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by

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ABSTRACT

Optimization of photoresist performance in the sub-micron domain is greatly facilitated by the availability of accurate simulation algorithms for the calculation of developed resist profiles. In this paper, a new procedure for the calculation of resist profiles is described. A numerically efficient version of the WKB approximation is implemented for the determination of standing wave intensity and PAC concentration in a model resist film on both silicon and aluminum substrates. Utilizing these PAC concentration profiles, the recently proposed dissolution algorithm based on the least action principle for solvent penetration through the exposed resist film is employed to calculate developed resist profiles.

INTRODUCTION

Numerical calculation of developed positive photoresist profiles plays a key role in the optimization of photoresist performance in VLSI lithography. The two simulation algorithms SAMPLE[1] and PROLITH[2] are widely utilized to perform such calculations and facilitate the search for optimal process conditions for a given resist. Both SAMPLE and PROLITH combine Dill's model[3] for the exposure-bleaching of the resist film with the string algorithm[4] to model the process of development of the latent image in the exposed resist.

The concentration M(x,z,t′) of the photoactive compound (PAC) at any location (x,z) in the two dimensional resist film after an exposure time t′ is obtained by solving a system of coupled, nonlinear partial differential equations that constitute the Dill's model. Both SAMPLE and PROLITH obtain the function M(x,z,t′) by solving the Dill's system of equations, but with different approximation and iteration schemes.

Dill's equations have been solved analytically for the case of a matched, i.e., non-reflecting, substrate[5] and this solution has proved useful in the investigation of the CEL[6] process[7,8].

This simple solution also led to several new insights regarding resist exposure optimization[9]. The exposure-bleaching model equations for a reflective substrate have also been solved exactly[10] but the solution is very complicated. Consequently, a WKB approximation scheme has been proposed to calculate the PAC concentration profile in the resist film in the presence of standing waves[11] and a numerically efficient version of this scheme has been implemented successfully[12].

It is the purpose of this paper to describe the preliminary results of resist profile calculation in two dimensions obtained by combining the new standing waves profiles with the recently presented[13] *least action principle* algorithm for developed resist profile prediction.

LEAST ACTION PRINCIPLE FOR RESIST PROFILE PREDICTION[13]

Let R[M(x,z)] be the dissolution rate of the exposed photoresist at any location (x,z). Then along any development path inside the resist,

$$t = \int_0^{s_f} \frac{ds}{R[M\{x(s), y(s)\}]} \tag{1}$$

where t is the development time and s is the arc length of the development trajectory measured from the initial resist surface. Thus s_f is the final length reached by the trajectory at the end of the development time t. During resist development the trajectory followed by the solvent starting from any arbitrary location on the resist surface must be such that the development time t is a minimum. This requirement leads to the following system of ordinary differential equations for the co-ordinates x(s) and y(s) of the solvent trajectory.

$$\frac{d^2x}{ds^2} = \frac{\partial logR}{\partial x}(\frac{dx}{ds})^2 + \frac{\partial logR}{\partial z}(\frac{dx}{ds})(\frac{dz}{ds}) - \frac{\partial logR}{\partial x} \tag{2}$$

$$\frac{d^2z}{ds^2} = \frac{\partial logR}{\partial x}(\frac{dx}{ds})(\frac{dz}{ds}) + \frac{\partial logR}{\partial x}(\frac{dz}{ds})^2 - \frac{\partial logR}{\partial z} \tag{3}$$

The solution of this pair of differential equations for various initial trajectory starting points on the resist surface z=0 for a fixed development time t yields the final developed

resist profile. The algorithm used for the solution of these equations contains the following steps:

1. Start with an initial profile, say z=0 for all x.

2. Develop each point, proceeding normal to the initial profile, for a time Δt using the two differential equations (2) and (3). Δt is chosen small enough that no two adjacent paths cross each other.

3. The new profile is used as the initial profile and the process is repeated.

The maximum allowable time interval Δt is determined by the curvature of the profile and the requirement that individual rays may not cross. Crossing rays would lead to either shock waves or a non-unique solution.

Implementation of this algorithm requires prior knowledge of the function M(x,z,t′) and R[M(x,z,t′)], where t′ is the specified exposure time. R[M] is obtained phenomenologically by fitting experimentally measured dissolution rate data. Calculation of M(x,z,t′) in the presence of standing waves is described briefly in the next section.

PAC CONCENTRATION PROFILE

The exact solution[10] of Berning's equation[14] for a thin photoresist film is very complicated and difficult to implement numerically. An approximation scheme has been developed based on a steepest descent analysis which resulted in a functional relation between the PAC concentration M and the electric field in the resist[10,11]. The classical WKB approximation[15] has been used to solve the Maxwell equation for the electric field E(x,z,t′) in the resist film.

$$\frac{\partial^2}{\partial z^2} E(x,z,t') = -\left[\frac{2\pi N(x,z,t')}{\lambda}\right]^2 E(x,z,t') \tag{4}$$

Here N(x,z,t′) is the complex refractive index of the photoresist defined as N = n - iK, where n is the real part of the refractive index and K is given by

$$K = \frac{\lambda}{4\pi}(AM + B) \tag{5}$$

Here A and B are the usual Dill's parameters for the photoresist and λ is the wavelength of the exposing radiation. The field equations for $z \leq 0$ and $z \geq D$, where D is the location of the resist- substrate interface, are obtained by replacing N with the refractive index of the ambient, n_a, and of the substrate, N_s, respectively.

Solving these equations and applying the continuity conditions for the electric field at the resist-air and resist-substrate interface, the electric field can be expressed[11] in terms of the PAC concentrations M(x,0,t') and M(x,D,t') and one global property of M, namely $\int_0^D M(x,z,t')dz$.

$$\begin{aligned} E(z,t) &= \frac{2n_a A_1}{n_a + N(0,t)} \left[\frac{N(0,t)}{N(z,t)}\right]^{\frac{1}{2}} \\ &\times \left\{1 + \left[\frac{n_a - N(0,t)}{n_a + N(0,t)}\right]\left[\frac{N(D,t) - N_s}{N(D,t) + N_s}\right] e^{-2iD\delta(t)}\right\}^{-1} \\ &\times \left\{e^{-i\frac{2\pi}{\lambda}\int_0^z N(z',t)dz'} + \left[\frac{N(D,t) - N_s}{N(D,t) + N_s}\right] e^{i\left[\frac{2\pi}{\lambda}\int_0^z N(z',t)dz' - 2D\delta(t)\right]}\right\} \end{aligned} \tag{6}$$

For simplicity, the co-ordinate x is suppressed from the arguments in the functions above. A_1 is related to the incident intensity I_0 by $I_0 = |A_1|^2$ and δ(t) is defined as

$$D\delta(t) = \frac{2\pi}{\lambda}\int_0^D dz N(z,t). \tag{7}$$

Substitution of the field equations into the Dill's kinetic equation for M provides a self-contained system of ordinary differential equations for the time evolution of the PAC concentration.

A numerically efficient version of the WKB approximation scheme has been implemented and will be described in detail elsewhere[12]. Briefly, a simultaneous solution of the second order differential equation for the electric field in the resist film and Dill's kinetic equation for M is generated. An initial iterate for the PAC concentration profile is obtained. Each iteration then consists of a one-dimensional finite element scheme to solve for a new electric field followed by a Runge-Kutta scheme to calculate the next iterate for M.

This algorithm converges extremely rapidly. Furthermore, it is conceptually and practically implementable in three dimensions. The three dimensional PAC concentration profiles are being combined with a three dimensional dissolution algorithm to provide realistic 3-D resist profile simulation in the near future.

The algorithm described above has been tested in two dimensions for both silicon and aluminum substrates. In both cases, the WKB approximation is found to be extremely accurate. Even after two iterations the numerical values of the PAC concentration have hardly changed. In fact, the only significant changes in the values of M occurred around the first two maxima, and even there the changes are only of the order of 2% to 3%.

The results of the calculations are presented in Figures 1 and 2 at two different x locations for silicon and aluminum substrates. The photoresist investigated is a model resist studied by Mack using PROLITH. It is used here only for demonstration purposes. The resist and exposure parameters are listed in Table 1.

IMPLEMENTATION AND RESULTS

The initial profile is taken as the x-axis, with 51 equally spaced points. A specific Runge-Kutta scheme is developed for the system of five ordinary differential equations that include the two coordinates, their arclength derivatives and the development time. For most processes tested, an average development time step, Δt, in the range of 0.03 to 0.05 sec has been found to be satisfactory. After each time step an optimizing cubic spline routine was implemented, resulting in a smooth representation of the profile. The new profile is divided into segments of equal arclength in order to maintain consistency with the previous profile. Thus the number of segments varies according to the shape of the profile. This process is repeated until the prescribed development time has elapsed.

Two dimensional profiles can be expressed either explicitly as functions of the coordinates[13] or parametrically. The profiles described here are obtained using parametric representation which also permits implementation in three dimensions.

The PAC concentration profiles on silicon and aluminum substrates have been calculated as described earlier. The dissolution rate function R(M) employed in this study has been proposed by Mack[16] and has the following parameters: R_{max} = 200 nm/s, R_{min} = 1 nm/s, m_{TH} = 0.5, and n = 5. Figure 3 illustrates the relative development rate as a function of the normalized PAC concentration.

The calculated profiles are presented in Figure 4 for a silicon substrate for development times of 30s, 45s, and 60s. Figure 5 contains the profiles calculated for an aluminum substrate. The bleaching of the resist film is significantly reduced due to the reflectivity at the valleys in the standing wave intensity distribution as can be seen from Figures 1 and 2. Consequently, clearing the space requires longer development times. Profiles obtained after 80s, 100s, and 120s are shown in Figure 5. The time step, Δt, used in obtaining these profiles is 0.03s.

SUMMARY AND CONCLUSIONS

A new procedure for the calculation of two dimensional resist profiles is described based on the least action principle. The requisite PAC concentration profiles have been obtained using a numerically efficient version of the WKB method. The algorithm has been tested for both silicon and aluminum substrates and it converges very rapidly. In both cases, the WKB approximation is found to be extremely accurate. Furthermore, both the dissolution and exposure algorithms are being extended to provide comprehensive three-dimensional profile simulations [17].

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REFERENCES

1. W.G. Oldham, S.N. Nandgaonker and A.R. Neureuther, "General simulator for VLSI lithography and etching processes: Part 1 - Application to projection lithography", IEEE Trans. Electron Dev., Ed-26, 717 (1979).

2. C.A. Mack, "PROLITH: A comprehensive optical lithography model", Optical Microlithography IV, Proceedings of SPIE, Vol. 538, 207 (1985).

3. F.H. Dill, "Optical lithography", IEEE Trans. Electron Dev., Ed-22, 440 (1975).

4. R.E. Jewett, P.I. Hagouel, A.R. Neureuther and T. Van Duzer,"Line-profile resist development simulation techniques"Poly. Engg. and Sci., 17, 381 (1977).

5. S.V. Babu and E. Barouch, "Exact solution of Dill's model equations for positive photoresist kinetics", IEEE Electron Dev. Lett., EDL-7, 252 (1986).

6. B.F. Griffing and P.R. West, "Contrast enhanced lithography", Solid State Technol., 28(5), 152 (1985)

7. W.G. Oldham, "The use of contrast enhancement layers to improve the effective contrast of positive photoresist", IEEE Trans. Electron Dev., ED-34, 247 (1987).

8. R.A. Ferguson, P.R. West and A.R. Neureuther, "Optimization of contrast enhanced lithography with SAMPLE", KTI Symposium Proceedings, (1987).

9. C.A. Mack, "Understanding focus effects in submicron optical lithography", in Optical Laser Microlithography, vol 922, SPIE Symposium Proceedings (1988).

10. S.V. Babu and E. Barouch, "An exact solution for the optical absorbance of thin films", Studies in App. Math., 77, 173 (1987).

11. S.V. Babu and E. Barouch, "Standing waves in optical positive photoresist films: A new approach", J. Opt. Soc. Am. 5, 1460 (1988).

12. B.D. Bradie, E. Barouch and S.V. Babu, "Calculation of photoactive compound profiles in the presence of standing waves", submitted to J. Vac. Sci. and Tech.

13. E. Barouch, B.D. Bradie and S.V. Babu, "Resist development described by least action principle - line profile prediction", J. Vac. Sci. and Tech. (in press); presented at the 32nd

IEEE International Conf. on Electron, Photon and Ion Beams, Fort Lauderdale, June 1988.

14. P.H. Berning, "Theory and calculations of optical thin films", in Physics of Thin Films, Vol 1, pp. 69, G. Hess (Editor), Academic Press (1963).

15. WKB approximation is discussed in many textbooks on quantum mechanics: see for example Quantum Mechanics by L.I. Schiff, McGraw-Hill Book Co.,Inc., New York 1955.

16. C.A. Mack, "Development of positive photoresists", J. Electrochem. Soc., 134, 148 (1987).

17. S.V. Babu, E. Barouch, and B. Bradie, Abstract submitted to SPIE Microlithography Conference, 1989.

Table 1

Resist parameters:

$A = 0.6\ \mu m^{-1}$

$B = 0.1\ \mu m^{-1}$

$C = 0.02\ cm^2/mJ$

refractive index = 1.65

thickness = 1.00 μm

Exposure parameters:

Wavelength = 436 nm

$NA_o = 0.35$

coherence = 0.5

defocus = 0.0 μm

Pattern = space

Width = 1.00 μm

Pitch = 2.00 μm

energy = 80 mJ/cm^2

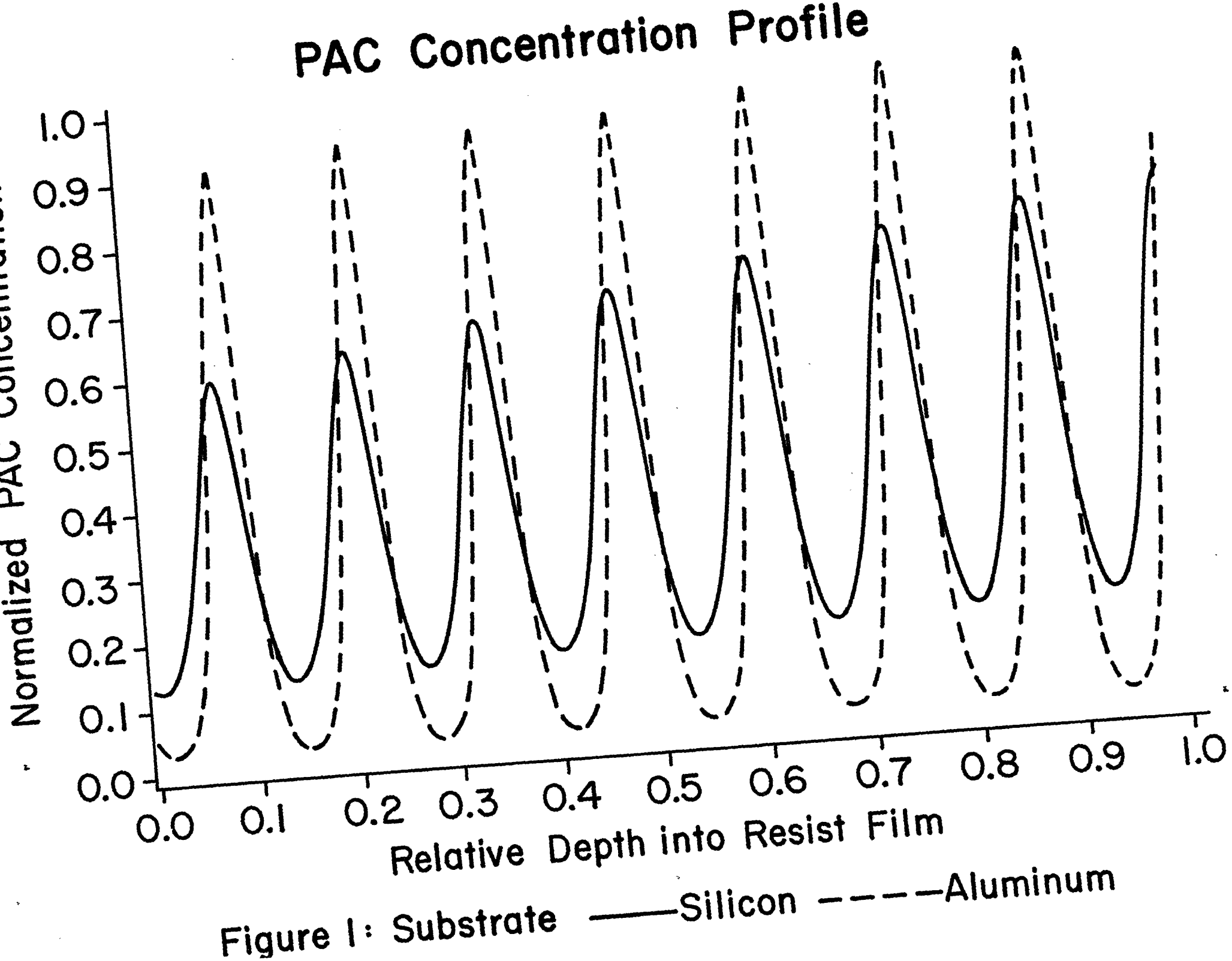

Figure 1: Substrate

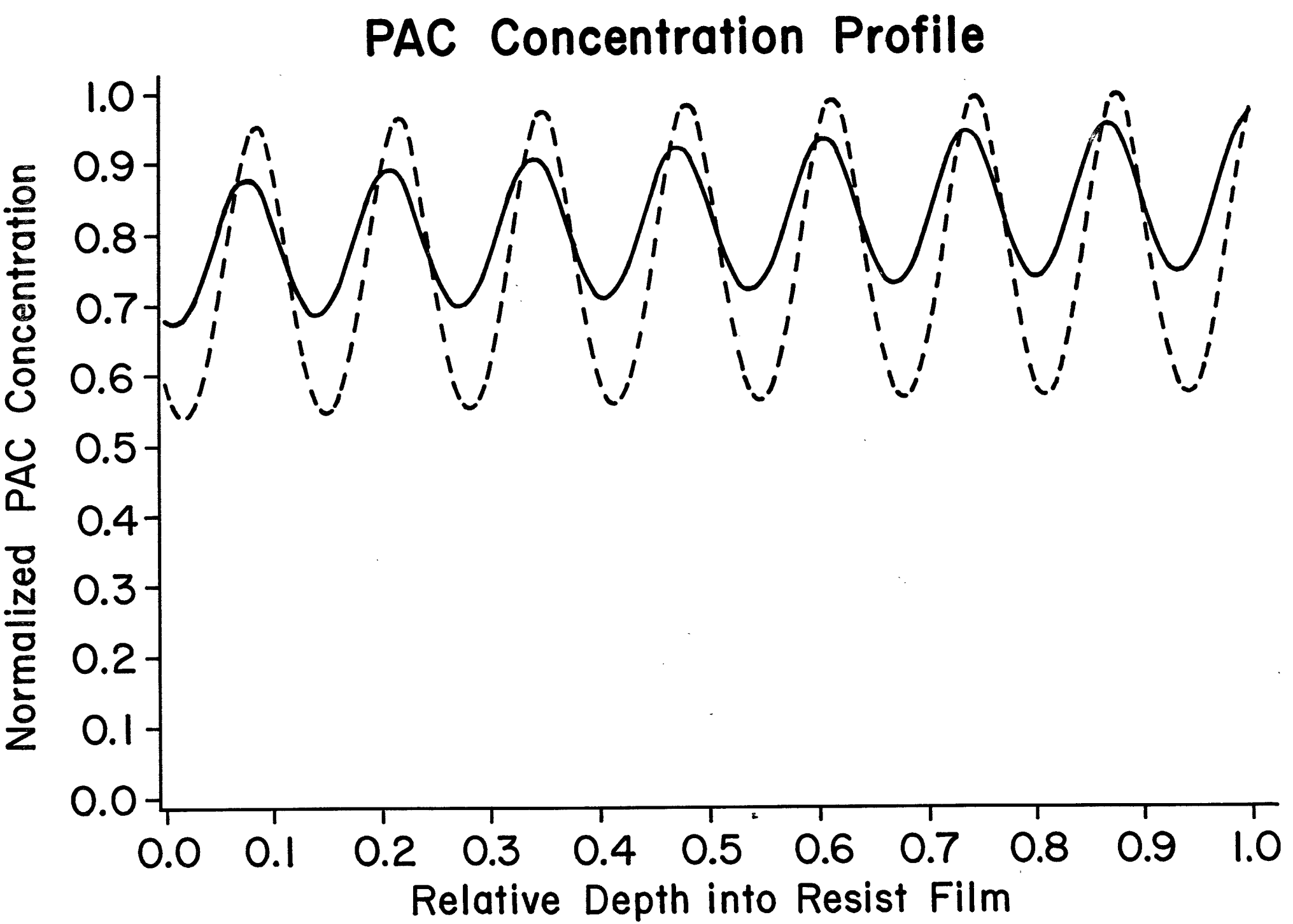

Figure 2: Substrate ——Silicon ----Aluminum

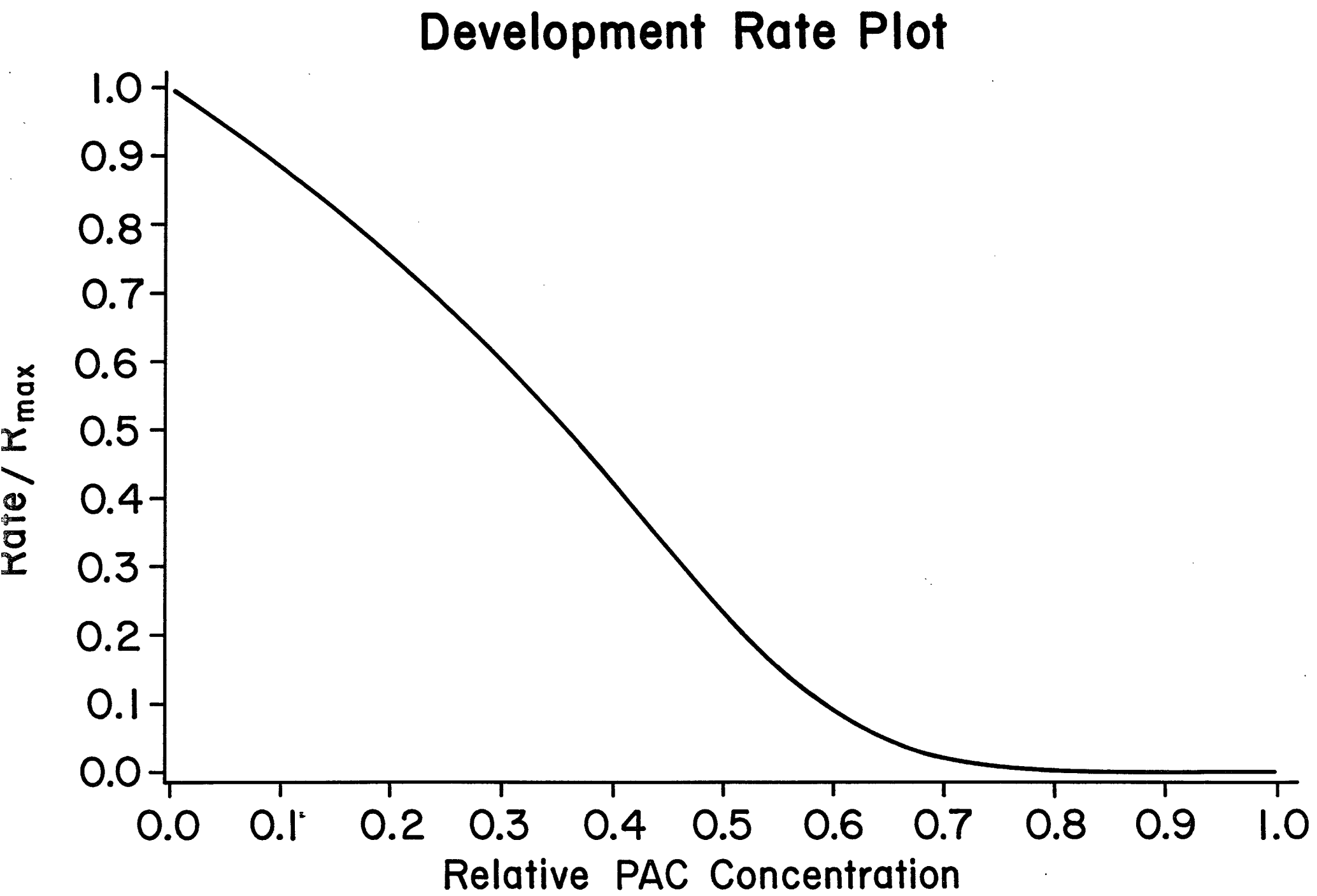

Figure 3: Dissolution rates calculated using Mack model

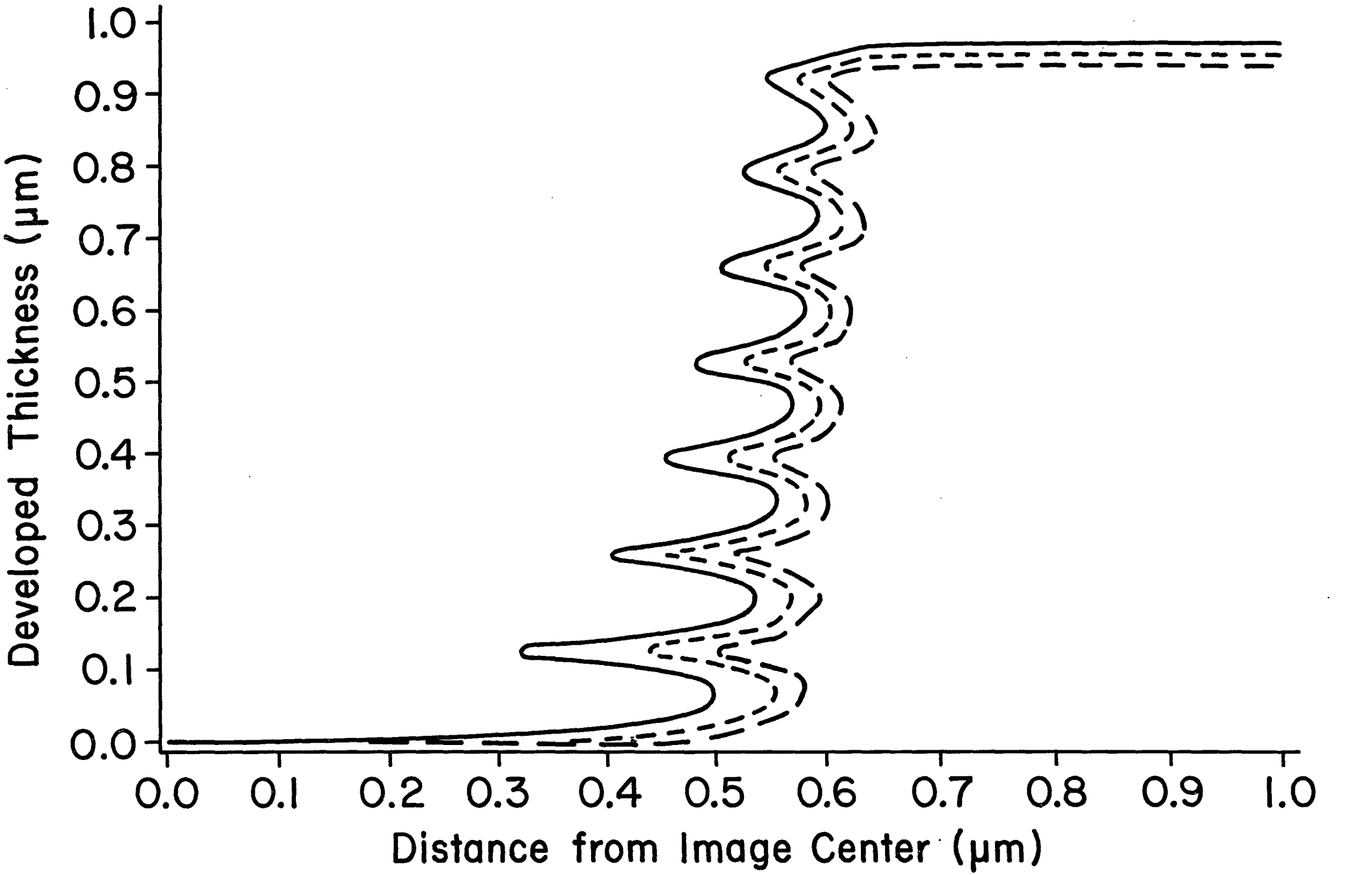

Figure 4: Development times ——30sec ----45sec — — —60s

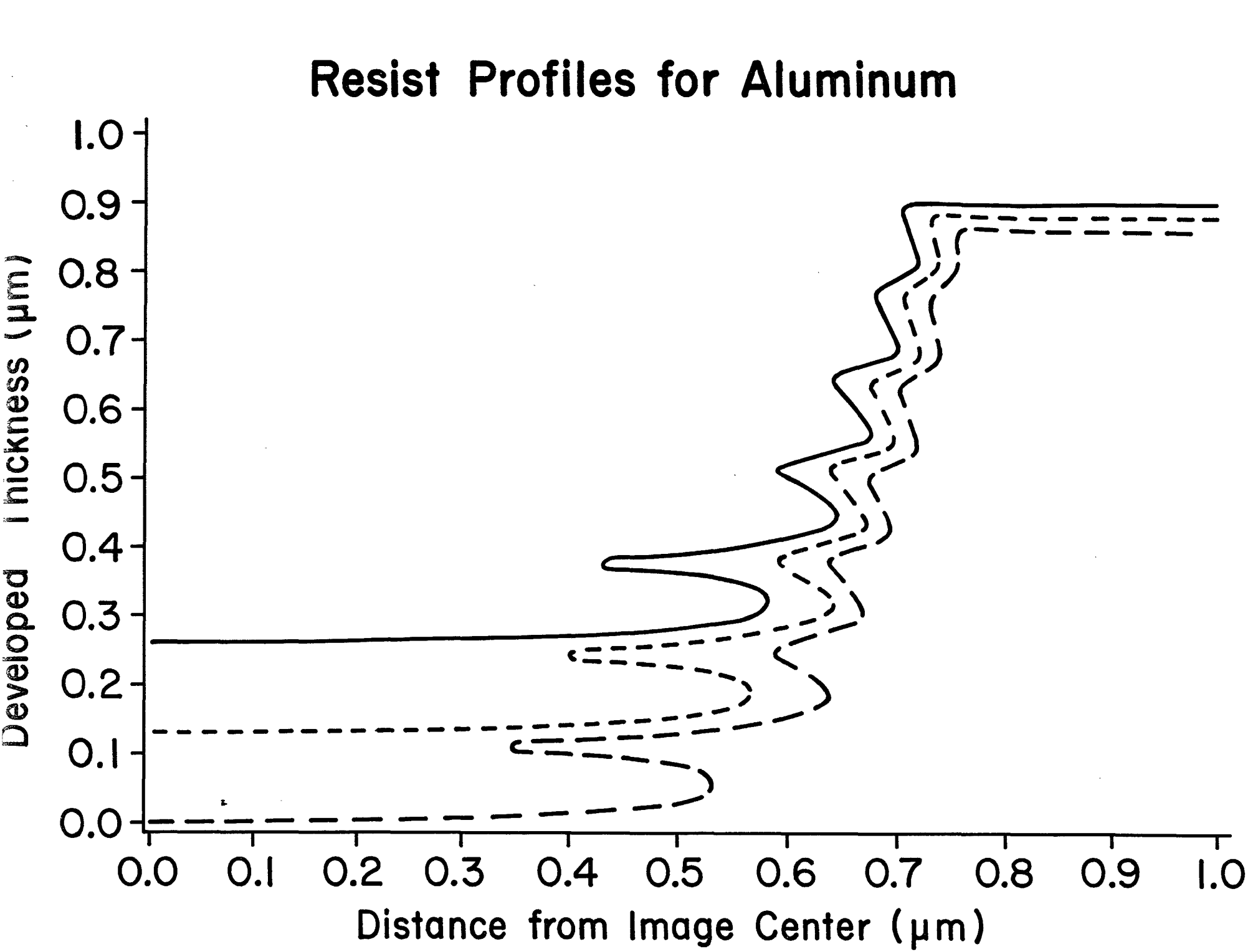

Figure 5: Development times ——100sec - - - -120sec — — —140s