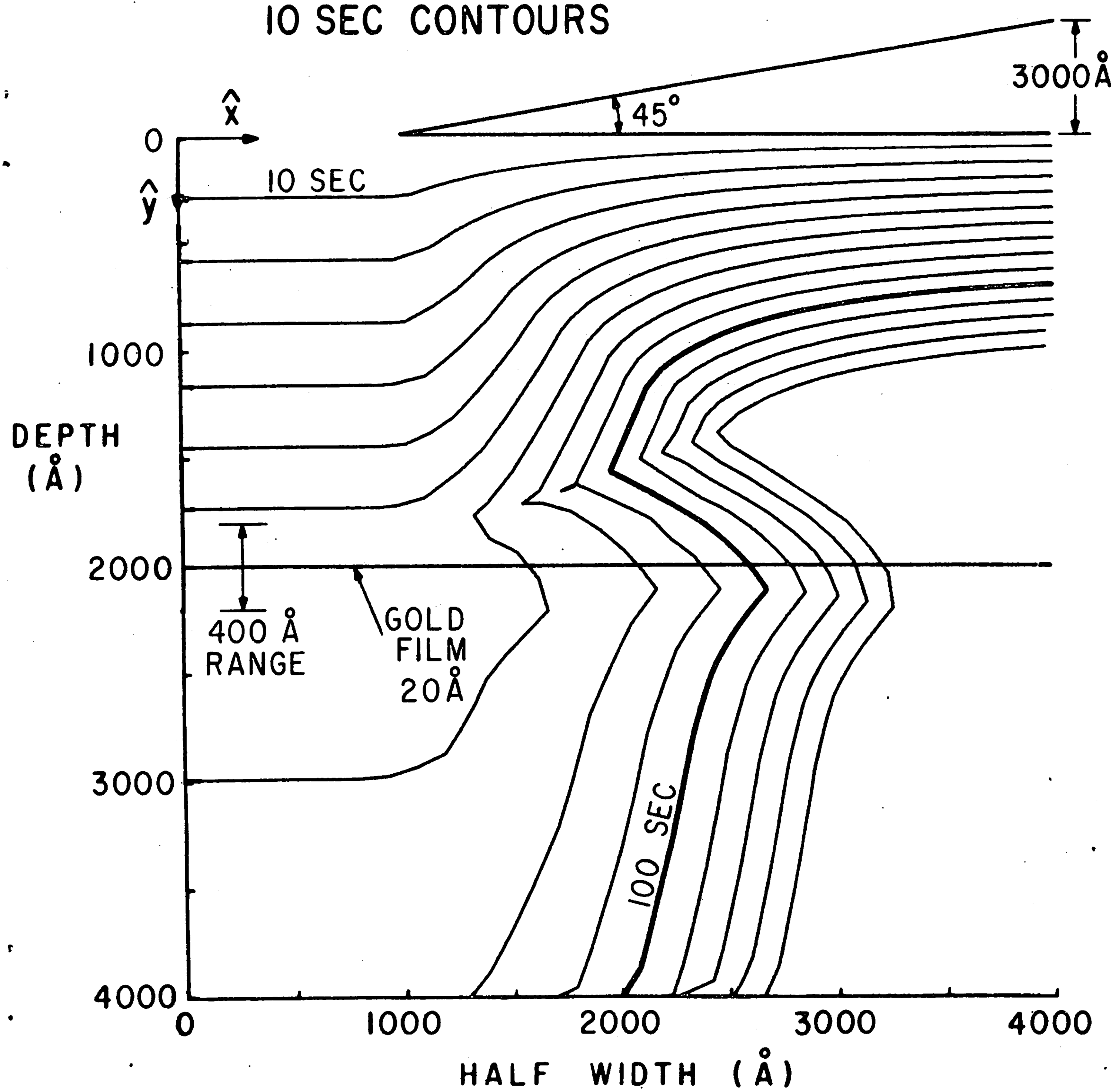

P(MMA-MAA) 5 WITH GOLD FILM
F = 10 mJ/cm2 TM=0.25 A=0.0672
30 SEC CONTOURS R=300 Å
MASK
x̂
ŷ
0
1000
2000
3000
4000
5000
6000
7000
8000
DEPTH (Å)
1 MIN
RESIST 5
RESIST 5
7 MIN
GOLD FILM 146 Å
600 Å RANGE
0
2000
4000
6000
8000
HALF WIDTH (Å)

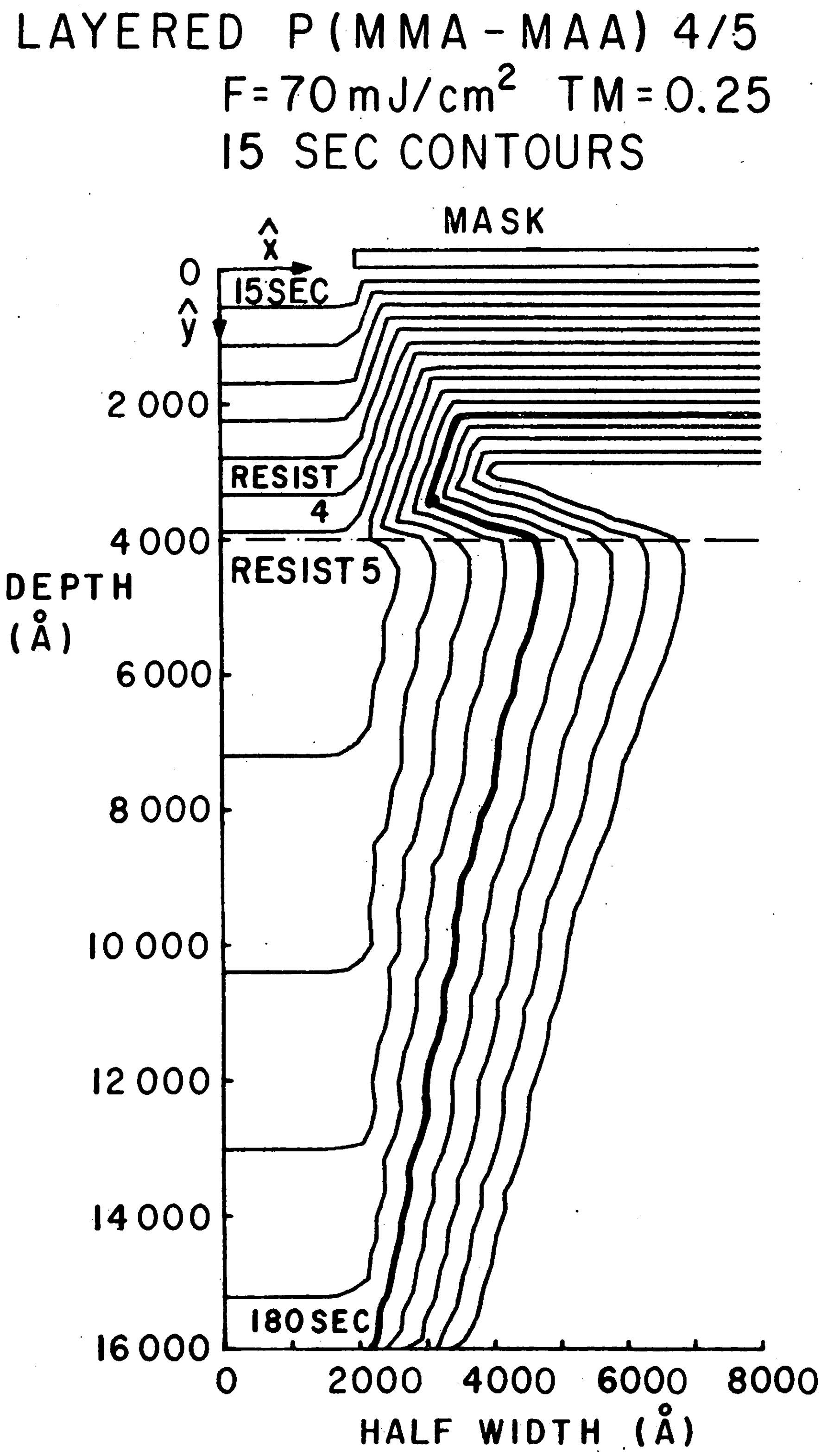

LAYERED P(MMA-MAA) 4/5
F = 40 mJ/cm2 TM=0.25 A=0.036
10 SEC CONTOURS R=300Å
MASK
x̂
ŷ
0
10 SEC
1000
DEPTH (Å)
RESIST 4
600Å RANGE
2000
GOLD FILM (80Å)
RESIST 5
3000
100 SEC
4000
0
1000
2000
3000
4000
HALF WIDTH (Å)



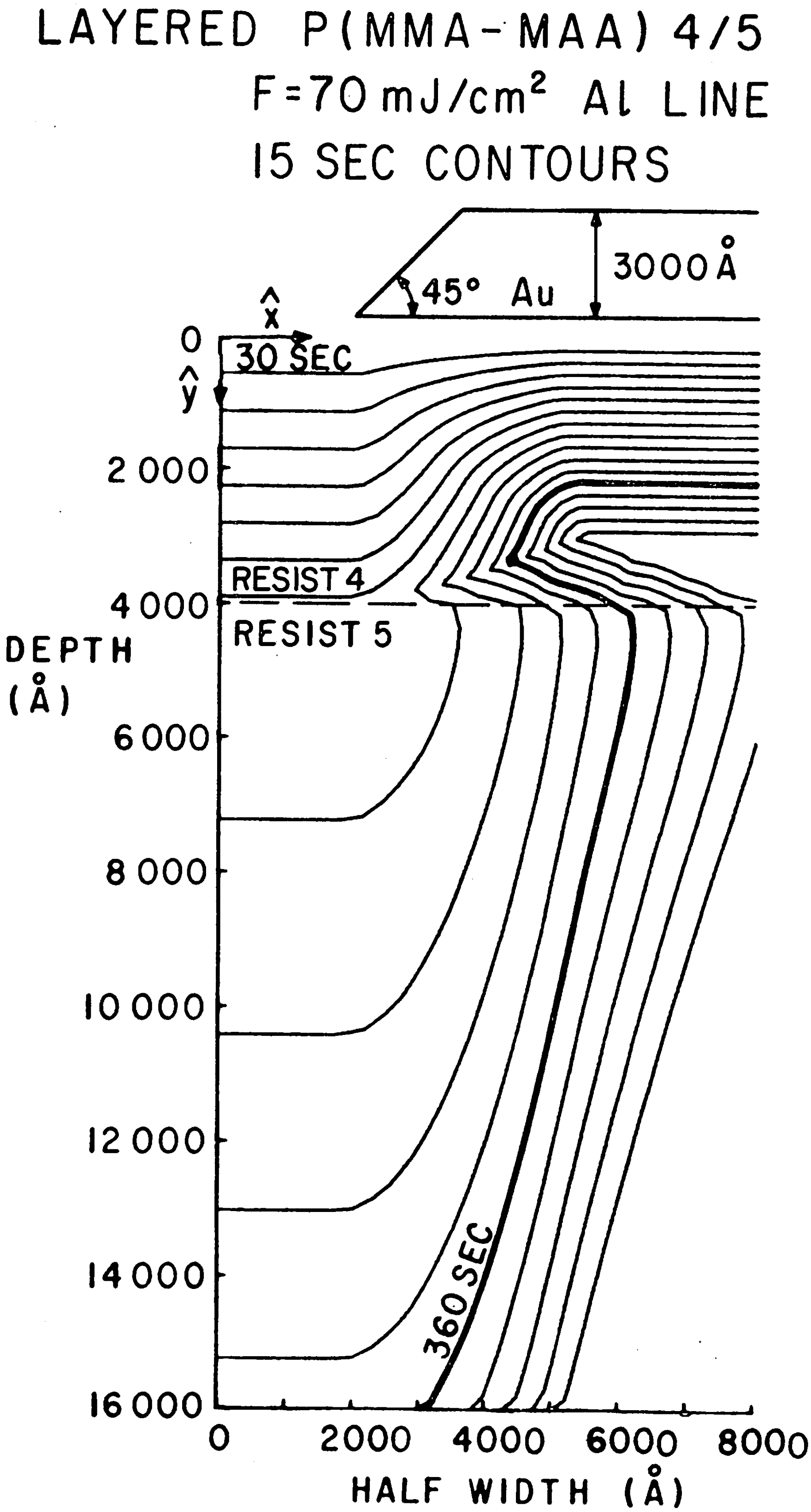
LAYERED P(MMA-MAA)
F = 40 mJ/cm2 A=0.036 Al LINE
10 SEC CONTOURS
3000Å
45°
Au
x̂
ŷ
10 SEC
RESIST 4
TH
)
600Å
RANGE
GOLD FILM
(80Å)
RESIST 5
100 SEC
0
1000
2000
3000
4000
0
1000
2000
3000
4000
HALF WIDTH (Å)

LAYERED P(MMA-MAA)
$F = 15\ mJ/cm^2$ A = 0.010 Cu LINE
10 SEC CONTOURS





LAYERED P(MMA-MAA) 4/5
F=70 mJ/cm2 TM=0.25
15 SEC CONTOURS
MASK
x̂
ŷ
15SEC
RESIST 4
RESIST 5
180SEC
DEPTH (Å)
0
2000
4000
6000
8000
10000
12000
14000
16000
0
2000
4000
6000
8000
HALF WIDTH (Å)



LAYERED P(MMA-MAA) 4/5
F=70 mJ/cm2 Al LINE
15 SEC CONTOURS
45°
Au
3000 Å
x̂
ŷ
30 SEC
RESIST 4
RESIST 5
360 SEC
DEPTH (Å)
0
2 000
4 000
6 000
8 000
10 000
12 000
14 000
16 000
0
2000
4000
6000
8000
HALF WIDTH (Å)

LAYERED RESIST P(MMA-MAA)4/5

$F = 20 mJ/cm^2$ Cu LINE

30 SEC CONTOURS