X RAY ELASTIC CONSTANTS IN TEXTURED TITANIUM SHEETS AND BARS

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INTRODUCTION

Hexagonal closed packed materials present strong crystallographic textures. A direct consequence of texture presence in these materials is the anisotropy of mechanical properties which influences the Residual Stress (R.S.) determination using diffraction technique. As a matter of fact, the evaluation of R.S. states requires the knowledge of the X-Ray Elastic Constants (XREC) which depend of the elastic properties of crystals, the crystallographic texture of the material and the family $\{hkl\}$ of diffracting planes.

For anisotropic elastic materials, the macroscopic behaviour can not anymore be described by only two XREC, as in the isotropic case. In that case, it is necessary to introduce the texture in the evaluation of XREC. It can be done either using a set of discrete orientations associated to the principal components of texture¹ or by means of the Orientation Distribution Function (O.D.F.), which gives a quantitative description of textures. Barralet al² used the O.D.F. and the Reuss assumptions for XREC calculations in cubic materials.

The aim of this work is to study the case of textured Titanium sheets for all the $\{hkil\}$ crystalline planes which can be used in X-Ray diffraction stress measurements. Their XREC are also calculated using the O.D.F. and Reuss hypothesis in the case of Titanium thin sheet and also for Titanium extruded bars.

CALCULATION OF X-RAY ELASTIC CONSTANTS

In a general case, the constitutive equations for elasticity in the laboratory system are given by:

$$\epsilon_{33} = R_{33ij} \cdot \sigma_{ij} \quad (1)$$

where R_{33ij} are the X-Ray compliances. It can be referred to the sample system as:

$$\epsilon_{33} = R_{33ij} \cdot a_{ik} \cdot a_{j1} \cdot \sigma_{k1} = F_{ij} \cdot \sigma_{ij} \quad (2)$$

a_{ij} being the components of the rotation matrix, described in an Eulerian space, which allows to link the laboratory system to the sample system. F_{ij} are the XREC to be determined. Assuming an orientation (ϕ, ψ) of the laboratory system and a given family of planes $\{hkl\}$ contributing to diffraction, under Reuss hypothesis, the R_{33k1} values are calculated from²:

$$R_{33k1} = (1/V_d) \int S_{33k1} \cdot dV_d \quad (3)$$

where V_d is the diffracting volume of the material. The knowledge of V_d requires the determination of the fraction of volume associated to grains so that the normal directions to the $\{hkl\}$ planes verify the diffraction conditions. Then, it is evident that a quantitative description of texture must be introduced in the resolution of eq. (3). The representation of texture used in this work is given by the ODF, $F(g)$ ³. For the resolution of eq.(3), it is necessary to consider that any rotation $d\theta$ around the L3 direction does not change the diffraction conditions. Then, this equation can be written as:

$$R_{ij k1} = \frac{\int S_{ij k1} \cdot F(g) \cdot dg \cdot d\theta}{\int F(g) \cdot dg \cdot d\theta} \quad (4)$$

The resolution of this equation in the Euler space requires the description of the rotation $d\theta$ around L3 and the elastic compliances in the laboratory systems ($S_{ij k1}$). Details about the calculation of this equation are given in another publication⁴. The Ti single crystals elastic constants used in this paper correspond to those obtained by Fisher and Renken⁵.

RESULTS

Crystallographic textures.

In this work, the ODF for Ti samples were calculated for

an expansion order $l=16$ without considering the odd part of the function⁶. The ODF analysis put in evidency that for Ti sheets the c axes are concentrated around the plane defined by the normal direction and the transversal direction being reinforcements observed for the components $\{10\bar{1}3\}\langle 1\bar{2}10\rangle$ and $\{2\bar{1}\bar{1}5\}\langle 10\bar{1}0\rangle$. These components direct the c axes near 30° from the normal direction. In the case corresponding to extruded bars, a distribution of $[0002]$ directions concentrated around the plane formed by the radial and tangential directions is observed. The ODF reinforcements are near the $\{1\bar{1}00\}\langle 11\bar{2}0\rangle$ and $\{2\bar{2}01\}\langle 11\bar{2}0\rangle$ components, which are related to the c axes directed in positions close to the transversal direction. The weight of this distribution decreases when the orientation of c axes moves towards the rolling direction.

X-Ray Elastic Constants

In the case of Ti sheets and bars two cases can be clearly distinguished:

1) F_{ij} vs $\sin^2\psi$ curves for a given family of diffracting planes $\{hkl\}$ can be represented by straight lines, fig.(1a). In these cases, the XREC can be treated as those corresponding to an isotropic material. Assuming this behaviour, only two XREC (S_1 and $\frac{1}{2}S_2$) are needed. Table 1 shows the predicted values of these constants for sheets and bars, which are calculated from the equations corresponding to the isotropic case⁷:

$$\begin{aligned} F_{11} &= \frac{1}{2} S_2 \cos^2\phi \sin^2\psi + S_1 & (\text{at } \phi=0^\circ) \\ F_{22} &= \frac{1}{2} S_2 \sin^2\phi \sin^2\psi + S_1 & (\text{at } \phi=90^\circ) \end{aligned} \quad (6)$$

2) F_{ij} vs. $\sin^2\psi$ curves for different diffracting planes present an anisotropical behaviour and they can not be reduced to the isotropical case. Fig.(1.b-c) show F_{11} and F_{22} vs. $\sin^2\psi$ curves for two cases corresponding to different $\{hkl\}$ diffracting planes and samples.

DISCUSSION

XREC calculations indicate that in some cases, they can be treated as those corresponding to isotropic materials. This results are similar to those obtained for Zr alloys, where a good agreement between experiments and predictions was observed [4]. It must be remarked that this "isotropic treatment" does not imply that the material has elastic isotropy. The predicted S_1 and $\frac{1}{2}S_2$ values at $\phi=0^\circ$ and $\phi=90^\circ$ present differences, as shown in Table 1, in which they are ordered according increasing differences. Taking into

Table 1: S_1 and $\frac{1}{2}S_2$ values (in 10^{-5} Mpa^{-1}) for different families of diffracting planes in (a) Ti sheets and (b) Ti extruded bars. r is the correlation factor related to the straight line drawn on the graphs F_{ij} vs. $\sin^2 \psi$.

{hkil}	Coefficient	Calc. $\phi=0^\circ$	Calc. $\phi=90^\circ$	Mean value
{10 $\bar{1}$ 3}	S_1	-0.238	-0.239	-0.239
	$\frac{1}{2} S_2$	1.134	1.067	1.100
	r	0.9991	0.9994	
{10 $\bar{1}$ 4}	S_1	-0.212	-0.229	-0.220
	$\frac{1}{2} S_2$	1.022	1.026	1.024
	r	0.9985	0.9988	
{11 $\bar{2}$ 4}	S_1	-0.268	-0.233	-0.250
	$\frac{1}{2} S_2$	1.211	1.092	1.152
	r	0.9995	0.9998	
{12 $\bar{3}$ 3}	S_1	-0.347	-0.247	-0.297
	$\frac{1}{2} S_2$	1.356	1.157	1.256
	r	0.9999	0.9996	
{20 $\bar{2}$ 3}	S_1	-0.319	-0.219	-0.269
	$\frac{1}{2} S_2$	1.331	1.081	1.206
	r	0.9990	0.9985	

(a)

{hkil}	Coefficient	Calc. $\phi=0^\circ$	Calc. $\phi=90^\circ$	Mean value
{10 $\bar{1}$ 3}	S_1	-0.239	-0.224	-0.231
	$\frac{1}{2} S_2$	1.177	0.985	1.081
	r	0.9994	0.9999	
{10 $\bar{1}$ 4}	S_1	-0.213	-0.217	-0.215
	$\frac{1}{2} S_2$	1.076	0.954	1.015
	r	0.9992	0.9999	
{11 $\bar{2}$ 4}	S_1	-0.263	-0.232	-0.248
	$\frac{1}{2} S_2$	1.223	1.015	1.119
	r	0.9990	0.9998	
{12 $\bar{3}$ 3}	S_1	-0.366	-0.232	-0.299
	$\frac{1}{2} S_2$	1.387	1.112	1.249
	r	0.9999	0.9999	
{20 $\bar{2}$ 3}	S_1	-0.332	-0.224	-0.278
	$\frac{1}{2} S_2$	1.378	1.060	1.219
	r	0.9986	0.9985	

(b)

Figure 1: F_{11} and F_{22} vs. $\sin^2 \psi$ calculated values for a Titanium sheet: (a) {1014} planes, (b) {1010} planes and for a Titanium extruded bar (c) {1120} planes ($\diamond \phi=0^\circ$, $+\phi=48^\circ$, $\times \phi=66^\circ$ and $\blacksquare \phi=90^\circ$).

account the error introduced by the ODF serie expansion (10-15%) and the fact that under the isotropic approximation only $\frac{1}{2}S_2$ values are needed in Residual Stress analysis, we believe that the $\frac{1}{2}S_2$ mean values presented in table 1, which are similar for both textures, can be used in experiments.

It can be demonstrated that, under Reuss approximation, $\{0002\}$ XREC calculated values are not affected by any rotation around the c axis and consequently these values are independent of texture. Our results show that textures can have an important effect when $\{hkl\}$ XREC are calculated for planes next to $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$, as it is illustrated in fig. (1.b-c) for Ti sheets and bars respectively. We believe that the $\{12\bar{3}3\}$ and $\{20\bar{2}3\}$ XREC are in a limit condition for using the "isotropic" approximation.

Taking into account our predictions, we finally suggest to utilize the XREC calculated values given in Table 1 for the isotropic treatment. Nevertheless, it must be remarked that, even if crystallographic texture does not affect the calculated values of the constants, they play an important role in order to assure a good diffracted intensity during experiments⁴.

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