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DETERMINATION OF THE ELASTIC CONSTANTS OF INHOMOGENEOUS

MATERIALS WITH X-RAY DIFFRACTION

BY

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DETERMINATION OF THE ELASTIC CONSTANTS OF INHOMOGENEOUS MATERIALS WITH X-RAY DIFFRACTION

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ABSTRACT

Experimental determination of the elastic constants is of fundamental importance in residual stress analysis with x-rays. Such constants are usually termed "x-ray elastic constants". In certain materials changes have been observed in these elastic constants as a result of plastic deformation. However, since for some of such cases the "d" vs. $\sin^2\psi$ plots used in the analysis were not linear, as predicted by theory, but oscillatory, the meaning of these variations was not fully understood. In this paper the meaning of "x-ray elastic constants" obtained from materials with oscillatory "d" vs. $\sin^2\psi$ plots is examined. It is shown that x-ray diffraction analysis is a powerful tool that can be used to determine the "effective elastic constants" of the material under investigation, even when the material is inhomogeneous.

INTRODUCTION

X-ray diffraction techniques are used widely in non-destructive measurement of residual stresses caused during production operations such as shot-peening, grinding, quenching[1]. Currently there are several x-ray methods for measuring residual stresses that utilize different assumptions as to the stress state existing in the near-surface layers sampled by the x-ray beam[1-5]. All of these techniques, however, utilize an interatomic spacing "d" in the material as an internal strain gage and determine the strain tensor existing in the surface layers from the slope of the "d" vs. $\sin^2\psi$ line. The residual stress tensor is then calculated through the use of Hooke's law.

This procedure, of course, requires that the appropriate elastic constants of the material be known accurately. The elastic constants used in the x-ray determination of residual stress are called "x-ray elastic constants" and are usually measured by x-ray diffraction[1]. When measured data is not available, these constants can be calculated from single crystal elastic constants using procedures given by Voigt , Reuss , Hill , or Kroner[3,6]. A review of the literature shows that in some cases the measured values do not fall between the Reuss and Voigt limits as postulated by theory[7]. In other cases a large dependence of measured elastic constants on plastic deformation (35-40 % for hardened steel undergoing uniaxial plastic deformation[8]) has been observed, while in other studies no such dependence was found[2]. Since in most of the cases discussed

above no error analysis of the results are given or, in some cases, elastic constants are calculated from oscillatory "d" vs. sin data, the causes of these anomalies are not clear.

In this paper the meaning of the "x-ray elastic constants" obtained from analysis of oscillatory "d" vs. $\sin^2\psi$ data is investigated. It will be shown that even for oscillatory "d" vs. $\sin^2\psi$ data, current techniques for x-ray elastic constant determination measure the total linear elastic response of the material in question to an applied load. The x-ray elastic constants determined from such data are 'effective elastic constants' and contain contributions from the shape and orientation distributions of the constitutive grains of the material. The possible causes for the variation of x-ray elastic constants with plastic deformation are also discussed.

THEORY

Assume that a homogeneous, normal stress σ_{ii}^{o}, which is below the elastic limit, is applied to the boundary of a residual-stress-free textured material. At a point A in the interior of the material σ_{ij}^{o} will cause the strains ε_{ij}. The strain ε_{ij} may be expressed as the sum of two components:

$$\varepsilon_{ij} = \varepsilon_{ij}^{o} + \varepsilon_{ij}^{in.} \tag{1}$$

Here ε_{ij}^{o} is the homogeneous elastic strain that would be observed if the stress was applied to a homogeneous isotropic

material. $\varepsilon_{ij}^{ia.}$, the reaction strain component, arises because of the variation of elastic constants along a given direction in the surface plane of the sample. Consider figure 1 where six grains of various orientations along a surface direction ($\underline{S}_1$) are shown. If these grains were subjected seperately to $\sigma_{ii}^{\bullet}$ on their boundaries, each would have a different strain $\varepsilon_{11}^{\bullet}$ along $\underline{S}_1$, related to $\sigma_{ii}^{\bullet}$ through the general Hooke's law[6,9],

$$\varepsilon_{11}^{\bullet} = S_{11kl} \, \sigma_{kl}^{\bullet} \qquad (2)$$

These different strains indicate different displacements in the different grains. However in a solid body where grains are in rigid contact, displacements across a grain boundary along $\underline{S}_1$ must be constant in order to avoid having voids, and a reaction stress field constraining the possible displacements arises and causes the reaction strains $\varepsilon_{ij}^{ia.}$. The magnitude of the reaction stresses (and hence the reaction strains) depend on the difference between the displacements that have to be made compatible at a point and varies from point to point since the effect of surrounding grains at each point is different. However as long as the total stress at a point is lower than the microscopic elastic limit at any point, the magnitude of the reaction stresses and strains at any point will be directly proportional to the applied stress.

Thus if a homogeneous stress $\sigma_{11}^{\bullet}$ in the $\underline{S}_1$ direction is applied at the boundary

of the material, the components of the strain tensor at any point A in the material may be expressed as:

$$\varepsilon_{11}(x,y,z) = \sigma_{11}^{0} \cdot \left\{ \frac{1}{E} + K_{1}'(x,y,z) \right\}$$

$$\varepsilon_{22}(x,y,z) = \sigma_{11}^{0} \cdot \left\{ -\frac{\nu}{E} + K_{2}'(x,y,z) \right\}$$

$$\varepsilon_{33}(x,y,z) = \sigma_{11}^{0} \cdot \left\{ -\frac{\nu}{E} + K_{3}'(x,y,z) \right\} \tag{3}$$

$$\varepsilon_{13}(x,y,z) = \sigma_{11}^{0} \cdot K_{4}'(x,y,z)$$

$$\varepsilon_{23}(x,y,z) = \sigma_{11}^{0} \cdot K_{5}'(x,y,z)$$

$$\varepsilon_{21}(x,y,z) = \sigma_{11}^{0} \cdot K_{6}'(x,y,z)$$

here x, y, z are the coordinates of the point A with respect to a coordinate system describing the surface, and $K_{j}'(x,y,z)$ are the proportionality constants at A between the applied load and the resulting reaction strains. The constants K_{4}', K_{5}', K_{6}' may be finite depending on the symmetry of the constitutive grains of the material[9]. Also in certain cases the local symmetry changes as one approaches a grain boundary[10]. In the following discussion it is assumed that $K_{4}' = K_{5}' = K_{6}' = 0$.

If the material also has an inhomogeneous residual stress distribution the total elastic strain ε_{ij}^{t} at a point will also have a residual strain component in addititon to the strains caused by the applied stress. Thus for this case equations (3) become:

$$\varepsilon_{ij}^{t}(x,y,z) = \varepsilon_{ij}(x,y,z) + \varepsilon_{ij}^{r}(x,y,z) \tag{4}$$

where $\varepsilon_{ij}^{r}(x,y,z)$ is the residual strain at the point (x,y,z).

Now assume that this material is placed, applied stress and

all , on a diffractometer and a beam of x-rays, (whose edges
extend from X_1 to X_2 along $\underline{S}_1$, Y_1 to Y_2 along $\underline{S}_2$ and
which penetrates a distance τ along $\underline{S}_3$ into the material), is
used to measure the average strain along $\underline{L}_3$ in the
$\underline{L}_i$ coordinate system, which makes the angles ϕ and γ with the
sample coordinate system $\underline{S}_i$ (fig.2). This is done by measuring
the lattice spacing $d_{\phi\gamma}$ along $(\underline{L}_3)_{\phi\gamma}$, and then obtaining the
average strain along $(\underline{L}_3)_{\phi\gamma}$ from:

$$\langle \varepsilon'_{33} \rangle_{\phi\gamma} = \frac{\langle d_{\phi\gamma} \rangle - d_o}{d_o} \qquad (5)$$

where d_o is the unstressed lattice spacing, and carats
represent averages over the diffracting volume.

The relationship between the average strains $\langle \varepsilon_{ij} \rangle$ in the
sample coordinate system and the average strains measured by
x-rays in the laboratory coordinate system is given by the
transformation rule for tensors of second rank:

$$\langle \varepsilon'_{33} \rangle_{\phi\gamma} = a_{3k} a_{3l} \langle \varepsilon_{kl}^t \rangle \qquad (6)$$

For $\phi = 0$, and $\gamma = \gamma_j$, substituting the actual values for the
direction cosines a_{3k} , a_{3l} into the above equation:

$$\langle \varepsilon'_{33} \rangle_{\gamma_j} = \frac{\langle d_{\gamma_j} \rangle - d_o}{d_o} = \left\{ \langle \varepsilon_{11}^t \rangle_{\gamma_j} - \langle \varepsilon_{33}^t \rangle_{\gamma_j} \right\} \cdot \sin^2 \gamma_j \quad (7)$$

$$+ \langle \varepsilon_{33}^t \rangle_{\gamma_j}$$

The average strains $\langle \varepsilon_{ij} \rangle$ in equation (7) are related to the strains at a point (equations 3,4) through equations of the form:

$$\langle \varepsilon_{ij}^t \rangle_{\psi_j} = \frac{\sum_{i=1}^{N_j} \frac{\int_{V_i} \varepsilon_{ij}^t (x,y,z) \cdot f(z) \cdot dV}{\int_{V_i} f(z) \, dV}}{\sum_{i=1}^{N_j} V_i} \qquad (8)$$

Here $\varepsilon_{ij}(x,y,z)$ is the strain at point (x,y,z) in a diffracting grain in the irradiated volume, V_i is the volume of this grain, $f(z)$ is a function relating the variation of diffracted intensity to depth (z), and N_j is the total number of grains diffracting at a tilt angle ψ_j. The summation is used instead of an integral since the diffracting grains are not necessarily contiguous. It must also be noted that because x-rays may penetrate to a different depth (z) for each ψ-tilt due to absorbtion[4] and, for finite beam sizes, the intersection of the tilting specimen with the beam changes the dimensions $x_2 - x_1$, $y_2 - y_1$ the total irradiated volume is also a function of the tilt angle "ψ_j". This means that parameters that are a function of volume can also be expressed as a function of ψ.

The evaluation of the average x-ray strains in terms of the strains at a point is exteremely complicated since, to date, the exact nature of the coupling terms in equation (8) is not known[6]. However by inspection of equations (8), (3) and (4) it can be seen that the average strain may be written in terms of

the average strain components contributing to it:

$$\langle \varepsilon_{ij} \rangle^t = (\mathcal{E}_{ij}^o) + \langle \varepsilon_{ij} \rangle^{in.} + \langle \varepsilon_{ij} \rangle^r \qquad (9)$$

or, from equations 3,8,9:

$$\langle \varepsilon_{11} \rangle^t = \sigma_{11}'^o \cdot \left\{ \frac{1}{E} + K_1(\psi) \right\} + \langle \varepsilon_{11} \rangle^r$$

$$\langle \varepsilon_{23} \rangle^t = \sigma_{11}'^o \left\{ -\frac{\nu}{E} + K_3(\psi) \right\} + \langle \varepsilon_{33} \rangle^r \qquad (10)$$

and similar equations may be written for the other terms of the strain tensor. Here $K_i(\psi)$ is the average proportionality constant describing the average response (described by equations 3,8) of the population of grains diffracting at tilt angle ψ_j to an applied load, and $\langle \varepsilon_{ij} \rangle^r$ is the average (inhomogeneous) residual strain in this population.

By substituting equations (10) into equation (7) the relationship between the applied stress and the measured strain is obtained:

$$\langle \varepsilon_{33}' \rangle_{\psi_j} = \frac{d_{\gamma_j} - d_o}{d_o} = \left[\sigma_{11}'^o \left\{ \frac{1+\nu}{E} + K_1(\psi_i) - k_3(\psi_i) \right\} \right.$$

$$\left. + \langle \varepsilon_{11} \rangle^r - \langle \varepsilon_{33} \rangle^r \right] \cdot \sin^2 \psi_j + \sigma_{11}'^o \left\{ -\frac{\nu}{E} + K_3(\psi_j) \right\} \qquad (11)$$

$$+ \langle \varepsilon_{33} \rangle^r_{\psi_j}$$

Since $K_i(\psi), \langle \varepsilon_{ij} \rangle^r$ are not constant in $\sin^2 \psi$, equation 11 describes a function that is non-linear in $\sin^2 \psi$. On the other hand, in a homogeneous material the interaction terms are zero by

definition and for a homogeneous residual stress distribution the terms $\langle \varepsilon_{ij} \rangle'$ are constant for all ψ tilts, thus for this case a linear "d" vs. $\sin^2 \psi$ plot will be obtained.

If a linear least-squares line is fitted to the data, described by equation (11), (as is usually done in practice), it is assumed that the function,

$$d_{\psi_j} = \beta_0 + \beta_1 \sin^2 \psi_j + e \qquad (12)$$

describes the relationship between d and $\sin^2 \psi$. Here e is the random error component. The regression parameters β_i are then obtained from the equation:

$$\beta_1 = \frac{\sum_{j=1}^{n} (\sin^2 \psi_j - \overline{\sin^2 \psi_j})(d_{\psi_j} - \overline{d_{\psi_j}})}{\sum_{j=1}^{n} (\sin^2 \psi_j - \overline{\sin^2 \psi_j})} \qquad (13\text{-}a)$$

$$\beta_0 = \overline{d_{\psi_j}} - \beta_1 \cdot \overline{\sin^2 \psi_j} \qquad (13\text{-}b)$$

where n is the number of ψ tilts and:

$$\overline{\sin^2 \psi_j} = \frac{\sum_{j}^{n} \sin^2 \psi_j}{n}$$

$$\overline{d_{\psi_j}} = \frac{\sum_{j}^{n} d_{\psi_j}}{n} \qquad (14)$$

It must be noted that, because a "linear" fit is forced on oscillatory data, the parameters β_0, β_1 can not be called "slope" and "intercept" of the least-squares line in the traditional sense (e.g. as in the conventional analysis of linear "d" vs. $\sin^2\psi$ plots). Here they are simply mathematical functions described by equations (13 a,b).

Substituting equation (11) into equation (13-a) we obtain:

$$\beta_1 = \frac{d_0}{\sum\limits_{j=1}^{n} c_j^2} \cdot \left\{ \sigma_{11}^0 \sum_{j=1}^{n} c_j \left[\left\{ \left(\frac{1+\nu}{E}\right) + K_1(\gamma_j) - K_3(\psi_j) \right\} \cdot \sin^2\psi_j \right. \right.$$

$$+ K_3(\gamma_j) - \frac{\nu}{E} \sum_{j=1}^{n} \left\{ \left(\frac{1+\nu}{E}\right) + K_1(\psi_j) - K_3(\psi_j) \right\} \cdot \sin^2\psi_j \qquad (15)$$

$$\left. + K_3(\gamma_j) - \frac{\nu}{E} \right] + \sum_{j=1}^{n} c_j \left[\left\{ \langle \varepsilon_{11} \rangle_{\psi_j} - \langle \varepsilon_{33} \rangle_{\psi_j} \right\} \cdot \sin^2\psi_j + \langle \varepsilon_{33} \rangle_{\gamma_j} + 1 \right.$$

$$\left. \left. - \sum_{j=1}^{n} \left\{ \langle \varepsilon_{11} \rangle_{\psi_j} - \langle \varepsilon_{33} \rangle_{\psi_j} \right\} \sin^2\psi_j + \langle \varepsilon_{33} \rangle_{\gamma_j} + 1 \right] \right\}, \quad C_j = \sin^2\psi_j - \overline{\sin^2\psi_j}$$

which can be written simply as:

$$\beta_1 = \sigma_{11}^0 \, \overline{S}_1\left(\frac{1+\nu}{E}, \, K_i(\gamma)\right) + \overline{S}_2\left(\langle \varepsilon_{ij} \rangle\right) \qquad (16)$$

Where the function $\overline{S}_1\left(\frac{1+\nu}{E}, K_i(\psi)\right)$ is an average, defined by equation 15, of the terms $\frac{1+\nu}{E}$, $K_1(\gamma)$, $K_3(\psi)$. The term $\overline{S}_2$ is an average residual stress term.

A similar equation can be written for β_0. However this case is more complicated and will not be treated here.

From equation 16 it is seen that the variation of the parameter β_1 with applied load σ_{11}^0 is linear. The slope of the β_1 vs. σ_{11}^0 : $\overline{S}_1\left(\frac{1+\nu}{E}, K_i(\gamma)\right)$ is a measure of the average elastic

response of the inhomogeneous material to an applied load and contains the interaction terms $K_i(\psi)$. Thus it is not an elastic constant (S_{ijkl} , C_{ijkl}) in the strict sense defined by linear elasticity theory. In figure 3, "d" vs. $\sin^2\psi$ plots for α-brass (a), β-brass (b), 1008 steel (c) and 1075 steel (d) loaded in-situ on a diffractometer to various elastic loads are shown. The variation of the parameter β_i calculated from these curves vs. applied load for these materials is shown in figure 4. The "x-ray elastic constants" obtained from figure 4, and average macroscopic elastic constants calculated from single crystal elastic constants for these materials in the Voigt[3] (constant strain in all grains), Reuss[3] (constant stress in all grains), and Kroner[3] (anisotropic precipitate coupled to an isotropic matrix) limits are given in table I.

DISCUSSION

The differences between the average elastic constants calculated from single crystal values without taking coupling effects into account, and those obtained from the experimental procedure described above are measures of the reaction stresses (and strains) caused by the inhomogeneity of the material in question. It is thus seen that a study in the variation of "x-ray elastic constants" with plastic deformation for a given specimen is really a study of the change in the inhomogeneous distribution of crystallographic directions (and the grains) along a direction in the surface coordinate system, and the constraining effect such a distribution has on the strains

caused by an applied stress. If during the study, the plastic deformation causes changes in this distribution such that the average reaction stresses, and hence $k_i(\gamma)$ changes, the "x-ray elastic constants" will change also. In fact one should not use the term "elastic constants" for these parameters when they have been evaluated from oscillatory "d" vs. $\sin^2\gamma$ plots, where the oscillations are due to the reaction stresses generated by $\sigma_{11}^{\bullet}$, since, in this case they are not fundamental material properties that depend only on the interatomic forces like E or ν, but also contain simple configurational parameters. If the plastic deformation is such that the inhomogeneous residual strains ε_{ij}^r change, but the coupling constants are not affected, then no change in the "x-ray elastic constants" will be observed since, even though such a residual strain (or stress) distribution causes oscillations in "d" vs. $\sin^2\gamma$, the residual strain distribution itself is not a function of the elastic loads applied (after plastic deformation) during the measurement and will affect only the intercept of the β_i vs. $\sigma_{11}^{\bullet}$ plot (equation (16)).

The configurational parameters contributing to such "effective elastic constants" may have two main components. The shape distribution of the grains in the material is one of the possible components. Wull has treated the effect of the inclusion shape on the average elastic moduli of a two phase material and determined that disk shaped precipitates cause a significant increase in the average Young's modulus. For a textured material the non-random distribution of crystallographic directions (and hence elastic moduli S_{ijkl})

within the material volume will also contribute to such "effective elastic constants".

One other conclusion from this line of reasoning is that even if the oscillations in "d" vs. $\sin^2\psi$ plots from two samples of the same material look alike, unless the shapes of any precipitates that might be present and the distribution of crystallographic directions in the constitutive grains of the matrix along surface directions are the same for both specimens, and in both cases the oscillations are due to the same effect, they may not have the same "x-ray elastic constants". In fact such effective elastic constants may be different along different surface directions of a given specimen.

It must be emphasized that, even though it is possible to measure the effective elastic constants of a textured material accurately along any direction in the specimen surface using x-ray methods, these constants may not be used to determine the residual stress state by x-rays. This is due to the fact that when "d" vs. $\sin^2\psi$ is oscillatory the stress/strain state is inhomogeneous[12] and an average value for an inhomogeneous distribution (where the distribution function is not known), is of dubious utility. Rather, one may utilize the x-ray elastic constant measurements for such materials to determine the effect of shape/orientation distributions on the elastic properties of a given material.

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CONCLUSIONS

1) Conventional methods of "x-ray elastic constant"
determination measure the total elastic response of the material
under analysis whether the "d" vs. $\sin^2\psi$ plots obtained from
this material are linear or oscillatory. For both of these
cases the plot of applied load
vs. linear-least-squares-regression-parameter will be linear as
long as the test is carried out within the elastic range.

2) "X-ray elastic constants" obtained from oscillatory "d"
vs. $\sin^2\psi$ plots, where the oscillations are due to the reaction
stresses (caused by an applied stress) contain configurational
parameters in addition to Young's modulus and Poisson's ratio
and are not, in a strict sense, "elastic" constants. A better
name for such constants may be 'effective elastic constants'.

3) The configurational parameters contributing to these
effective elastic constants may be due to shape and/or
crystallographic direction distributions of the constitutive
grains in the material.

4) If during plastic deformation the distribution of
crystallographic directions in individual grains, or the shape
of any precipitates along surface directions changes, such
change may reflect in the configurational parameters and cause
an apparent change of (x-ray) "elastic constants" with plastic
deformation.

5) If, on the other hand, in a given sample plastic deformation
only changes the residual stress distribution, but does not
affect the distribution of crystallographic orientations or
precipitate shapes along surface directions, there will be no

change in "x-ray elastic constants" with plastic deformation.

4) The average interaction parameters can not be evaluated easily from first principles since, in order to calculate the interaction among non-random composite elements, the boundary value problems of elasticity must first be solved . The x-ray average of the fields calculated by these solutions must then be calculated using a formula similar to (8).

ACKNOWLEDGEMENTS

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FIGURE CAPTIONS

Figure 1: Grains with various crystallographic orientations along a sample coordinate $\underline{S}_i$. The strains forming in each grain in response to a uniform applied stress at the boundary (σ_M°) will be different due to Hooke's law.

Figure 2: Definition of the specimen $\underline{S}_i$ and laboratory $\underline{L}_i$ coordinate systems.

Figure 3: "d" vs. $\sin^2\psi$ plots at various loads from alpha-brass (a), beta-brass (b), 1008 steel (c), 1075 steel (d). The specimens were loaded in-situ on the diffractometer. For a description of the apparatus see reference 7.

Figure 4: Variation of regression parameter β_i (determined from figures 3 a,b,c, d) vs. applied load

Table I: Bulk elastic constants $(1+v)/E$ (Mpa^{-1}) calculated from single crystal elastic compliances in various limits and obtained from figures 3 a,b,c,d.

Table I

| Calculation Limit	Alpha-Brass* (220)	Beta-Brass* (211)	1008 Steel** (211)	1075 Steel*** (211)
VOIGT[3]	9.99.10-6	9.42.10-6	5.63.10-6	5.63.10-6
REUSS[2]	1.20.10-6	1.75.10-6	5.84.10-6	5.84.10-6
KRONER[3]	1.07.10-6	1.14.10-6	5.71.10-6	5.71.10-6
EXPERIMENTAL+	9.90.10-6	4.494.10-6	6.19.10-6	6.84.10-6

*   Experimental data obtained from respective phases of a 60-40 Cu-Zn specimen, machined from cold-rolled sheet. This configuration maximizes the interaction coefficients $K_i(\psi)$.

**   Specimen machined from as-received cold-rolled plate.

***   Specimen solution-treated @ 760°C for 2 hrs. to facilitate carbide precipitation, then grit-blasted to randomize the surface and annealed at 450°C for 45 minutes.
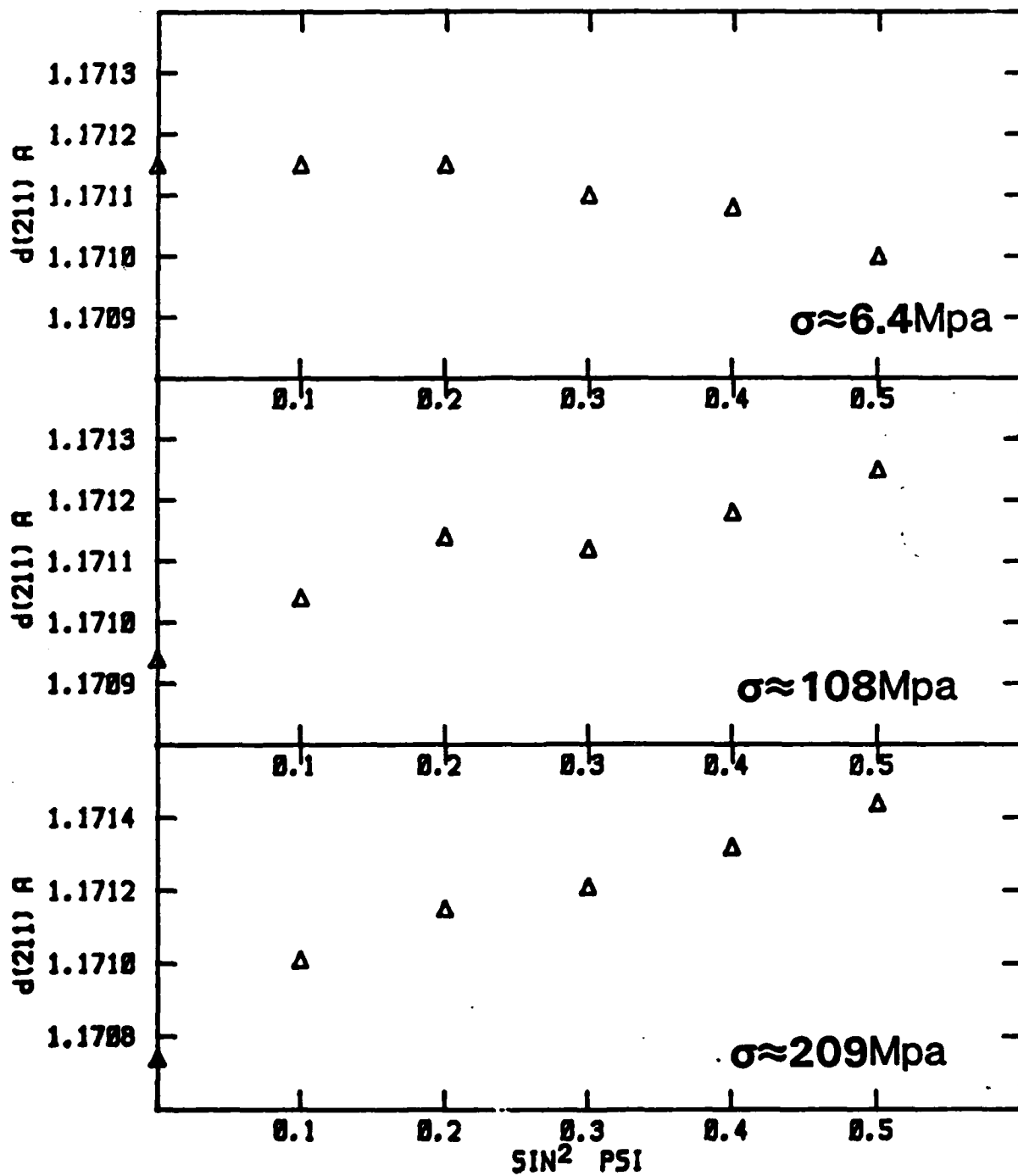
+   The total (statistical plus geometric) error associated with each value is less than 15%. The equations used in error calculations are from reference 7.
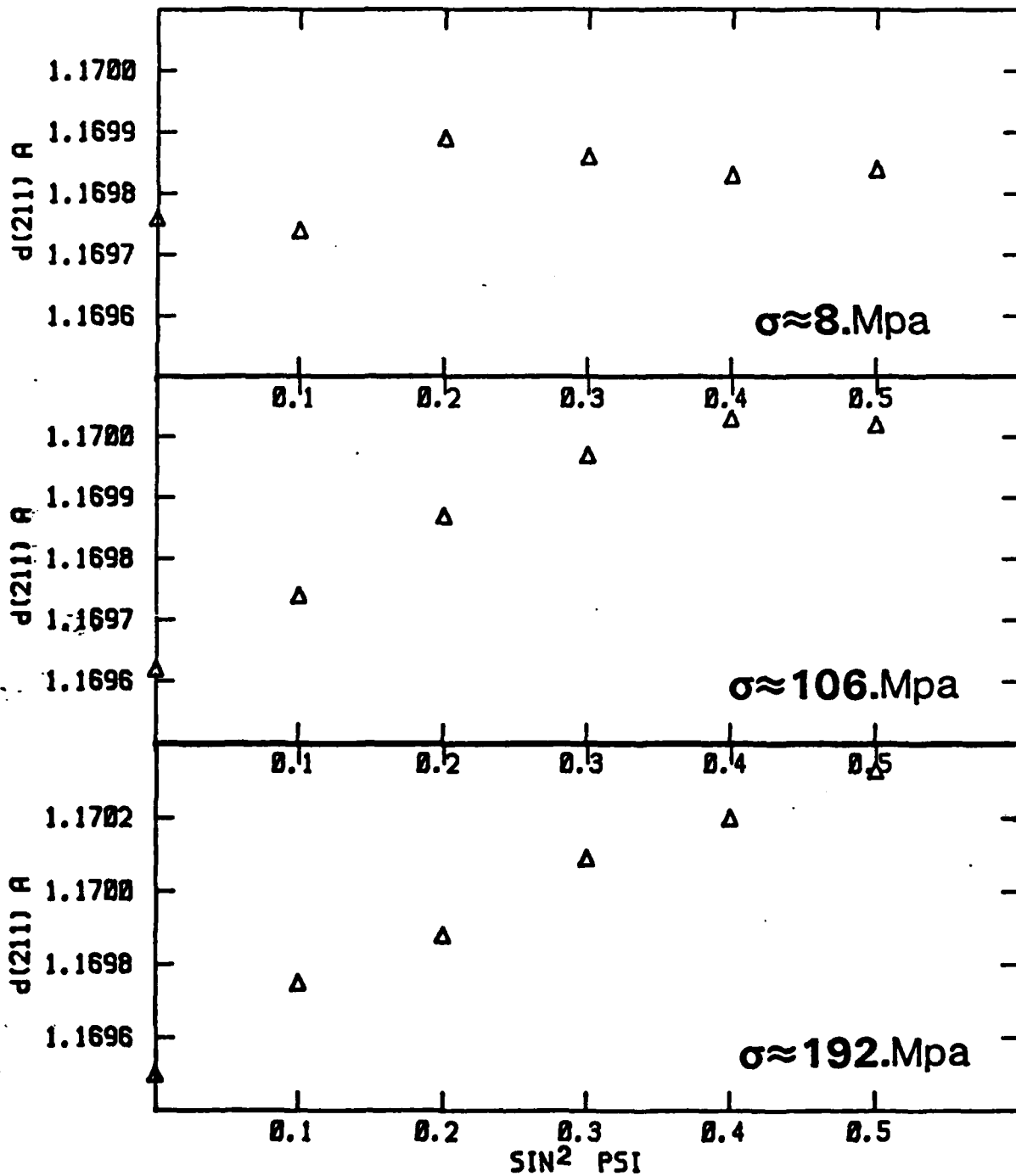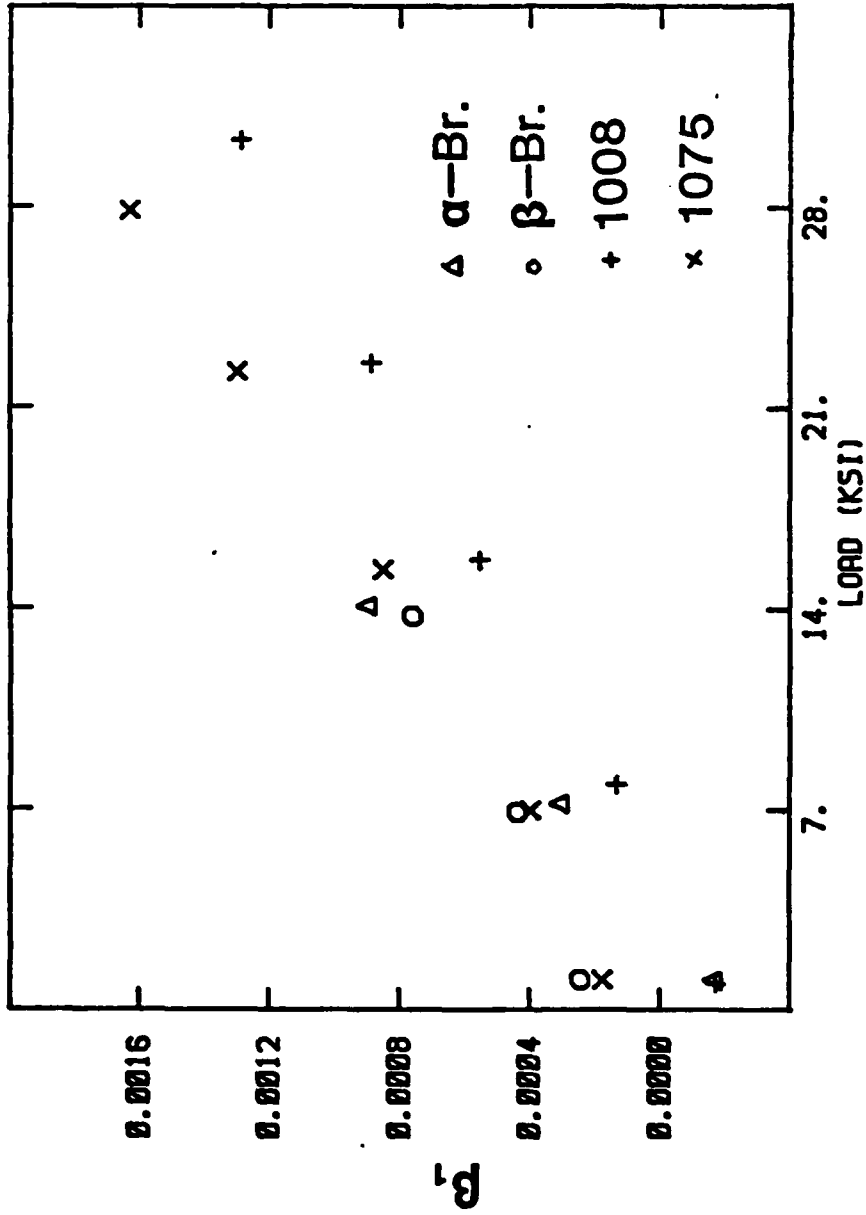
LOAD (KSI)

β_1

△ α—Br.
◦ β—Br.
+ 1008
× 1075
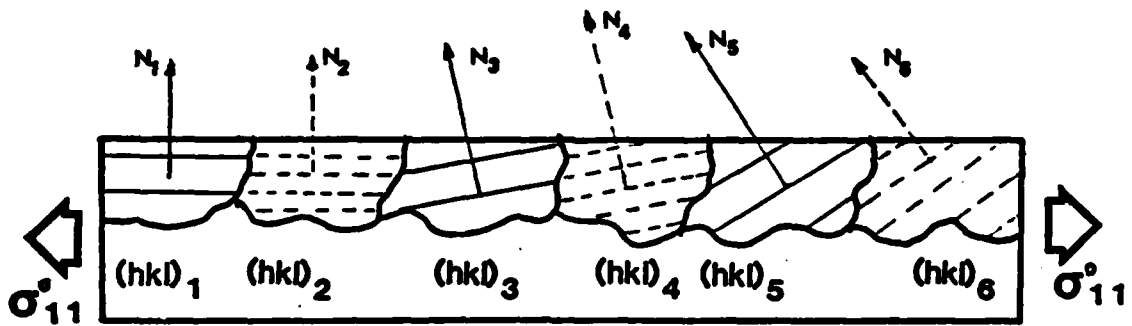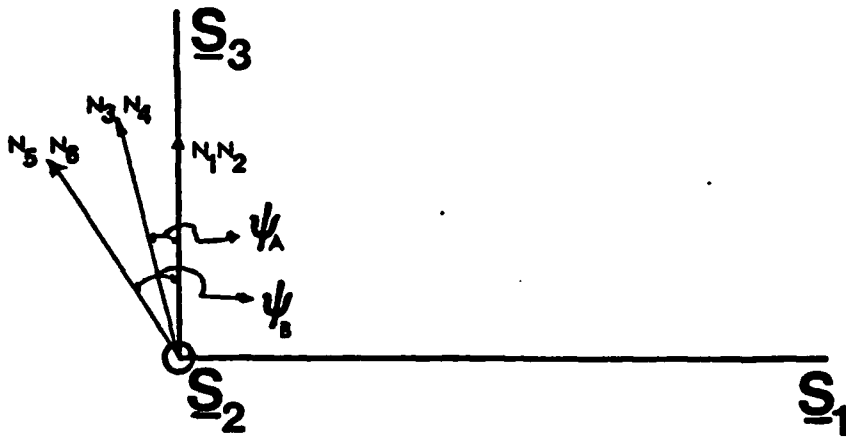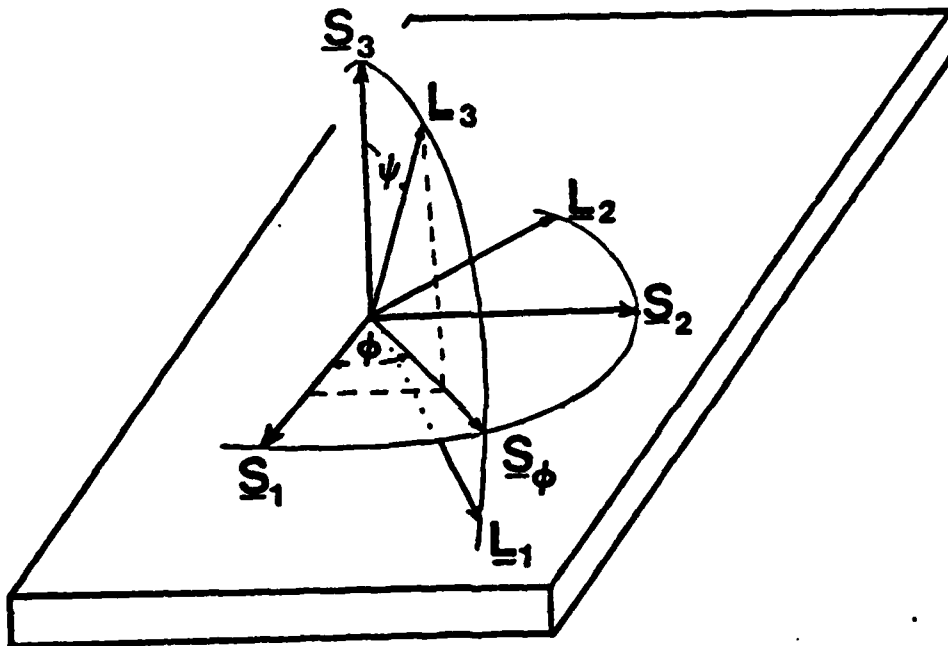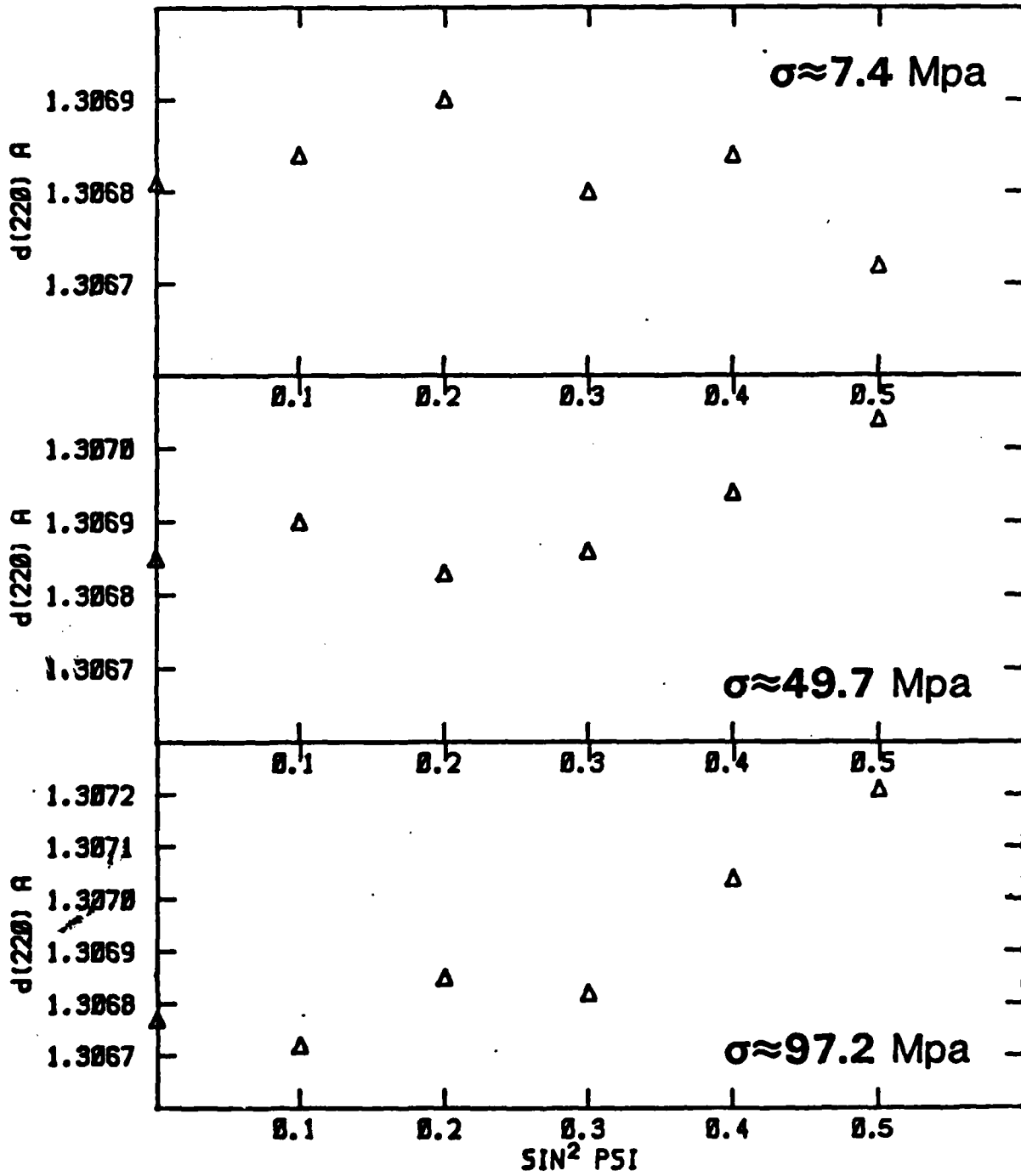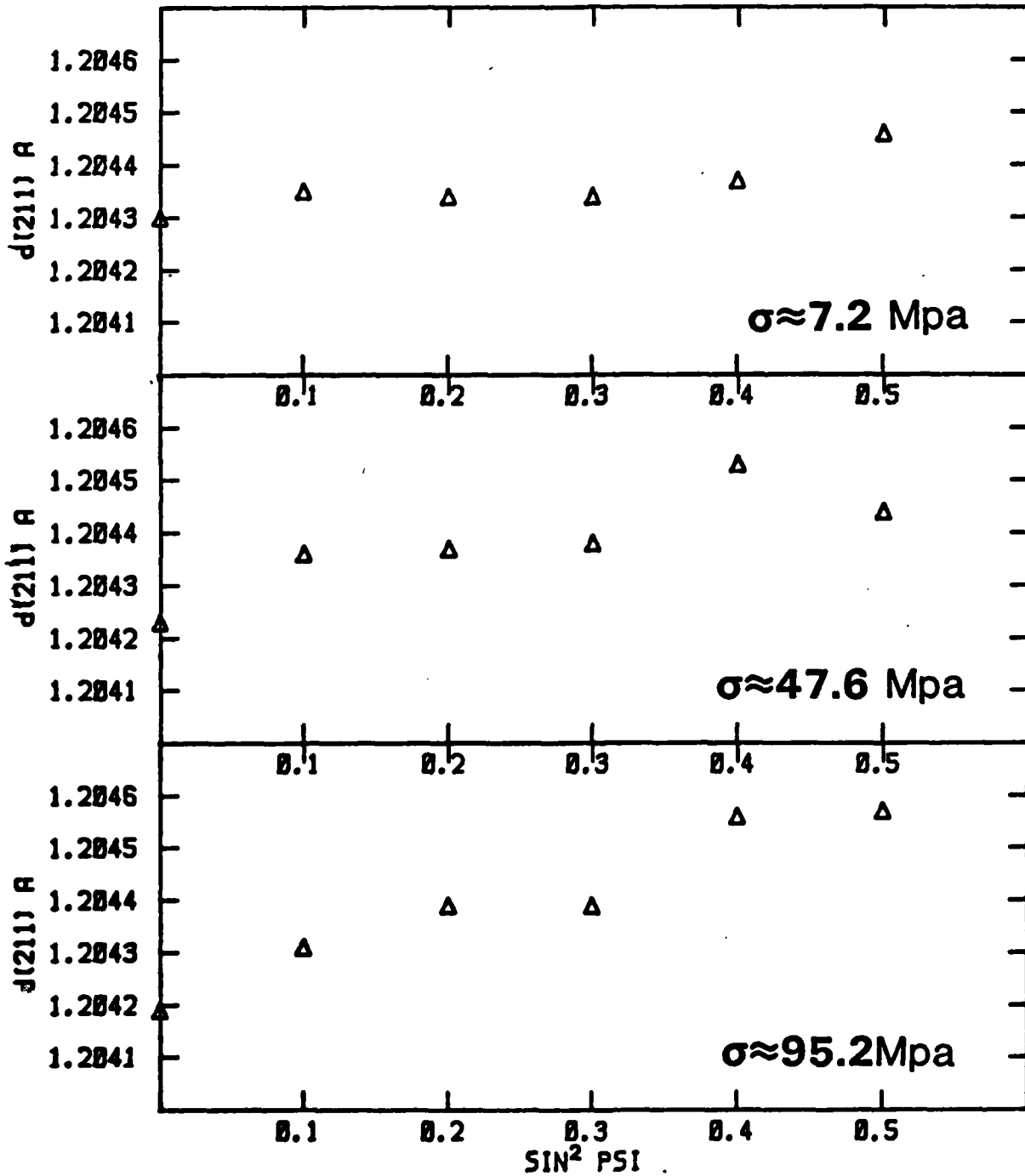
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13. ABSTRACT

Experimental determination of the elastic constants is of fundamental importance in residual stress analysis with x-rays. Such constants are usually termed "x-ray elastic constants". In certain materials changes have been observed in these elastic constants as a result of plastic deformation. However, since for some of such cases the "d" vs. $\sin^2\psi$ plots used in the analysis were not linear, as predicted by theory, but oscillatory, the meaning of these variations was not fully understood. In this paper the meaning of "x-ray elastic constants" obtained from materials with oscillatory "d" vs. $\sin^2\psi$ plots is examined. It is shown that x-ray diffraction analysis is a powerful tool that can be used to determine the "effective elastic constants" of the material under investigation, even when the material is inhomogeneous.

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14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
X-ray elastic constants						
elastic constants						

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