

REPORT

Assessment of Simple Models of the Cracking of Coatings Strained Under Tension

G Damerell

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National Physical Laboratory
Teddington, Middlesex TW11 0LW, UK

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Approved on behalf of Managing Director, NPL, by Dr M K Hossain,
Director, Centre for Materials Measurement & Technology.

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1 INTRODUCTION

Protection of materials from wear and corrosion has a major impact in the engineering and power generation industrial sectors. When thermal cycles are imposed on a substrate-coating system, stresses will be generated in the system if the two materials have different thermal expansion coefficients, for example, a metal and its oxide. The resistance of such a system to spallation is related to the strength of the interface between the substrate and the coating. There are various methods of measuring this. One such is to strain a sample in tension, and then model the resultant cracking and/or spallation.

This work attempts to assess the mathematics of various models of cracking in tension. The models are summarised and data for nickel oxide on nickel is used in each model to calculate the interfacial shear strength. Nickel oxide is a simple, one layer oxide which should correspond reasonably well with the ideal coatings used in the models, especially since the thermal expansion coefficients of nickel and nickel oxide are very similar, so very little thermal stresses are generated while cooling from growth to test temperature. The models are then analysed for their mathematical basis, validity of assumptions made, and validity of the results they give with the data for nickel oxide on nickel.

2 DESCRIPTION OF MODELS

2.1 MODEL 1: CALCULATION OF INTERFACIAL SHEAR STRENGTH FROM THE LONGITUDINAL STRAIN REQUIRED FOR INTERFACIAL DEBONDING

Ollivier and Matthews [1] assessed the model of Ting et al [2] which ignores the length of the segments occurring in the film when subjected to strain and instead considers the strain required for debonding. After finite element analysis, the shear stress is approximated by a curve, as in Figure 1, where τ_m is the maximum shear stress. It is assumed that

$$|\tau_m| = \epsilon \sqrt{\frac{E^c \cdot b \cdot G^s}{a}} F(\xi_1) \quad (1)$$

where

- ϵ is the longitudinal strain in the substrate
- E^c is the Young's modulus of the coating
- G^s is the modulus of rigidity of the substrate
- b is the thickness of the film
- a is the thickness of the substrate
- $F(\xi_1)$ is a stress distribution parameter to be found.

$$G^s = \frac{E^s}{2(1+\nu^s)}$$

where E^s is the Young's modulus of the substrate and ν^s is the Poisson's ratio of the substrate.

$F(\xi_1)$ is determined from

$$F(\xi_1) = \left[\frac{C-2}{2} \xi_1^{\frac{2(C-1)}{C-2}} - \frac{C}{2} \xi_1^2 + \xi_1 \right]^{1/2} \quad (2)$$

where ξ_1 is the root of the polynomial

$$(C-1) \xi^{\frac{C}{C-2}} - C \xi + 1 = 0 \quad (3)$$

and

$$C = \frac{E^s \cdot a}{E^c \cdot b} \quad (4)$$

When the film debonds under a certain strain ϵ_o , it is possible to calculate the maximum shear stress and it can be assumed that this is the interfacial shear strength τ_o .

However, the induced cracks in the coating change the length, L , of the coating. The influence of L on the interfacial shear stress is shown in a term $\tanh\left(\frac{\beta L}{2}\right)$ which is replaced by unity in eq (1)

$$\beta = \sqrt{\frac{G^s}{ab E^c}} F(\xi_1) \quad (5)$$

and is normally very large for thin coatings, and therefore the correction term is taken to be unity except if $\frac{\beta L}{2} < 3$ ($\tanh 3 = 0.995$) because the value of L then begins to have an effect on τ_o . However, in most thin coatings the correction term can be replaced by unity.

Parameters Needed

Young's moduli of both
Thickness of both
Longitudinal strain in substrate
Poisson's ratio of substrate.

2.2 MODEL 2: CALCULATION OF INTERFACIAL SHEAR STRENGTH FROM THE LIMITING CRACK SPACING

Ollivier and Matthews [1] also assessed the model put forward by Armitt *et al* [3] which assumes that the tensile strain in the coating ϵ^c is:

$$\epsilon^c = \epsilon + Ae^{y/\lambda} + Be^{-y/\lambda} \quad (6)$$

where

$$\lambda = b(1 + \nu^c)^{1/2} \quad (7)$$

where b is the coating thickness, ν^c is the Poisson's ratio of the coating.

$$\epsilon^c = 0 \text{ when } y = \pm L \quad (8)$$

as in Figure 2.

$$\epsilon^c = \epsilon \left[1 - \frac{\cosh y/\lambda}{\cosh L/\lambda} \right] \quad (9)$$

ϵ_k is the critical strain needed for failure at $y = 0$.

$$\epsilon_k = \epsilon \left[1 - \frac{1}{\cosh L/\lambda} \right] \quad (10)$$

so, for a given applied strain, ϵ , the crack spacing, $2L$, can be found if ϵ_k is known. Or, if crack spacing and applied strain are known, ϵ_k can be found.

It is then assumed that the maximum strain which can be sustained at the middle of an island of oxide is related to the interfacial shear stress as follows:

$$\epsilon_{\max} = \frac{L\tau_o}{bE^c} = \epsilon_k \quad (11)$$

$$\therefore \tau_o = \frac{\epsilon_k bE^c}{L} \quad (12)$$

where τ_o is the interfacial shear strength, E^c is the elastic modulus of the coating.

All that remains is to find ϵ_k , the critical strain for failure. It is assumed to be

$$\epsilon_k = \sqrt{\frac{0.5\gamma}{E^c \cdot d}} \quad (13)$$

where γ is the fracture surface energy density, d is the flaw size of the initial flaw.

Armitt *et al* suggest that γ/E^c has been shown to be about $0.4 \text{ \AA}$ for a range of ceramic materials.

Parameters needed

Crack spacing - minimum at the point of spallation

Thickness of coating

Elastic modulus of coating

critical strain for failure

- can be found from
 - 1) fracture surface energy density
flaw size of initial crack
 - 2) applied strain
Poisson's ratio of coating

2.3 MODEL 3: CALCULATION OF INTERFACIAL SHEAR STRENGTH FROM THE LENGTH OF THE LONGEST DEBONDED SEGMENT

The model of Wheeler and Osaki [4] (also assessed by Ollivier and Matthews [1]) begins by stating that under tensile strain, an interfacial shear stress $\tau(y)$ is produced. While the film is bonded to the substrate, the shear stress $\tau(y)$ at the interface causes a tensile stress $\sigma(y)$ in the film. When the strain is sufficient, the tensile stress will reach the ultimate tensile strength of the film σ_{ox} , and the film will then crack.

If the film is thin enough that $\sigma(y)$ is constant throughout its thickness, and if peeling normal to the film may be ignored, then the tensile and shear forces at any point, y , in the film must balance:

$$b \sigma(y) = \int_0^y \tau(\xi) d\xi \quad (14)$$

where b is the thickness of the film.

The function $\tau(\xi)$ is dependent on the properties of the material and represents the shear stress distribution. Assuming that $\tau(\xi)$ is a linear function of y with maximum τ_m at the segment edge decreasing to zero at some characteristic distance L_c as in Figure 3.

The segments will crack randomly until they are all of length $L_c \leq L \leq 2L_c$, they will then crack at the midpt. After that, the applied stress must increase until the interfacial shear stress at the edge of a crack, τ_m , reaches the interfacial shear strength τ_o at which point debonding will occur. This will happen first in the largest segment.

$$\tau_o = \frac{4 \sigma_{ox} b}{L} \quad (15)$$

where L is the length of the longest debonded segment.

The constant, 4, in this equation is dependent on the shear stress distribution. If the distribution is assumed to be linear, $C = 4$; sinusoidal, $C = \pi$ and arccosinusoidal, $C = \frac{2\pi}{\pi-2}$.

Parameters needed

Thickness of oxide

Length of largest debonded segment (which will be the 1st to spall)

Stress in oxide

It is not suggested how one finds the latter.

Evans [5] assessed the model of Tien and Davidson [6], who reached the same formula by a slightly different route, only their stress distribution was as in Figure 4.

They do, however, then go on to make some suggestion as to how σ_{ox} can be found, but only for thermal stresses.

$$\epsilon_{ox,ther} = \alpha_{ox} \Delta T \quad (16)$$

$$\epsilon_{s,ther} = \alpha_s \Delta T \quad (17)$$

where

$\epsilon_{ox,ther}$ is the thermal strain in the oxide
 $\epsilon_{s,ther}$ is the thermal strain in the substrate
 α_{ox} is the thermal expansion coefficient of the oxide
 α_s is the thermal expansion coefficient of the substrate
 ΔT is the temperature change producing the thermal stress.

Since the substrate and coating are joined together, the difference in their thermal strains will produce mechanical strains, and the sum of these must be constant across the interface.

$$\alpha_{ox} \Delta T + \sigma_{ox} \left[\frac{1 - \nu_{ox}}{E_{ox}} \right] = \alpha_s \Delta T + \sigma_s \left[\frac{1 - \nu_s}{E_s} \right] \quad (18)$$

E_{ox} and E_s are the Young's moduli of oxide and substrate, ν_{ox} and ν_s are the Poisson's ratios of oxide and substrate, σ_{ox} and σ_s are the biaxial stresses in oxide and substrate.

This assumes that the stresses in both phases are biaxial and parallel to the interface, with stress discontinuity at the interface. Also, that the strain is constant across the thickness of the oxide and substrate.

Combining the above expression with a force balance across a cross-section perpendicular to the interface, ie $\sigma_{ox} b = -\sigma_s a$, and assuming $\nu_{ox} = \nu_s = \nu$, one can obtain

$$\sigma_{ox} = \frac{-E_{ox} \Delta T (\alpha_s - \alpha_{ox})}{(1 - \nu) \left(1 + \frac{E_{ox} b}{E_s a} \right)} \quad (19)$$

$$\text{and } \sigma_s = \frac{E_s \Delta T (\alpha_s - \alpha_{ox})}{(1 - \nu) \left(1 + \frac{E_s a}{E_{ox} b} \right)} \quad (20)$$

where a and b are the thickness of the substrate and coating respectively.

This leads to the formula

$$\tau_o = \frac{4bE_{ox} \Delta T (\alpha_s - \alpha_{ox})}{L(1 - \nu) \left(1 + \frac{E_{ox} b}{E_s a} \right)} \quad (21)$$

Nagl (7) uses what is essentially Tien & Davidson's model, with a few changes as follows:

$$\tau_o = \frac{4b E_{ox} \epsilon}{L \left(1 - \nu_{ox} + (1 - \nu_s) \frac{E_{ox} b}{E_s a} \right)} \quad (22)$$

where ϵ is a strain which could be the thermal strain, $\Delta T (\alpha_s - \alpha_{ox})$, or a growth strain ϵ_{gr} , or an applied strain. The difference in the denominator is caused by the fact that Nagl does not assume that the Poisson's ratios are equal.

Parameters needed

Length of longest spalled segment (which should be the 1st to spall)

thickness of substrate and oxide

Young's modulus of both

Poisson's ratio of both

Strain - either applied strain

- or growth strain

- or $\Delta T (\alpha_s - \alpha_{ox})$

or the last need temp change and thermal expansion coefficients of both.

2.4 MODEL 4: CALCULATION OF INTERFACIAL SHEAR STRENGTH FROM A MODEL BASED ON FORCES

The model proposed by Burton [8] begins by assuming that the force required to cause cracks in the oxide is

$$F_f = wb\sigma_f \quad (23)$$

where

w is the width of the sample and therefore of the oxide

b is the thickness of the oxide

σ_f is the fracture strength of the oxide.

The force required to cause shear (ie spallation) over an area wL , where L is the crack spacing, is **assumed** to be

$$F_s = wL \tau_o \quad (24)$$

where τ_o is the interfacial shear strength.

When $L = L_k$, the critical crack spacing, spallation begins and it is **assumed** that $F_f = F_s$ at this point, ie

$$wL_c\tau_o = wb\sigma_f \quad (25)$$

$$\tau_o = \frac{b\sigma_f}{L_k} \quad (26)$$

There are no explanations given for these formulae.

σ_f may be taken as

$$\sigma_f = \epsilon_f \cdot E^c \quad (27)$$

where ϵ_f is the failure strain of the oxide and E^c is the Young's modulus of the oxide.

Parameters needed

Thickness of oxide and whole sample

Width of oxide, which is presumably the same as that of the whole sample

Critical crack spacing

Young's modulus of oxide

Failure strain.

2.5 MODEL 5: SHEAR-LAG MODEL FOR COATED SUBSTRATE IN TENSION

N McCartney [9] developed a shear-lag model for unidirectional composites and cross-ply laminates, which is readily adaptable to a coated substrate.

Consider the simple laminate (Figure 5), total thickness $2h$, with 2 outer coatings each of thickness b , and a substrate of thickness $2a$. A set of Cartesian co-ordinates (x, y) is located so that the origin is on the mid-plane of the laminate and is midway between the cracks, and so that the x -axis is normal to the mid-plane with the y -axis having the same direction as the loading.

For any variable $c(x, y)$ associated with the coating, the average across the coating is defined as

$$\bar{c}(y) = \frac{1}{b} \int_a^h c(x, y) dx, \quad (28)$$

and for any variable $s(x, y)$ associated with the substrate, the average across the substrate (assuming symmetry) is defined as

$$\bar{s}(y) = \frac{1}{a} \int_0^a s(x, y) dx. \quad (29)$$

In the following relations a superscript c will refer to variables associated with the coating, while a superscript s will refer variables to the substrate.

An equilibrium equation which must be satisfied in both the coating and the substrate is

$$\frac{\partial \sigma_{xy}}{\partial x} + \frac{\partial \sigma_{yy}}{\partial y} = 0, \quad (30)$$

where σ_{xy} is the shear stress and σ_{yy} is the axial stress. Averaging (3) over the coating yields

$$\frac{d\bar{\sigma}_{yy}^c}{dy} = \frac{\tau(y)}{b}, \quad (31)$$

since $\sigma_{xy}^c = 0$ on $x = h$. The function $\tau(y)$ is the limiting value of the shear stress on the interface $x = a$, i.e. $\tau(y) = \sigma_{xy}^c(a, y)$.

Averaging (30) over the substrate yields

$$\frac{d\bar{\sigma}_{yy}^s}{dy} = -\frac{\tau(y)}{a}, \quad (32)$$

since $\sigma_{xy}^s = 0$ on $x = 0$, so that the plane $x = 0$ is one of symmetry. The result (32) has made use of the fact that the shear stress σ_{xy} is continuous across the interface so that $\sigma_{xy}^s(a, y) \equiv \sigma_{xy}^c(a, y)$. It follows from (31) and (32) that

$$\frac{d}{dy} \left(\frac{b}{h} \bar{\sigma}_{yy}^c + \frac{a}{h} \bar{\sigma}_{yy}^s \right) = 0. \quad (33)$$

On integration the following relation is derived which is valid for all values of y .

$$b \bar{\sigma}_{yy}^c(y) + a \bar{\sigma}_{yy}^s(y) = h\sigma, \quad (34)$$

where σ is the effective axial stress (independent of y) applied to the laminate. The results (31), (32) and (34) are exact for any stress field which is symmetric about the plane $x = 0$.

The shear stress-strain relations for the coating and substrate may be written in the form:

$$\frac{\partial v^c}{\partial x} + \frac{\partial u^c}{\partial y} = \frac{\sigma_{xy}^c}{\mu^c}, \quad (35)$$

$$\frac{\partial v^s}{\partial x} + \frac{\partial u^s}{\partial y} = \frac{\sigma_{xy}^s}{\mu^s}, \quad (36)$$

where u^c , v^c , u^s and v^s are the displacement components for the coating and the substrate respectively. Also, μ^c and μ^s are the shear moduli for the coating and the substrate respectively. In order to develop a shear-lag model the relations (35) and (36) are approximated by the simpler forms,

$$\frac{\partial v^c}{\partial x} = \frac{\sigma_{xy}^c}{\mu^c}, \quad \frac{\partial v^s}{\partial x} = \frac{\sigma_{xy}^s}{\mu^s}. \quad (37)$$

The shear stress distribution is now assumed to be a linear function of x with the result that it must be of the form:

$$\sigma_{xy}^c = \tau(y) \frac{h-x}{b}, \quad \sigma_{xy}^s = \tau(y) \frac{x}{a}, \quad (38)$$

so that the shear stress is continuous at the interface and so that $\sigma_{xy}^s = 0$ on $x = 0$ and $\sigma_{xy}^c = 0$ on $x = h$. On multiplying (38)₁ by $h-x$ and integrating with respect to x over the range $a \leq x \leq h$ it can be shown using (37)₁ that

$$\int_a^h (h-x) \frac{\partial v^c}{\partial x} dx = \frac{b^2 \tau(y)}{3\mu^c}. \quad (39)$$

On integrating the LHS of (39) by parts it can be shown that

$$\bar{v}^c(y) - v^c(a, y) = \frac{b\tau(y)}{3\mu^c}. \quad (40)$$

On multiplying (38)₂ by x and integrating with respect to x over the range $0 \leq x \leq a$ it can be shown using (37)₂ that

$$\int_0^a x \frac{\partial v^s}{\partial x} dx = \frac{a^2 \tau(y)}{3\mu^s}. \quad (41)$$

On integrating the LHS of (41) by parts it can be shown that

$$v^s(a, y) - \bar{v}^s(y) = \frac{a\tau(y)}{3\mu^s}. \quad (42)$$

Since there is perfect bonding on the interface $x = a$

$$v^c(a, y) \equiv v^s(a, y), \quad (43)$$

and the addition of (40) and (42) leads to the result

$$\bar{v}^c(y) - \bar{v}^s(y) = \frac{1}{3} \left(\frac{b}{\mu^c} + \frac{a}{\mu^s} \right) \tau(y). \quad (44)$$

The axial stress-strain-temperature relations for the coating and substrate can be approximated as

$$\bar{\epsilon}_{yy}^c \equiv \frac{d\bar{v}^c}{dy} = \frac{\bar{\sigma}_{yy}^c}{E^c} + \alpha^c \Delta T, \quad (45)$$

$$\bar{\epsilon}_{yy}^s \equiv \frac{d\bar{v}^s}{dy} = \frac{\bar{\sigma}_{yy}^s}{E^s} + \alpha^s \Delta T, \quad (46)$$

where $\bar{\epsilon}_{yy}^c$ and $\bar{\epsilon}_{yy}^s$ are the average axial strain components, E^c and E^s the Young's moduli, and α^c and α^s the thermal expansion coefficients, all in the coating and substrate respectively.

The parameter ΔT is the temperature change from a given reference temperature at which the system is entirely stress free and at which the strain is defined to be zero everywhere.

On differentiating (45) and (46) with respect to y , and on making use of (31) and (32), it follows that

$$\frac{d^2 \bar{v}^c}{dy^2} = \frac{\tau(y)}{bE^c}, \quad \frac{d^2 \bar{v}^s}{dy^2} = -\frac{\tau(y)}{aE^s}. \quad (47)$$

Thus a subtraction together with the use of the result (44) leads to the following second order differential equation for the interfacial shear stress $\tau(y)$

$$\frac{d^2 \tau}{dy^2} = k^2 \tau, \quad (48)$$

where

$$k^2 = \frac{3\mu^c\mu^s(aE^s + bE^c)}{abE^cE^s(a\mu^c + b\mu^s)}. \quad (49)$$

The most general solution of (48) anti-symmetric about $y = 0$ is

$$\tau(y) = P \sinh ky, \quad (50)$$

and the corresponding average stresses in the coating and substrate are obtained by integrating (31) and (32) to give the results

$$\bar{\sigma}_{yy}^c = C + \frac{1}{kb} P \cosh ky, \quad (51)$$

$$\bar{\sigma}_{yy}^s = D - \frac{1}{ka} P \cosh ky. \quad (52)$$

The parameters P , C and D must now be determined.

Consider an uncracked plate, (Figure 6), and the stress-strain-temperature relations

$$\epsilon_{yy}^c = \frac{\sigma_{yy}^c}{E^c} + \alpha^c \Delta T, \quad (53)$$

$$\epsilon_{yy}^s = \frac{\sigma_{yy}^s}{E^s} + \alpha^s \Delta T. \quad (54)$$

However, since now the plate is not cracked, $\epsilon_{yy}^c = \epsilon_{yy}^s = \epsilon$ the applied strain and it follows that
and

$$\sigma_{yy}^c = E^c (\varepsilon - \alpha^c \Delta T), \quad (55)$$

$$\sigma_{yy}^s = E^s (\varepsilon - \alpha^s \Delta T). \quad (56)$$

Moreover, if the plate is uncracked, $\tau(y) \equiv 0$ and $\bar{\sigma}_{yy}^c = \sigma^c$, $\bar{\sigma}_{yy}^s = \sigma^s$, and as a result from (51) and (52) the parameters C and D have the values σ^c and σ^s respectively, giving for a cracked plate

$$\bar{\sigma}_{yy}^c = \sigma^c + \frac{1}{kb} P \cosh ky, \quad (57)$$

$$\bar{\sigma}_{yy}^s = \sigma^s - \frac{1}{ka} P \cosh ky. \quad (58)$$

For a cracked plate, (Figure 5), $\bar{\sigma}_{yy}^c = 0$ at the crack locations $y = L$ or $-L$ and, from (57), it follows that

$$P = - \frac{kb \sigma^c}{\cosh kL}. \quad (59)$$

The equation (50) for the interfacial shear stress then reduces to

$$\tau(y) = - \frac{kb \sigma^c \sinh ky}{\cosh kL}. \quad (60)$$

The axial stresses in the coating and substrate are then given by

$$\bar{\sigma}_{yy}^c = \sigma^c \left(1 - \frac{\cosh ky}{\cosh kL} \right), \quad (61)$$

and

$$\bar{\sigma}_{yy}^s = \sigma^s + \frac{b}{a} \frac{\cosh ky}{\cosh kL} \sigma^c. \quad (62)$$

2.6 MODEL 6: ANOTHER MATHEMATICAL SHEAR-LAG MODEL, STARTING FROM DIFFERENT ASSUMPTIONS

Evans [5] also assessed the model of Mahmood [10], who developed another shear-lag model which involves considering the simple laminate (Figure 9).

Starting from the **assumption** that for thin, flat specimens the applied load will be

$$F = \sigma_y^s A^s + \sigma_y^c A^c \quad (63)$$

where σ_y^s and σ_y^c are the stresses in the y direction in substrate and coating respectively, and A^s and A^c are the cross-sectional areas of substrate and coating respectively.

Assuming that the metal as a whole is strained homogeneously, but locally the state of uniform stress and strain is disturbed by transfer of stress in the oxide.

If F^c is the load shared by the coating, then at distance y from edge, it is assumed that

$$\frac{dF^c}{dy} = H (u - v) \quad (64a)$$

$$= -\tau(y) \cdot w \quad (64b)$$

where H is a constant depending on properties of coating and substrate, u is the longitudinal displacement of the coating, v is the displacement the substrate would undergo if the coating were not present, $\tau(y)$ is the shear stress along the interface $x = a$, and w is the width of the specimen.

Moreover,

$$F^c = E^c A^c \left(\frac{du}{dy} \right) \quad (65)$$

differentiating 64(a) and substituting from (65) for $\left(\frac{du}{dy} \right)$ we obtain

$$\frac{d^2 F^c}{dy^2} = k^2 (F^c - A^c E^c \epsilon) \quad \text{since } \epsilon = \frac{dv}{dx} \quad (66)$$

where

$$k^2 = \frac{H}{A^c E^c} \quad (67)$$

The solution of which is

$$F_c = E^c A^c \epsilon + R \sinh(ky) + S \cosh(ky) \quad (68)$$

since $F^c = 0$ when $y = 0$ and $y = 2L$

$$S = -E^c A^c \epsilon \quad (69)$$

$$\text{and } R = \frac{E^c A^c \epsilon}{\sinh(k \cdot 2L)} (\cosh(k \cdot 2L) - 1) \quad (70)$$

$$\therefore F^c = E^c A^c \epsilon \left(1 - \frac{\cosh k(L-y)}{\cosh kL} \right) \quad (71)$$

and assuming $\frac{F^c}{A^c} = \sigma_y^c$ (72)

$$\sigma_y^c = E^c \epsilon \left(1 - \frac{\cosh k(L-y)}{\cosh kL} \right) \quad (73)$$

Returning to equations (64),

$$H = - \frac{\tau(y) \cdot w}{u-v} \quad (74)$$

Assuming that shear strain in the substrate away from the interface will be

$$\frac{v-u}{a/2} = \frac{\tau(y)}{\mu^s} \quad (75)$$

where a is the thickness of the substrate, and μ^s its shear modulus

$$H = \frac{2 \mu^s w}{a} \quad (76)$$

Since $k^2 = \frac{H}{A^c E^c}$, and $A^c = b.w$, where b is the thickness of the coating,

$$k^2 = \frac{2\mu^s}{E^c \cdot b \cdot a} \quad (77)$$

In equation (64b),

$$\frac{dF^c}{dy} = - \tau(y) \cdot w \quad (78)$$

and it has already been assumed that

$$F^c = \sigma_y^c \cdot A^c \quad (79)$$

$$\therefore \frac{dF^c}{dy} = A^c \cdot E^c \cdot \epsilon \cdot k \left(\frac{\sinh k(L-y)}{\cosh kL} \right) \quad (80)$$

and since $A^c = b.w$

$$\tau(y) = -E^c \cdot b \cdot \epsilon \cdot k \left(\frac{\sinh k(L-y)}{\cosh kL} \right) \quad (81)$$

This is essentially the same as the previous model (model 5). The only difference is in the constant, k , and in the fact that the previous model takes account of thermal stresses.

The difference in the final equations of $\sinh k(L-y)$ as opposed to $\sinh ky$, is due to the difference in where y is measured from.

Parameters needed

Applied strain

Crack spacing

Thickness of both

Young's modulus of coating

Shear modulus of substrate

Shear Stress Distribution of Model 1

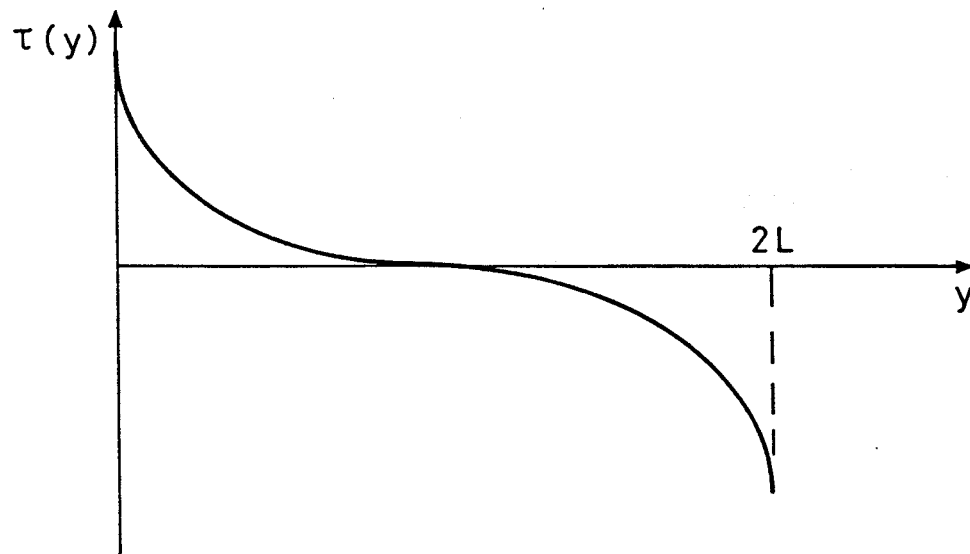


Figure 1

Basic Parameters of Models 1, 3 & 5

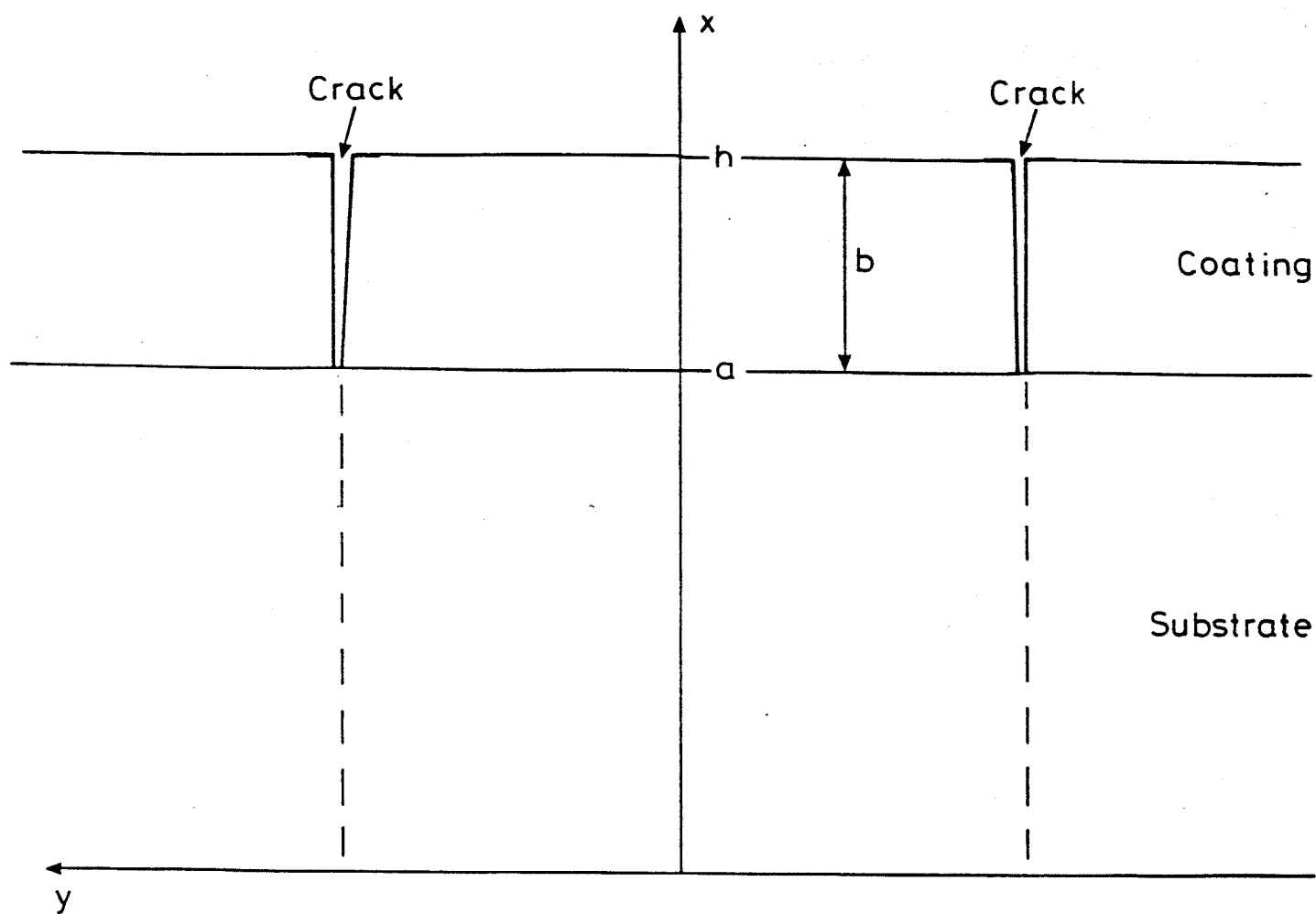


Figure 2

Model 3

Stress Distribution after Wheeler and Osaki (4)

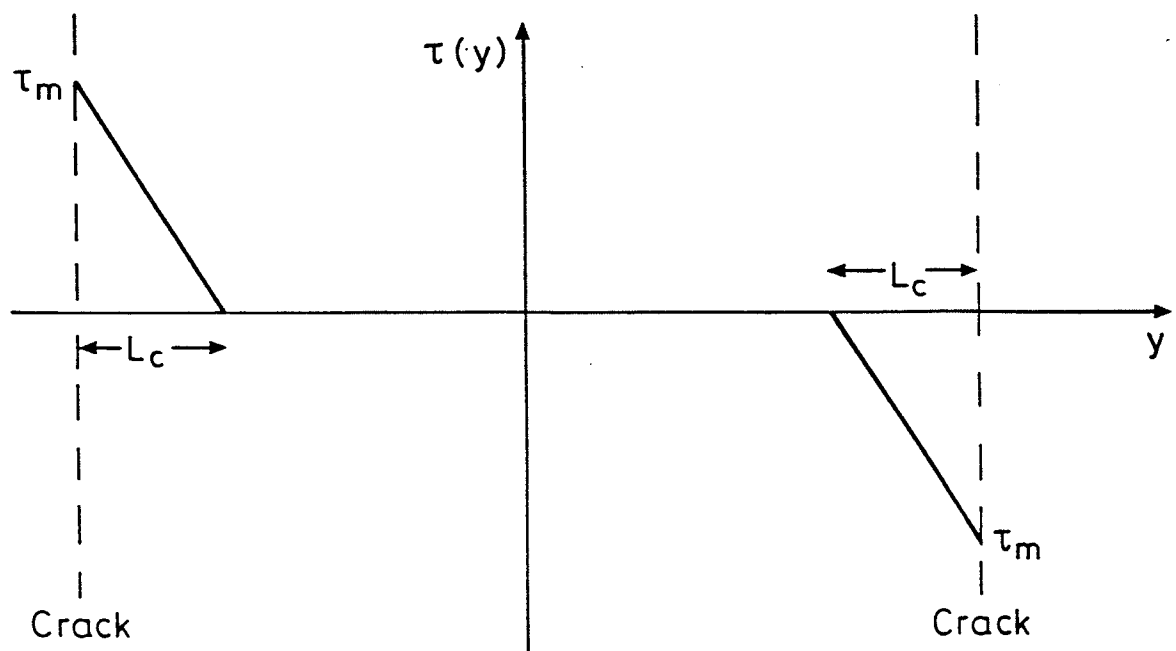


Figure 3

Model 3

Stress Distribution after Tien and Davidson (6)

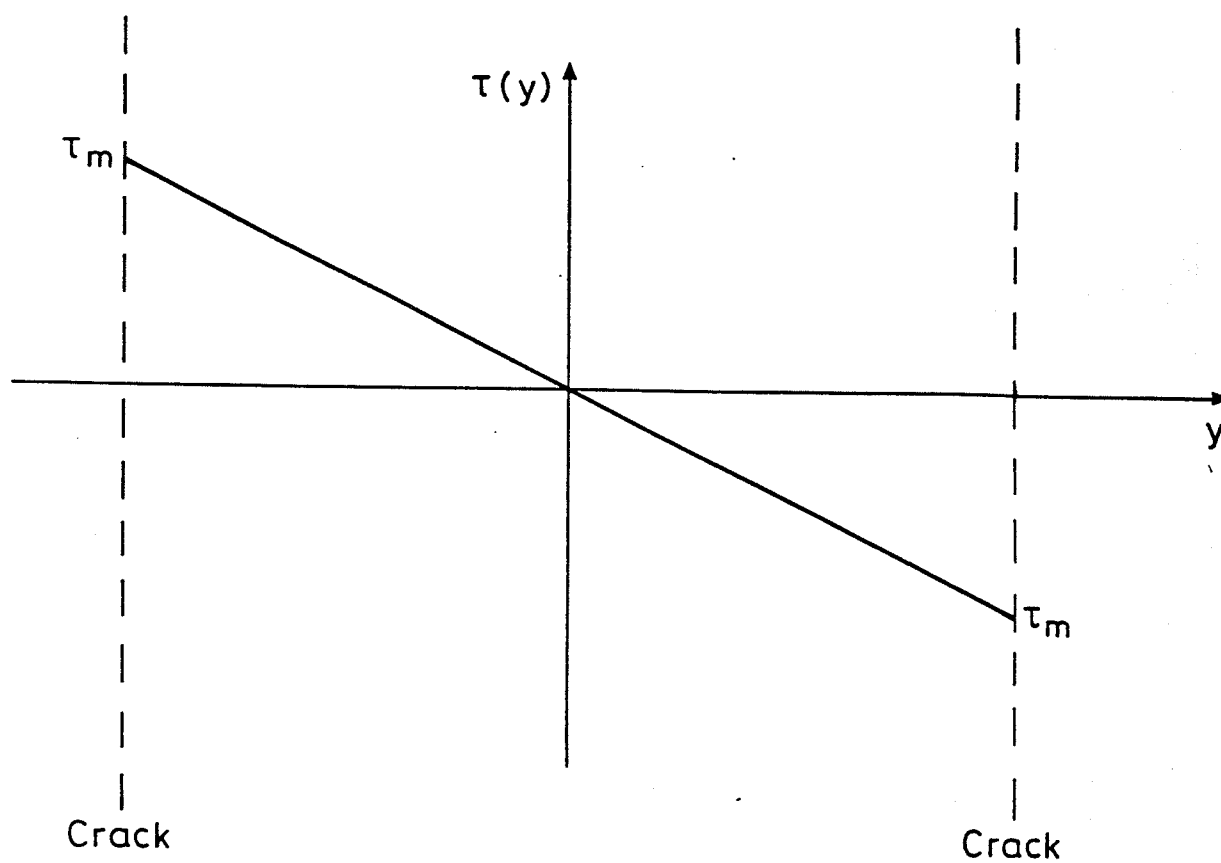


Figure 4

Model 5

Cracked Plate

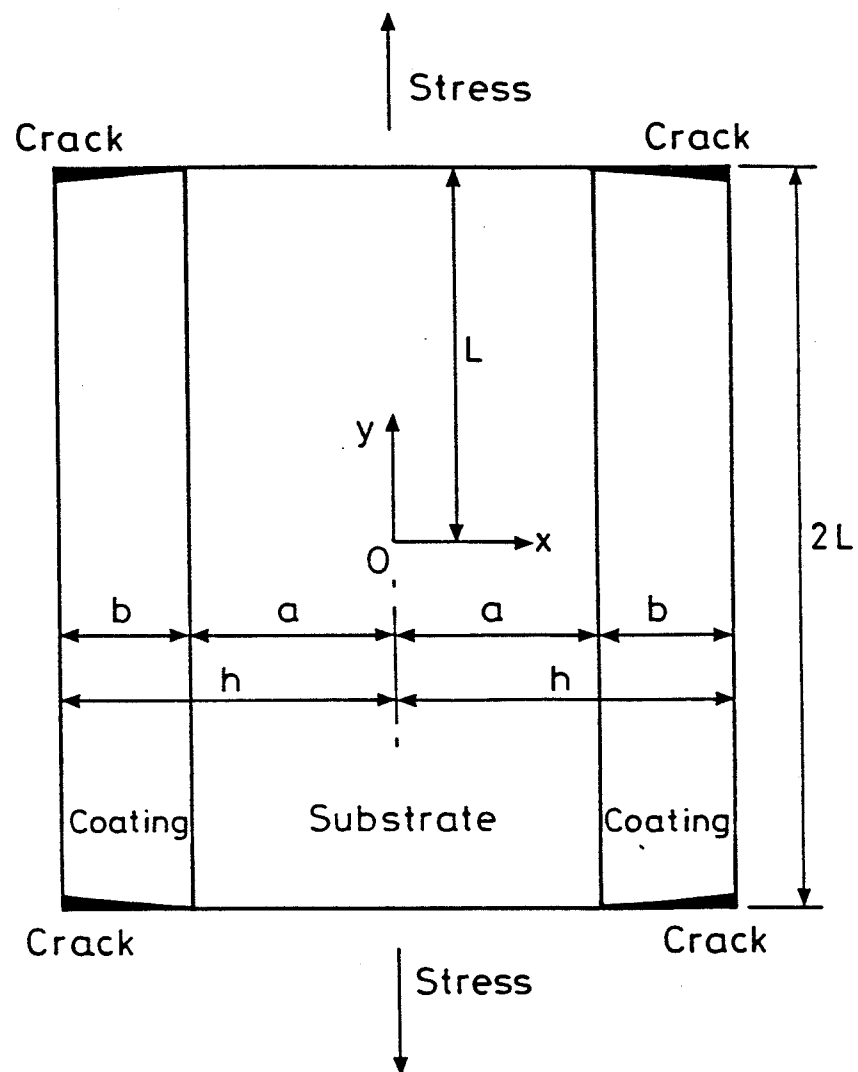


Figure 5

Model 5

Uncracked Plate

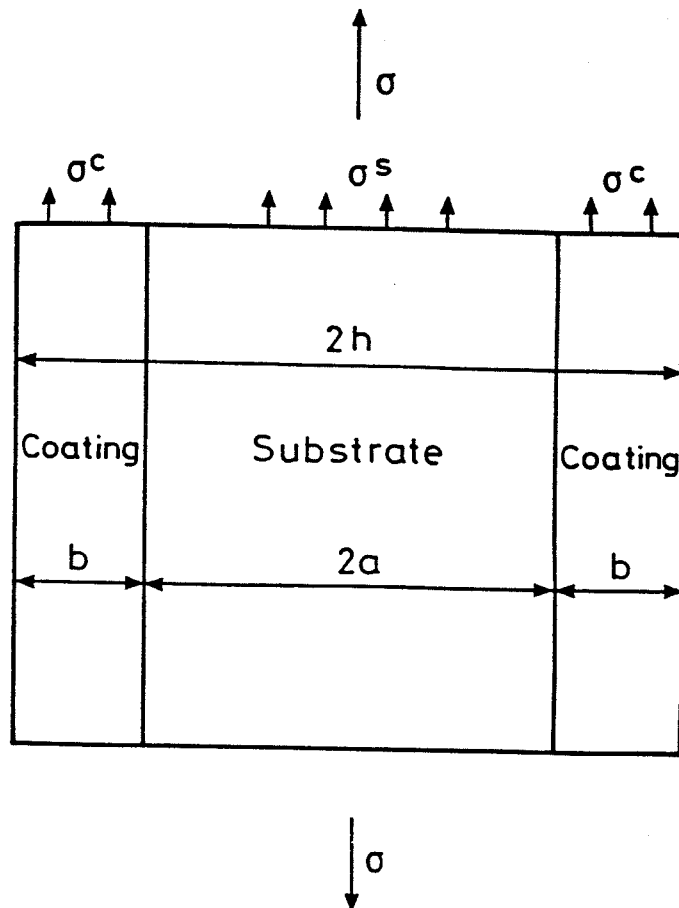


Figure 6

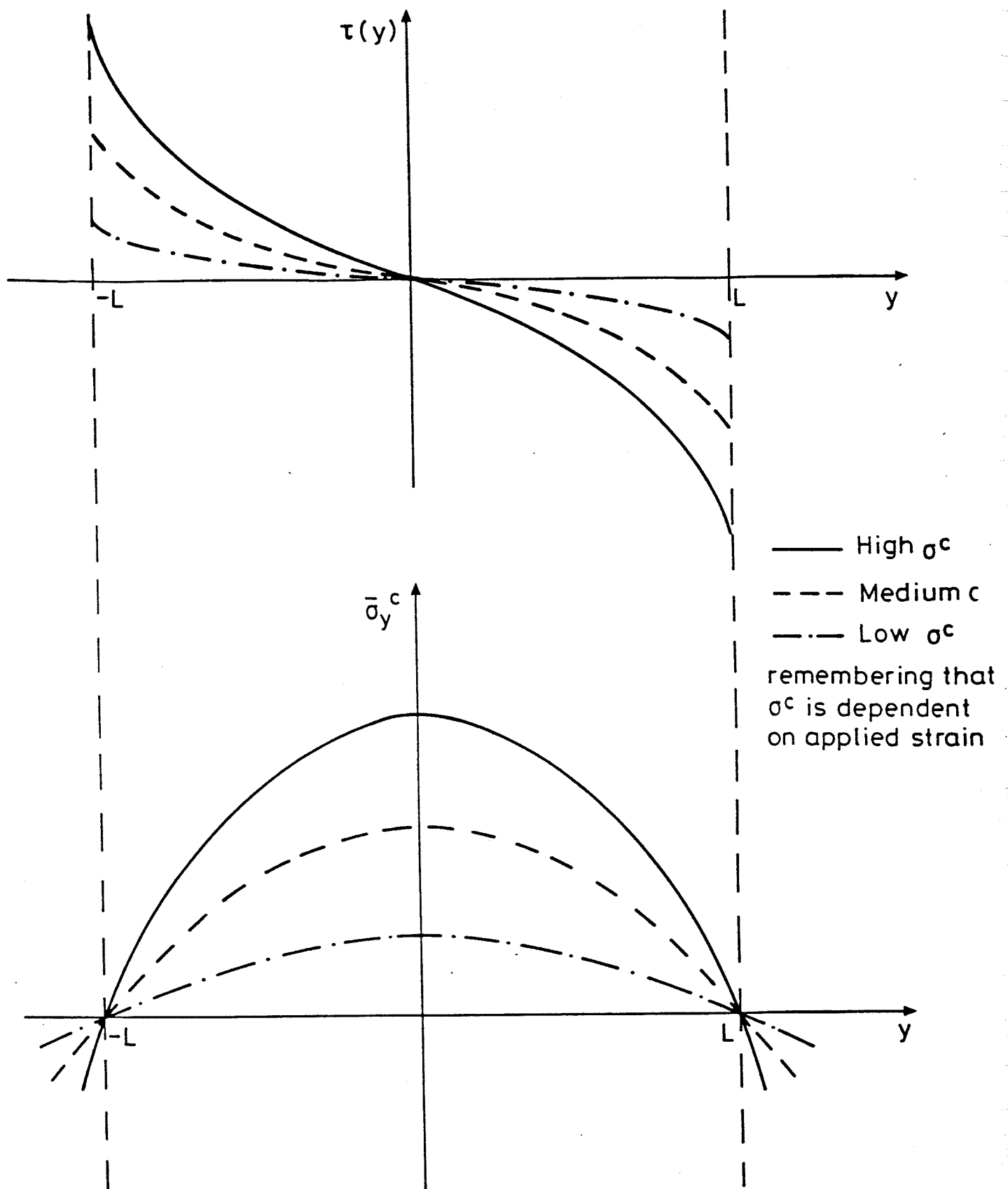
Model 5Stress Distributions with respect to y 

Figure 7

Model 6

Basic Parameters

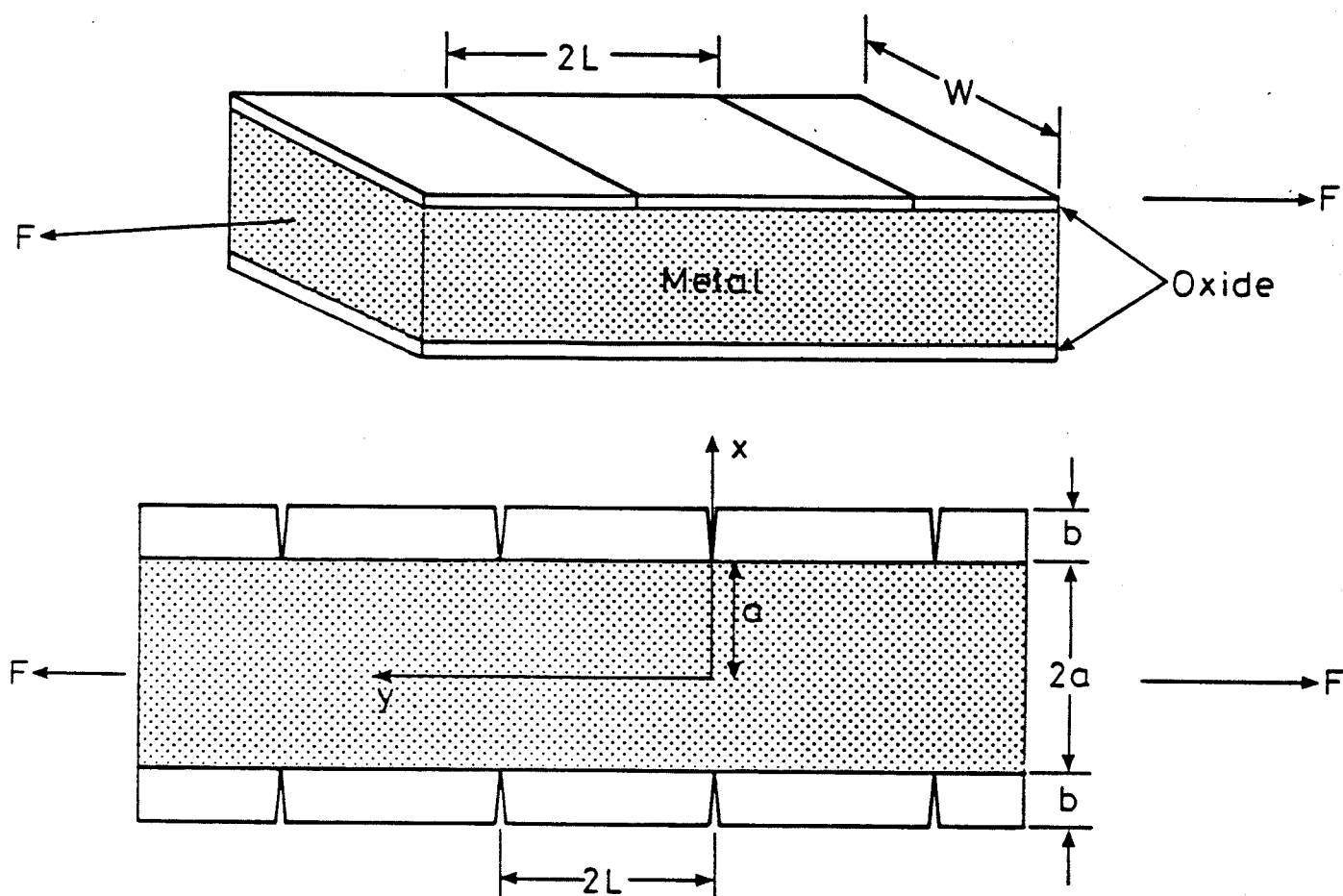


Figure 8

3 DATA, CALCULATIONS AND GRAPHS

The data come from the work of Nagl [7], who carried out a large number of 4 point bend tests on various materials. The tensile side of a 4 point bend test is generally taken as being approximately equivalent to straining a sample in tension in one dimension.

Unfortunately, it is not known whether the data points correspond to spallation or not. The thicker oxides almost undoubtedly have spalled, in line with the results of Nagl *et al* [11], but the thinner ones may not have done so. Models 2, 3 and 4 are intended for use with the crack spacing at the point of spallation, and the values calculated may therefore be somewhat inaccurate.

Figure 9 shows the variation of crack spacing with thickness of oxide. Figures 10-15 show the variation of interfacial shear stress calculated from Models 2-4 with thickness and average crack spacing. However, the variation with average crack spacing is not really significant because it merely shows the linear variation of average crack spacing with thickness.

Figures 16-19 show the variation of interfacial shear stress calculated from Models 5 and 6 with thickness and average crack spacing. The apparent perfect linearity of their relationship with average crack spacing is systematic and not significant. Both of them include a term $\tanh kL$, where L is the average crack spacing. However, kL is small enough that $\tanh kL \approx kL$, and therefore the interfacial shear stress varies linearly with average crack spacing. Figure 20 shows the interfacial shear stress calculated from Model 5 while making the above assumption. Figure 21 is a comparison between the interfacial shear stress calculated from Models 5 and 6.

Nickel oxide on nickel at room temp. from M.M. Nagl's progress report 16

test no.	thickness (m)	Crack Spacing			Failure strain (%)	max strain (%)
		Minimum (m)	Maximum (m)	Average (m)		
1	7.5E-6	20.0E-6	60.0E-6	40.0E-6	0.18	1.12
3	27.5E-6	40.0E-6	130.0E-6	80.0E-6	0.14	1.12
5	45.0E-6	50.0E-6	200.0E-6	125.0E-6	0.11	1.12
7	20.5E-6	40.0E-6	120.0E-6	75.0E-6	0.16	1.12
9	4.3E-6	15.0E-6	40.0E-6	25.0E-6	0.06	1.12
10	4.3E-6	15.0E-6	40.0E-6	30.0E-6	0.03	1.12
11	3.5E-6	15.0E-6	30.0E-6	25.0E-6	0.015	1.12
12	3.8E-6	20.0E-6	30.0E-6	27.0E-6	0.07	1.12
13	42.0E-6	40.0E-6	200.0E-6	120.0E-6	0.10	1.12
14	42.0E-6	40.0E-6	190.0E-6	115.0E-6	0.14	1.12
15	19.0E-6	40.0E-6	140.0E-6	85.0E-6	0.16	1.12

Y's mod (GPa) Ni	Y's mod (GPa) NiO	Shr mod (GPa) Ni	Shr mod (GPa) NiO	Poisson's ratio Ni	Poisson's ratio NiO	Thickness (m) Ni
200	220	76.92308	84.61538	0.3	0.3	1.5E-3

Max. Interfacial Shear Stress calculated from the various Models (GPa)

	Armitt et al	Tien et al	Burton	McCartney	Mahmood
Model no.	2	3	4	5	6
test no.					
1	0.453407	2.625559	0.07425	0.034071	0.022786
3	0.715718	4.744323	0.105875	0.068234	0.045538
5	0.733011	4.906873	0.08712	0.106142	0.070842
7	0.619154	3.791534	0.096213	0.063763	0.042624
9	0.418636	2.414147	0.022704	0.021369	0.014278
10	0.351619	2.011789	0.00946	0.025549	0.017092
11	0.343648	1.966154	0.00462	0.021326	0.01426
12	0.345422	1.976123	0.021674	0.023016	0.015393
13	0.722581	4.780753	0.077	0.101885	0.068019
14	0.738189	4.988612	0.112487	0.097796	0.065255
15	0.529009	3.104044	0.078682	0.071818	0.048112

Accurate and Approximate Shear Stress from model 5

thickness (m)	Shear Stress (GPa)	Approx. Stress (GPa)
3.5E-6	0.021326	0.021548
3.8E-6	0.023016	0.023273
4.3E-6	0.021369	0.02155
4.3E-6	0.025549	0.02586
7.5E-6	0.034071	0.034494
19.0E-6	0.071818	0.073406
20.5E-6	0.063763	0.064782
27.5E-6	0.068234	0.06916
42.0E-6	0.101885	0.103924
42.0E-6	0.097796	0.099593
45.0E-6	0.106142	0.108293

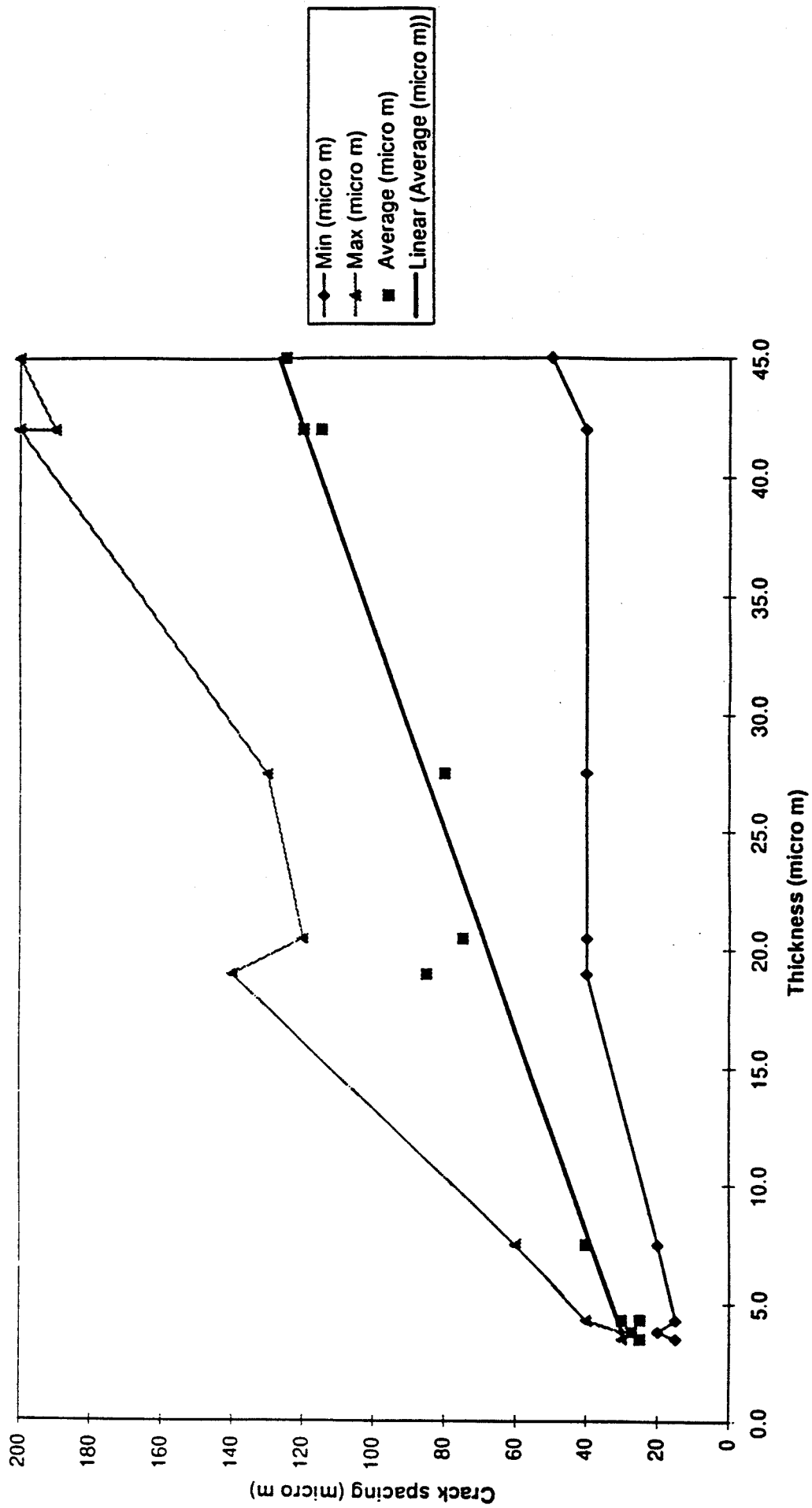


Figure 9 Crack Spacings versus Thickness for Nickel Oxide in Tension

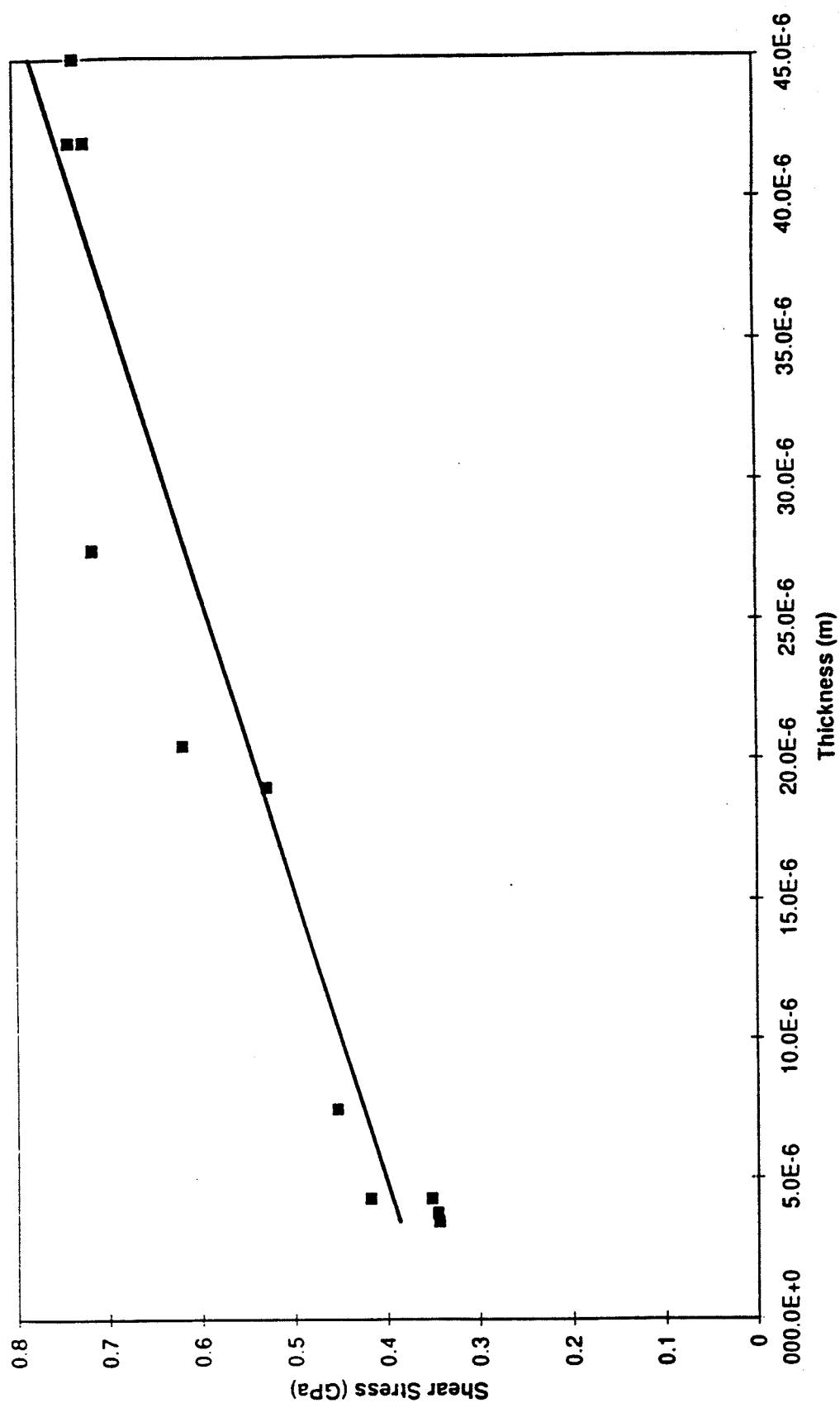


Figure 10 Max. Int. Shear Stress (calculated from Armitt et al's Model, no. 2) versus Thickness of Oxide

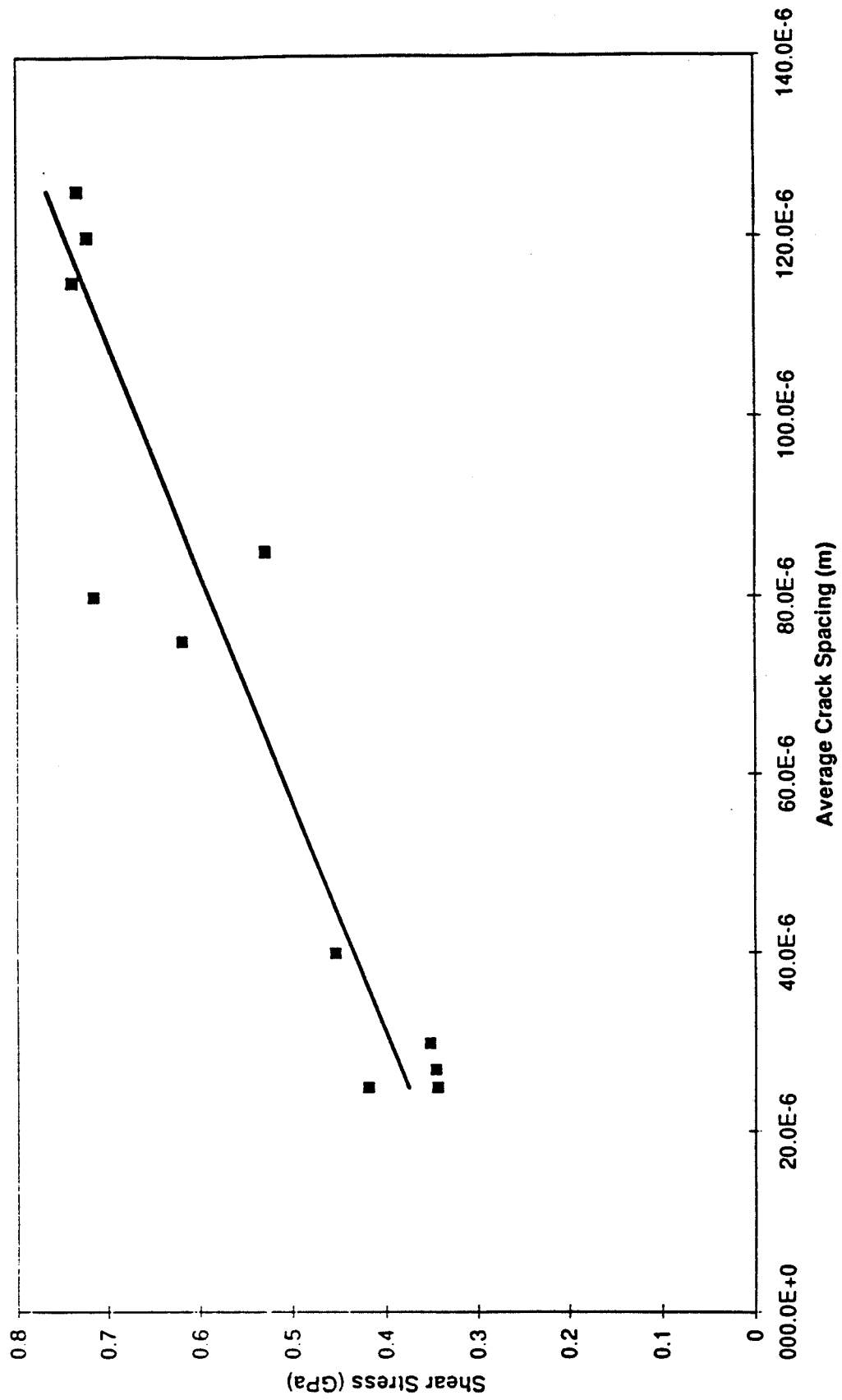


Figure 11 Max. Int. Shear Stress (calculated from Armitt et al's Model, no. 2) versus Average Crack Spacing

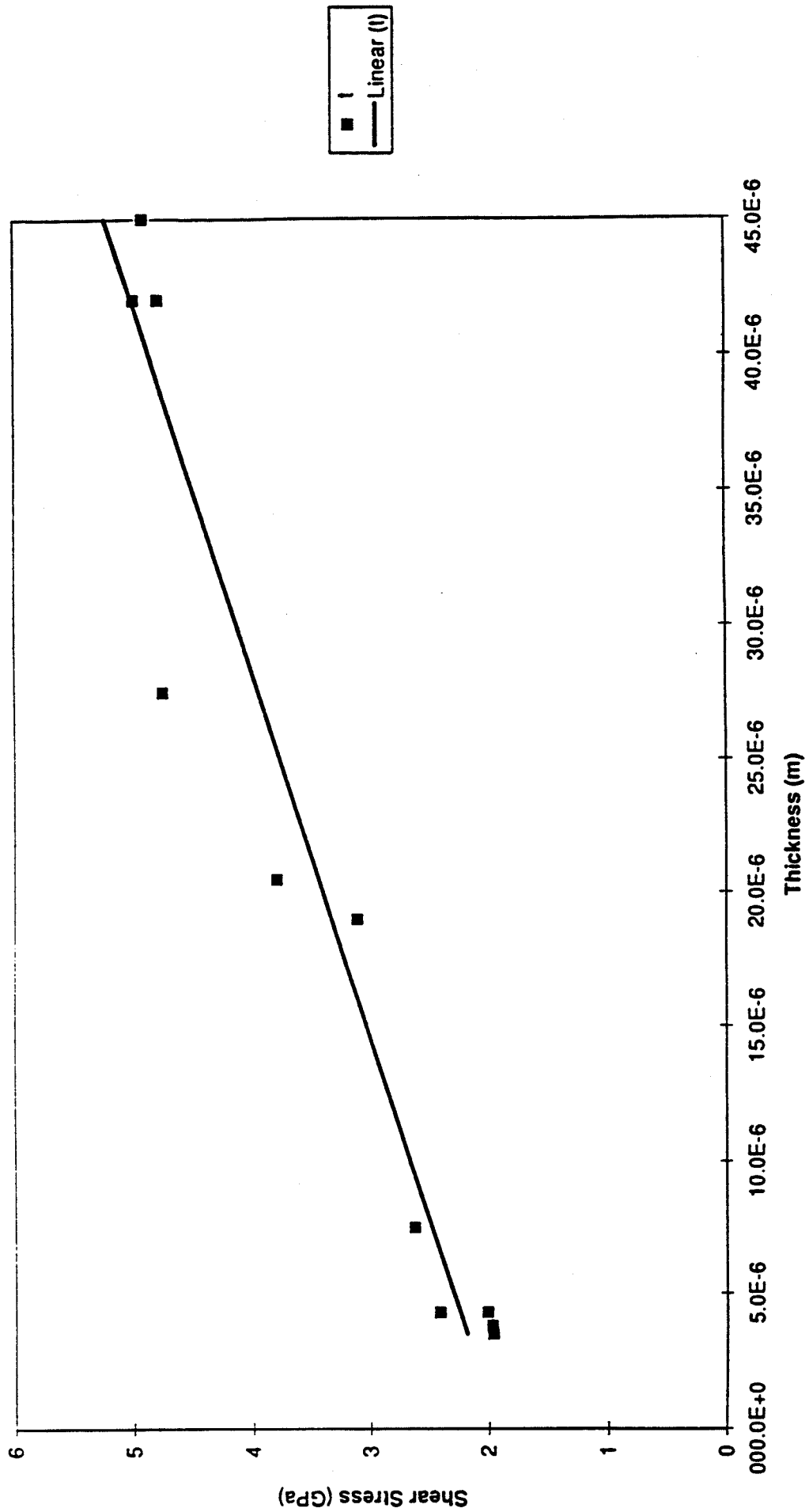


Figure 12 Max. Int. Shear Stress (calculated from Tien et al's Model, no. 3) versus Thickness of Oxide

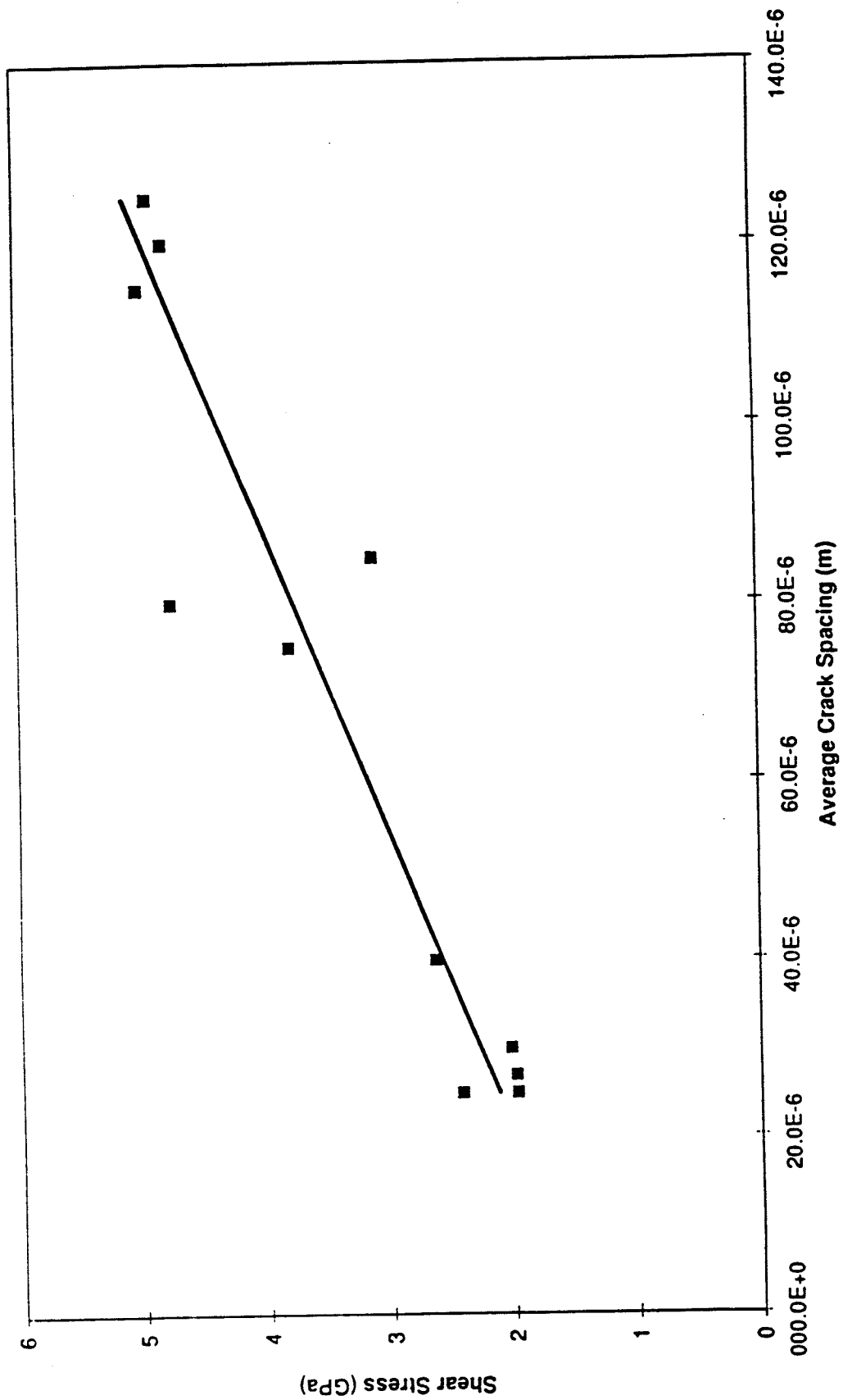


Figure 13 Max. Int. Shear Stress (calculated from Tien et al's Model, no. 3) versus Average Crack Spacing

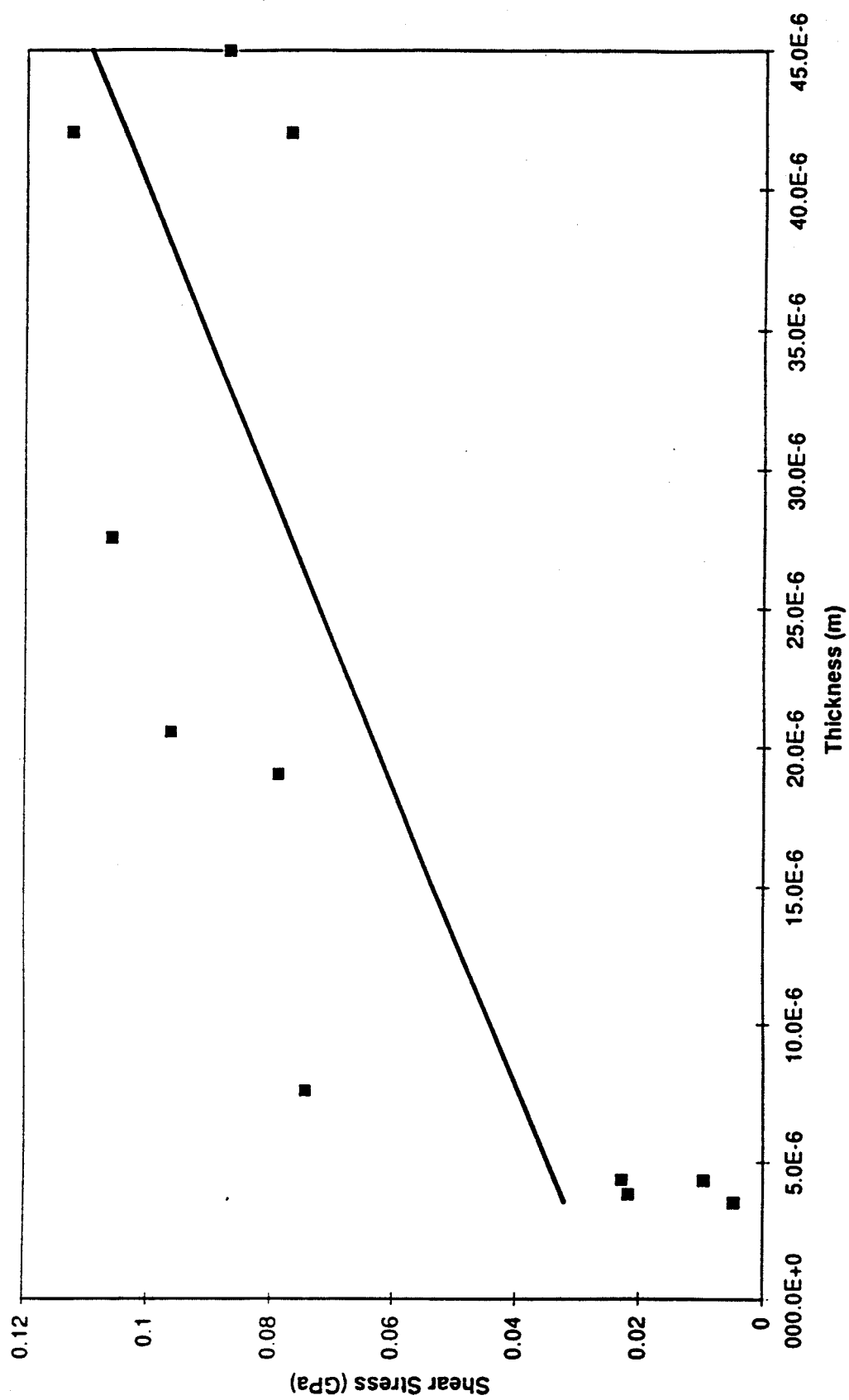


Figure 14 Max. Int. Shear stress (calculated from Burton's Model, no. 4) versus Thickness of Oxide

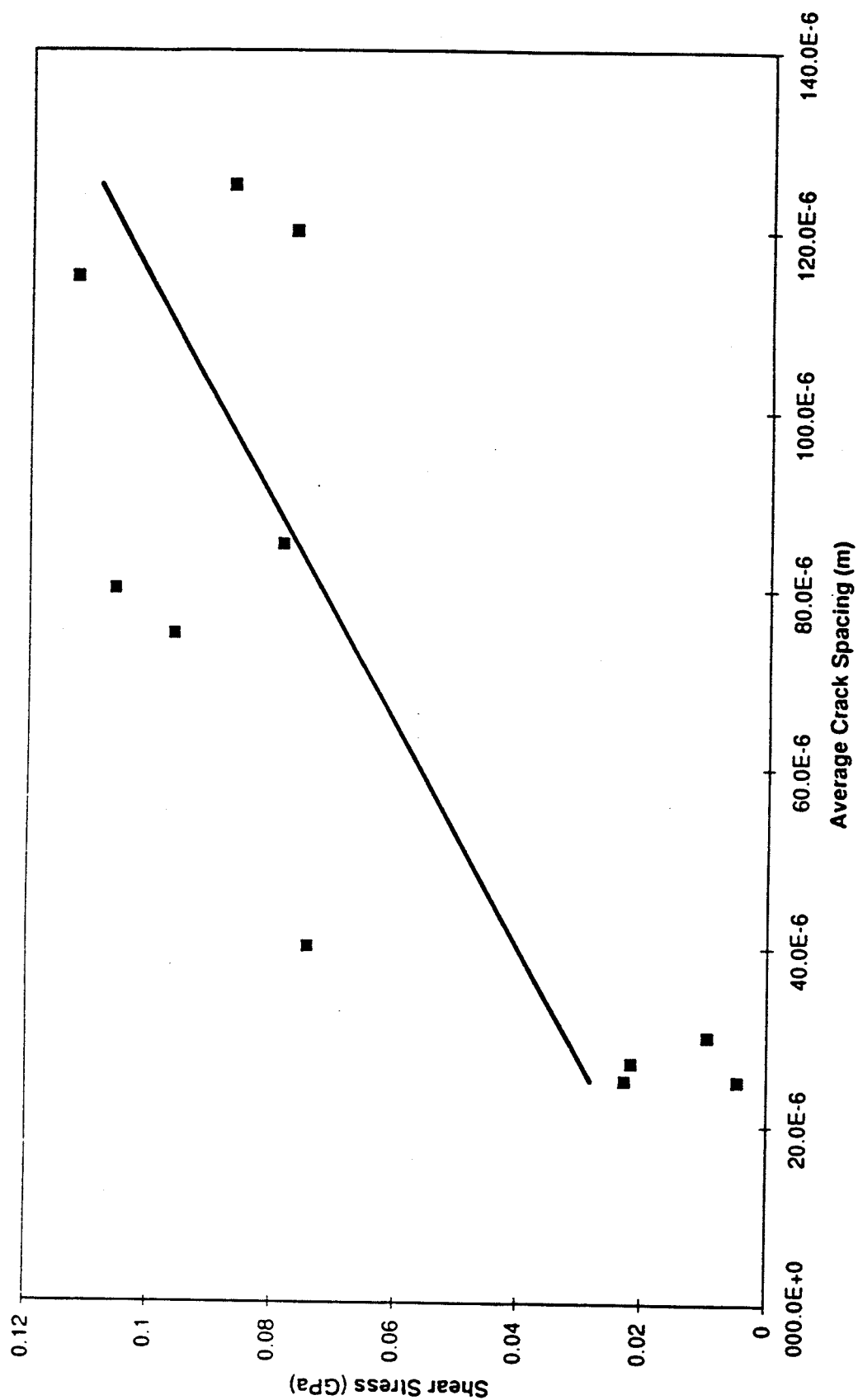


Figure 15 Max. Int. Shear Stress (calculated from Burton's Model, no. 4) versus Average Crack Spacing

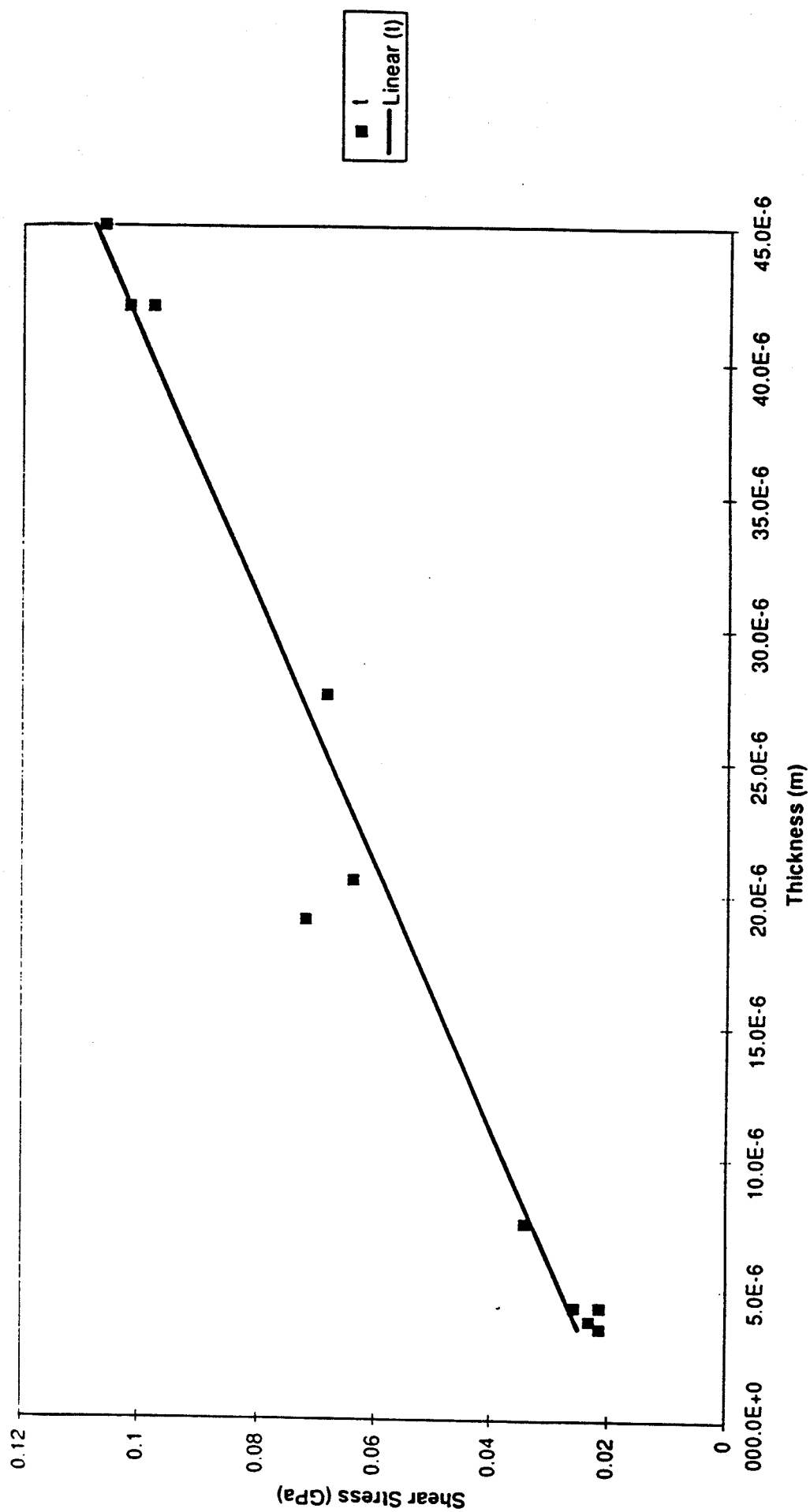


Figure 16 Max. Int. Shear Stress (calculated from McCartney's Model, no. 5) versus Thickness of Oxide

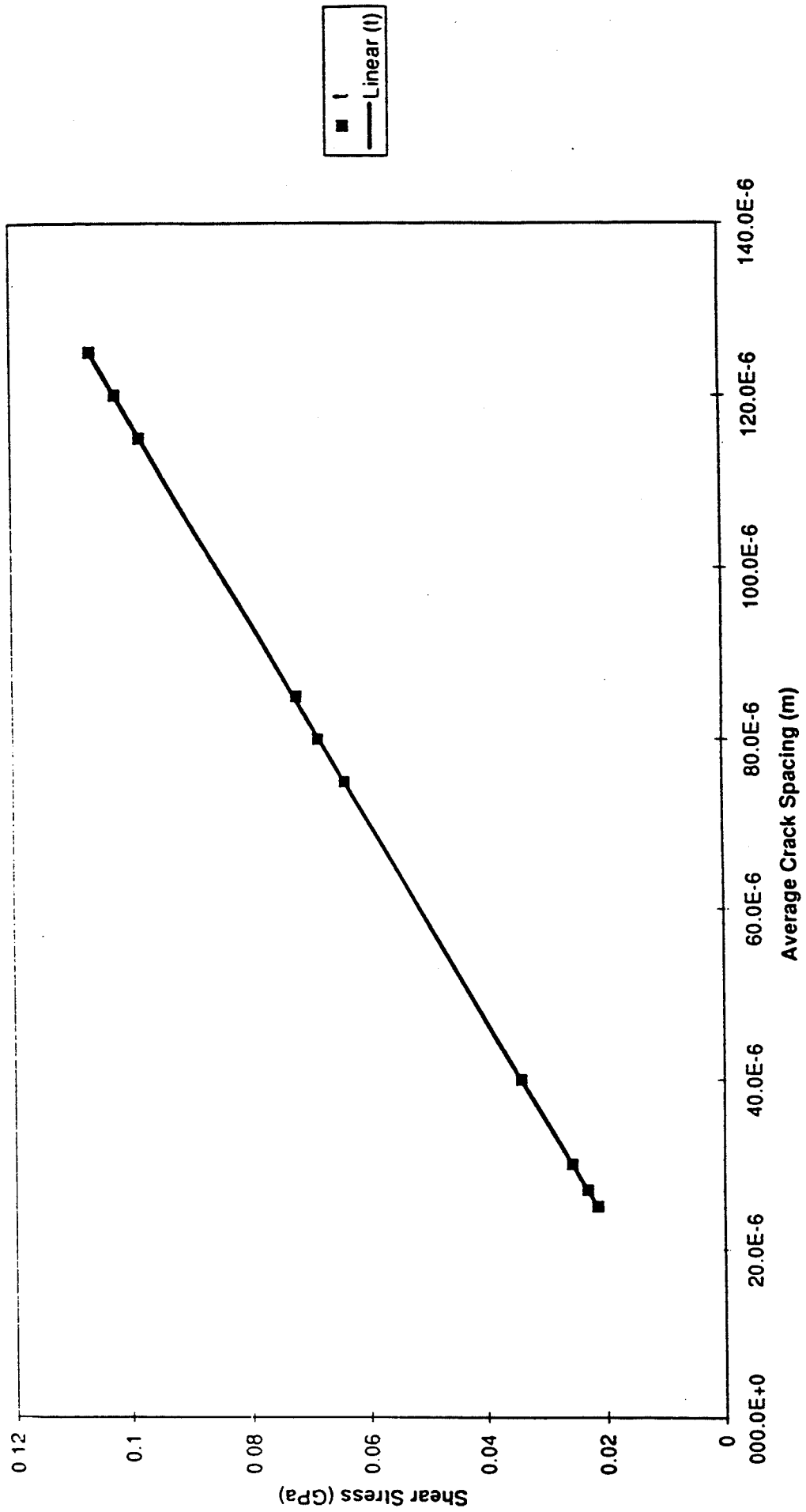


Figure 17 Max. Int. Shear Stress (calculated from McCartney's Model, no. 5) versus Average Crack Spacing

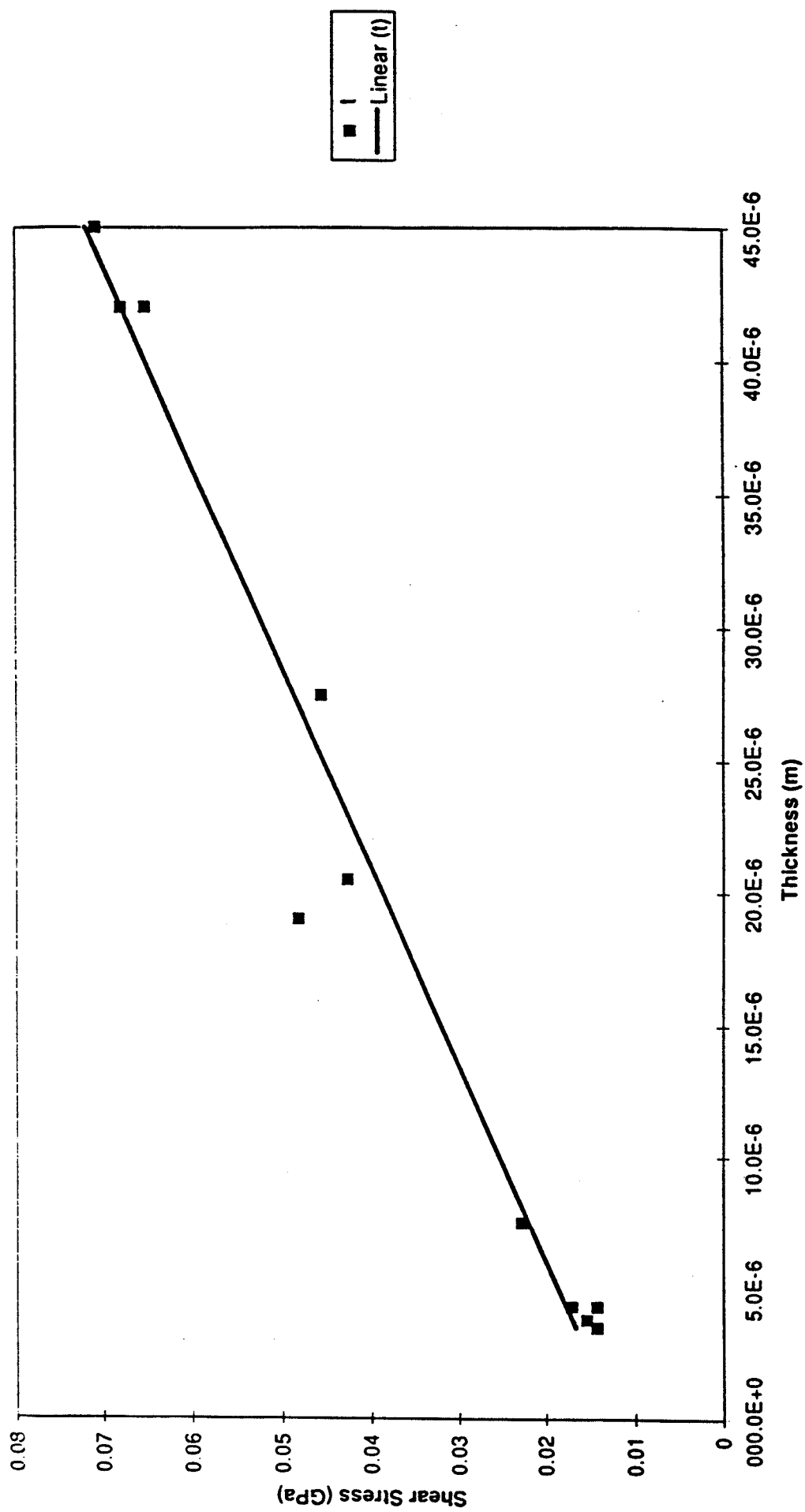


Figure 18 Max. Int. Shear Stress (calculated from Mahmood's Model, no. 6) versus Thickness of Oxide

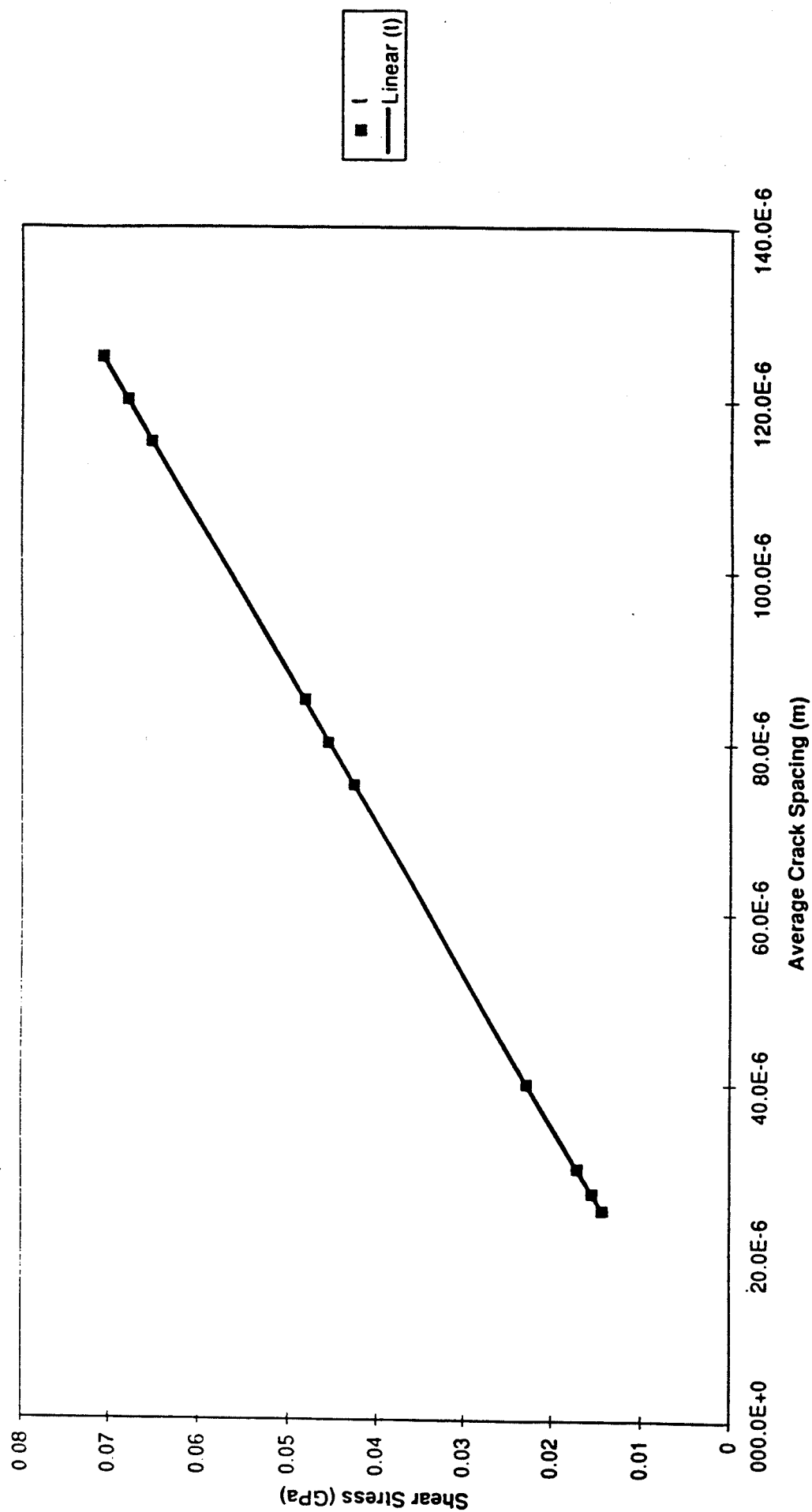


Figure 19 Max. Int. Shear Stress (calculated from Mahmood's Model, no. 6) versus Average Crack Spacing

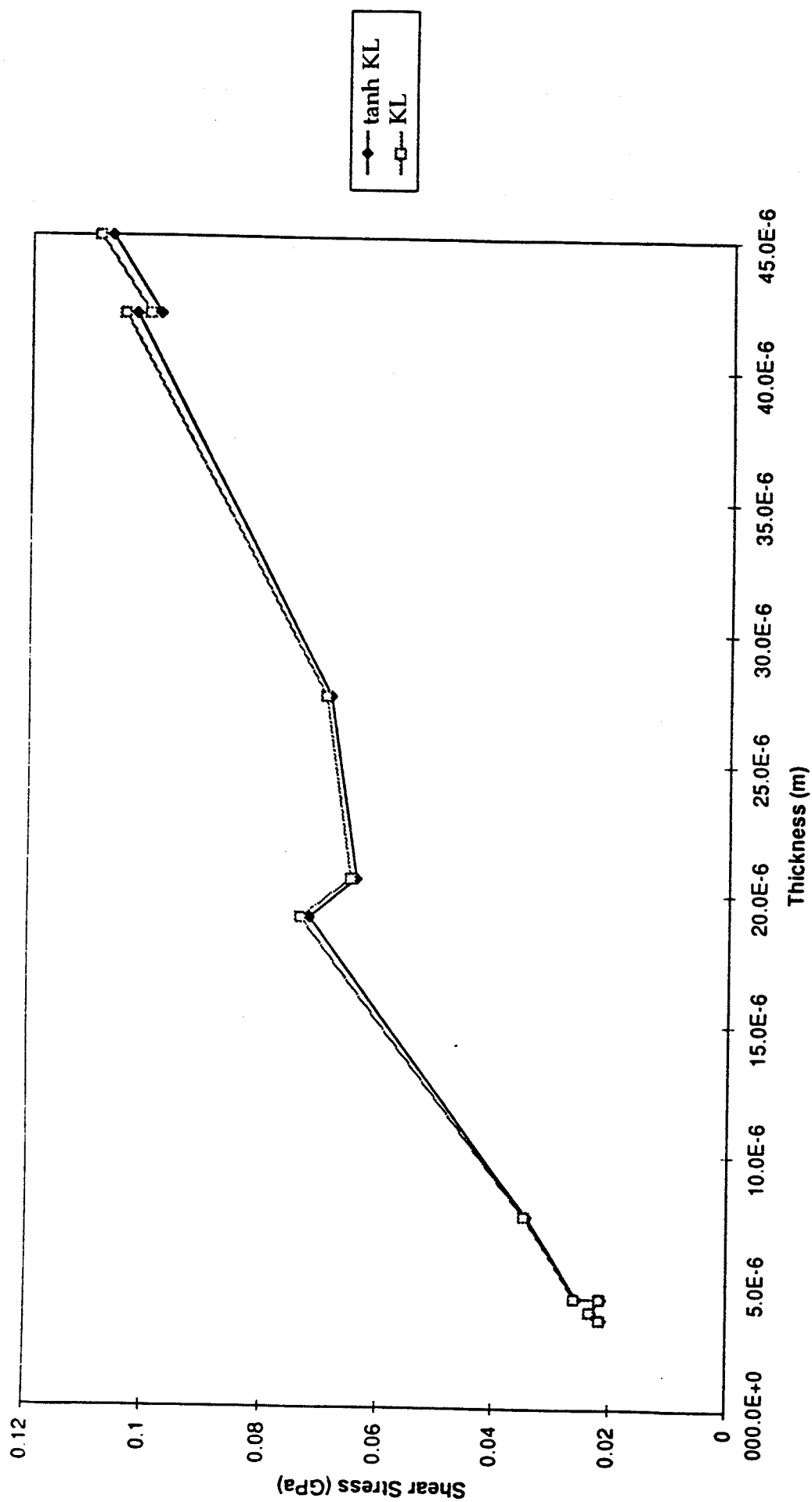


Figure 20 Accurate and Approximate Max. Int. Shear Stress (calculated from McCartney's model, no. 5)

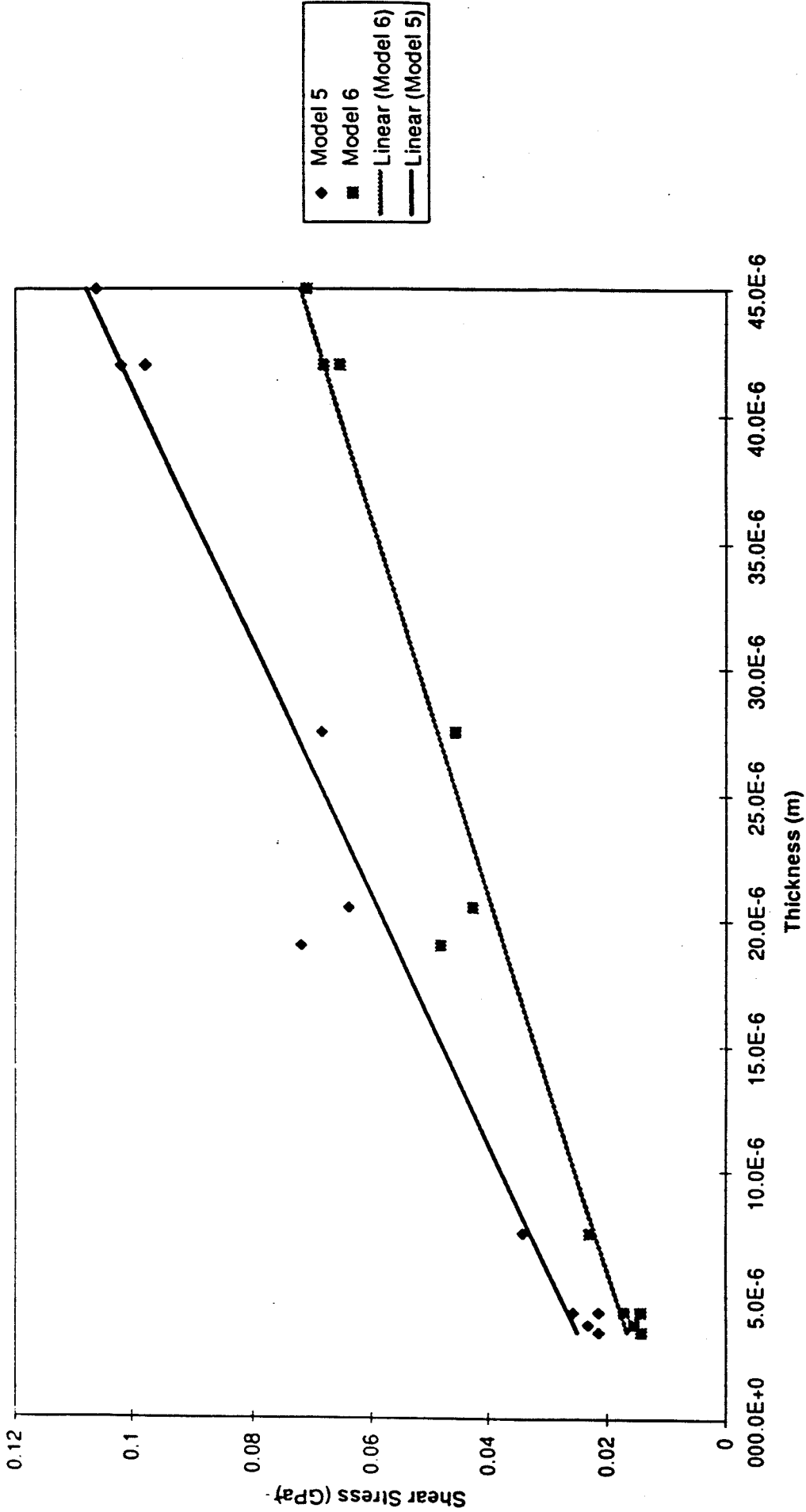


Figure 21 Max. Int. Shear Stress (calculated from Models 5 and 6) versus Thickness of Oxide

4 DISCUSSION AND CONCLUSION

4.1 DISCUSSION AND CONCLUSIONS

Model 1 - Ting et al

The papers which contain this model give no mathematical basis for it; the final equations are effectively assumptions, which throws a great deal of doubt on the model. Moreover, equation (3)

$$(C - 1) \xi^{C/(C-2)} - C \xi + 1 = 0$$

is said to be a polynomial, whereas in fact it is not. The values of C calculated from this model vary between about 30 and 400. For each value of C , it would be possible to perform a zero finding routine and find ξ , but the value might not be unique, or might not exist for some values of C . It was not possible to attempt such calculations in the time available for this work.

Model 2 - Armitt et al

The initial equation (6)

$$\epsilon^c = \epsilon + Ae^{y/\lambda} + Be^{-y/\lambda}$$

is assumed with no basis given, as is equation 11.

$$\epsilon_{\max} = \frac{L\tau_0}{bE^c} = \epsilon_k$$

Since these two equations are the basis of the entire model, doubt is cast on the validity of the model because they are assumed. The mathematics linking the two equations is perfectly valid, however. The values of τ_0 calculated from this model (see Figure 10) are rather larger than those of other models, but not unreasonably so. This model also requires the calculation of ϵ_k , the critical strain for failure. It is suggested that it could be found from equation 13.

$$\epsilon_k = \sqrt{\frac{\gamma}{2E^c d}}$$

Values of γ , the fracture surface energy density, and d , the flaw size of the initial crack, are both very difficult to find. However, ϵ_k can also be found from the applied strain and Poisson's ratio of the coating.

Model 3 - Tien et al

The assumption that the interfacial shear stress is a linear function of y is unjustified, as is the assumption that the strain is constant across the thickness of coating and substrate. However, Model 5 can justify the former. The term $\sinh ky$ in Model 5 can be replaced by ky when ky is very small. This is shown on Figure 20. Although Model 3 begins to sound more reasonable, the values of τ_0 found from it are ridiculously high, by about 2 orders of magnitude. (See Figures 12 and 13.) The failure strain of nickel oxide is at most 0.5%, according to Nagl *et al* [11], and this corresponds to a tensile fracture strength of at most 1 GPa (using a Young's modulus of 220 GPa.) It is unlikely that the interfacial shear stress would ever reach a value of 6 GPa as the calculations from this model suggest. It may be

that there is some systematic error which gives these values, but it has not been possible to find any such errors in the time available for this work.

Model 4 - Burton

This model is so simplistic that it bears very little resemblance to reality. Every assumption is a gross simplification, and every equation on which the model is based is assumed. The values of τ_0 obtained from Nagl's data show an enormous scatter (see Figures 15 and 16) and any discernable trends need to be viewed with care.

Model 5 - McCartney and Damerell

This model is the optimum shear-lag model, but any shear-lag model has inherent problems due to the simplifications involved. It neglects an important equilibrium equation, neglects Poisson's ratio effects, assumes that there is a linear relationship of shear stress across both coating and substrate, (although not necessarily the same relationship), and assumes that the materials involved behave elastically. However, these assumptions are more reasonable than those of the previous models, and the values calculated from this model are more realistic (see Figures 19 and 20 and page 22). Figure 21 shows the approximate shear stress, calculated under the assumption that kL is small enough than $\tanh kL \approx kL$. The close correlation between the two lines shows that it is a reasonable assumption. Under the assumption that this model is reasonably accurate, interfacial shear stress is shown to vary linearly with y . This supports the work of Tien *et al* (model 3), but does not explain why their final equation is so different.

Model 6 - Mahmood

This is another shear-lag model much like Model 5. It makes almost the same assumptions, but proceeds by a different route which involves some contradictions. Firstly, it is stated that the applied load will be shared between the coating and substrate according to their areas of cross-section only, whereas in fact the Young's moduli will also affect the load distribution. Secondly, the initial equation 63 states that

$$F = \sigma_y^s A^s + \sigma_y^c A^c$$

which is a statement of equilibrium only. Although this equation is correct, it does not, on its own, fully describe the relationship between the axial stresses in coating and substrate. Moreover, it is later assumed that the shear strain in the substrate away from the interface is expressed by the following relationship (equation 75)

$$\frac{v - u}{a/2} = \frac{\tau(y)}{\mu^s}$$

and there is no proven physical basis for this assumption. Although the values of interfacial shear stress calculated from this model are very similar to those in Model 5, (see Figure 22), the mathematics behind it is much more suspect.

4.2 CONCLUSION

Model 5 (McCartney) appears to be the most appropriate of the models discussed. Model 1 (Ting *et al*) is not currently in a usable state, models 2, 3 and 4 (Armitt *et al*, Tien *et al* and Burton, respectively) make excessive assumptions and produce suspect values. Model 6 (Mahmood) produces similar, although not identical, values to Model 5, but the mathematics behind it is not as rigorous. A useful piece of future work would be to compare the results given with those of more accurate, fracture mechanics based models such as those developed by McCartney (12) for composites.

5 ACKNOWLEDGEMENTS

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6 REFERENCES

1. B Ollivier and A Matthews, "Adhesion Assessment of Diamond-Like Carbon Films on Polyethyleneterephthalate using a simple tensile tester; Comparison of Different Theories", *Journal of Adhesion Science and Technology*, Vol 9, 1995, pp 769-784.
2. B Y Ting, S Ramalingam, W O Winer, "An Experimental Investigation of the Film-to-Substrate Bond Strength of Sputtered Thin Films Using a Semi-Quantitative Test Method", *Journal of Tribology*, Vol 107, 1985, pp 478-482.
3. J Armitt, D R Holmes, M I Manning, D B Meadowcroft, E Metcalfe, "The Spalling of Steam-Grown Oxide from Superheater and Reheater Tube Steels", *Epri report FP 686*, 1978, pp 4-13 to 4-17.
4. D R Wheeler, H Osaki, "Intrinsic Bond Strength of Metal Films on Polymer Substrates - A New Method of Measurement", *American Chemical Society, ACS Symposium Series 440*, 1990, Ch 36, p 500.
5. H E Evans, "Stress Effects in High Temperature Oxidation of Metals", *International Materials Review*, Vol 40, 1995, No. 1.
6. J K Tien, J M Davidson, "Oxide Spallation Mechanisms", *Proc. Symp. on Stress Effects and the Oxidation of Metals*, AIME 1974, pp 200-219.
7. M M Nagl, "Identification of the Mechanism of Oxide Scale Fracture, and its Correlation with Strain using Acoustic Emission", *PhD Thesis*, 1992.
8. B Burton, "The Low Stress Creep of Aluminium Near to the Melting Point: the Influence of Oxidation and Substructural Changes", *Philosophical Magazine*, Vol 25, 1992, p 645.
9. L N McCartney, "Analytical Models of Stress Transfer in Unidirectional Composites and Cross-Ply Laminates, and their Application to the Prediction of Matrix/Transverse Cracking", *Local Mechanical Concepts for Composite Material Systems*, 1992, pp 251-282.
10. K Mahmood, *PhD Thesis*, 1988, (Cranfield).
11. M M Nagl, S R J Saunders, W T Evans, D J Hall, "The Tensile Failure of Nickel Oxide Scales at Ambient and at Growth Temperature", *Corrosion Science*, Vol 35, 1993, Nos 5-8, pp 965-977.
12. L N McCartney, *Proceedings of IUTAM Symposium on Non-Linear Analysis of Fracture*, Cambridge 3-7 Sept 1995, 379-390, Kluwer Academic, Dordrecht, Boston and London, 1997.

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