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PREDICTION OF THE THERMAL EXPANSION OF TEXTURED ZINC ALLOYS

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I. Introduction

During studies on zinc alloy products it has been observed that the thermal expansion coefficients of zinc alloy sheets measured in different directions from the rolling direction are anisotropic.

This thermal expansion anisotropy also varies with the sheets which have been elaborated through different rolling schemes and strong correlations between this anisotropy and the corresponding crystallographic textures have been observed. Assuming that among a number of parameters, the texture is principally involved in the bulk properties of the polycrystals, the thermal expansion of the polycrystal was modelled by averaging the intrinsic thermal behavior of the single crystals with the Orientation Density Function (ODF) used as a weighting function. The comparison between the experimental thermal expansion coefficients and the predictions allow estimates for very different textures to be checked.

II. Mean value modelling

The thermal expansion of a Zinc single crystal is very anisotropic and is conveniently represented by a tensor of second rank :

$$\alpha_{ij} = \begin{pmatrix} \alpha_{11} & & \\ & \alpha_{11} & \\ & & \alpha_{33} \end{pmatrix} \qquad (1)$$

For hexagonal material the thermal behavior is isotropic in the basal plane ($\alpha_{11} = \alpha_{22}$). Within a temperature range from 0°C to 100°C α_{33} is about four times higher than

α_{11} (α_{11} = 13.1 x 10^{-6}/C° ; α_{33} = 63.1 x 10^{-6}/C°) /1/.

The corresponding strain reads

$$\varepsilon_{ij} = \alpha_{ij} \Delta T \tag{2}$$

It is assumed that the thermal expansion of the polycrystal can also be represented by a second rank tensor (A_{ij}). The macroscopical symmetry due to the rolling is orthorhombic, therefore this tensor expressed in the principal reference frame reads :

$$A_{ij} = \begin{pmatrix} A_{11} & & \\ & A_{22} & \\ & & A_{33} \end{pmatrix} \tag{3}$$

According to our assumptions the A_{ij}'s are estimated by the simple mean value in the aggregate of the single crystal property :

$$A_{ii} = \langle \alpha_{ii} \rangle = \frac{1}{V} \int \alpha_{ii}(r)\, d^3r = \frac{1}{V} \int dg \int_{V(g)} \alpha_{ii}(r)\, d^3r \tag{4}$$

$$= \int \alpha_{ii}(g)\, f(g)\, dg$$

$\alpha_{ii}(g)$ are the components of the tensor of the single crystal (in a given orientation g) which are expressed in the macroscopical reference frame according to the tensor transformation law

$$\alpha_{ii}(g) = a_{ik}(g)\ a_{il}(g)\ \alpha_{kl} \tag{5}$$

where the a_{mn}'s are the direction cosines of the crystal axes in the macroscopical reference frame.

In the previous integral it can be shown that total ODF f(g) can be replaced by its even part $\tilde{f}(g)$ directly accessible from pole figure.

Integral (4) can be numerically calculated provided that $\tilde{f}(g)$ be known at nodes of a grid in orientation space. One can

also develop $\tilde{f}(g)$ and $\alpha_{ij}(g)$ into series expansion /2/.

Taking advantage of the hexagonal symmetry of the Zinc crystal it can be shown that

$$A_{ii} \approx \langle \alpha_{ii} \rangle = \alpha_{11} + F_i (\alpha_{33} - \alpha_{11}) \tag{6}$$

Where the F_i 's are the anisotropy parameters /3/ which can be directly calculated from the complete $\vec{c}$ axis pole figure : $P_{00.2}(\alpha, \beta)$.

$$F_i = \frac{1}{4\pi} \int_{\beta=0}^{2\pi} \int_{\alpha=0}^{\pi} P_{00.2}(\alpha, \beta) \cos^2 \alpha_i \sin\alpha \, d\alpha \, d\beta$$

with
$$\begin{aligned} \cos\alpha_1 &= \sin\alpha \cos\beta \\ \cos\alpha_2 &= \sin\alpha \cos\beta \\ \cos\alpha_3 &= \cos\alpha \end{aligned} \tag{7}$$

of course the anisotropy parameters F_i are related to the coefficients C_l^{mn} of the series expansion of the ODF /4/.

$$\begin{aligned} F_1 &= \frac{1}{3} - \frac{1}{15} C_2^{00} + \frac{1}{5}\sqrt{\frac{2}{3}} \, \mathrm{Re}\, C_2^{02} \\ F_3 &= \frac{1}{3} + \frac{2}{15} C_2^{00} \\ F_2 &= 1 - F_1 - F_3 \end{aligned} \tag{8}$$

The knowledge of the A_{ii}'s allows the thermal expansion $A(\vec{y})$ and the consecutive strain in a given direction $\vec{y}$ of the polycrystal to be calculated by applying the relation :

$$A(\vec{y}) = A_{11} \cos^2 \alpha_1 + A_{22} \cos^2 \alpha_2 + A_{33} \cos^2 \alpha_3 \tag{9}$$

where the $\cos\alpha_i$ are the direction cosines of the $\vec{y}$ direction and have the same definition as in relation (7).

III. Results

Sample

The results presented in this contribution concern three sheets the principal caracteristics of which are given in table I.

SAMPLE	type of alloy	rolling reduction
I	Cu : 0.16% Ti : 0.076%	down to 0.65 mm in several passes
II	Ti	down to 0.65 mm in several passes
III	Ti	down to 0.65 mm rolling in TD from 0.8 mm to 0.65 mm

Table I

Texture

The even part $\tilde{f}(g)$ of the ODF has been obtained /5/ from 4 complete pole figures (00.2, 10.0, 10.1, 10.2) which have been measured by X-Ray diffraction according to the composite sample technique /6,7/. A particular attention has been paid to the intensity corrections and especially to the background scattering evaluation in order to minimize the experimental errors.

Figure 1 shows the 00.2 and 10.0 recalculated pole figures of each sample. Sample 1 has a relatively sharp texture with $\vec{c}$ axis localized in the centre of the pole figure. Sample 2 presents a texture of the same type but of a very low sharpness. The texture of sample 3 is quite different with $\vec{c}$ axis in RD and residual $\vec{c}$ axis in ND.

Thermal expansion predictions

Figure 2 presents the comparison between the

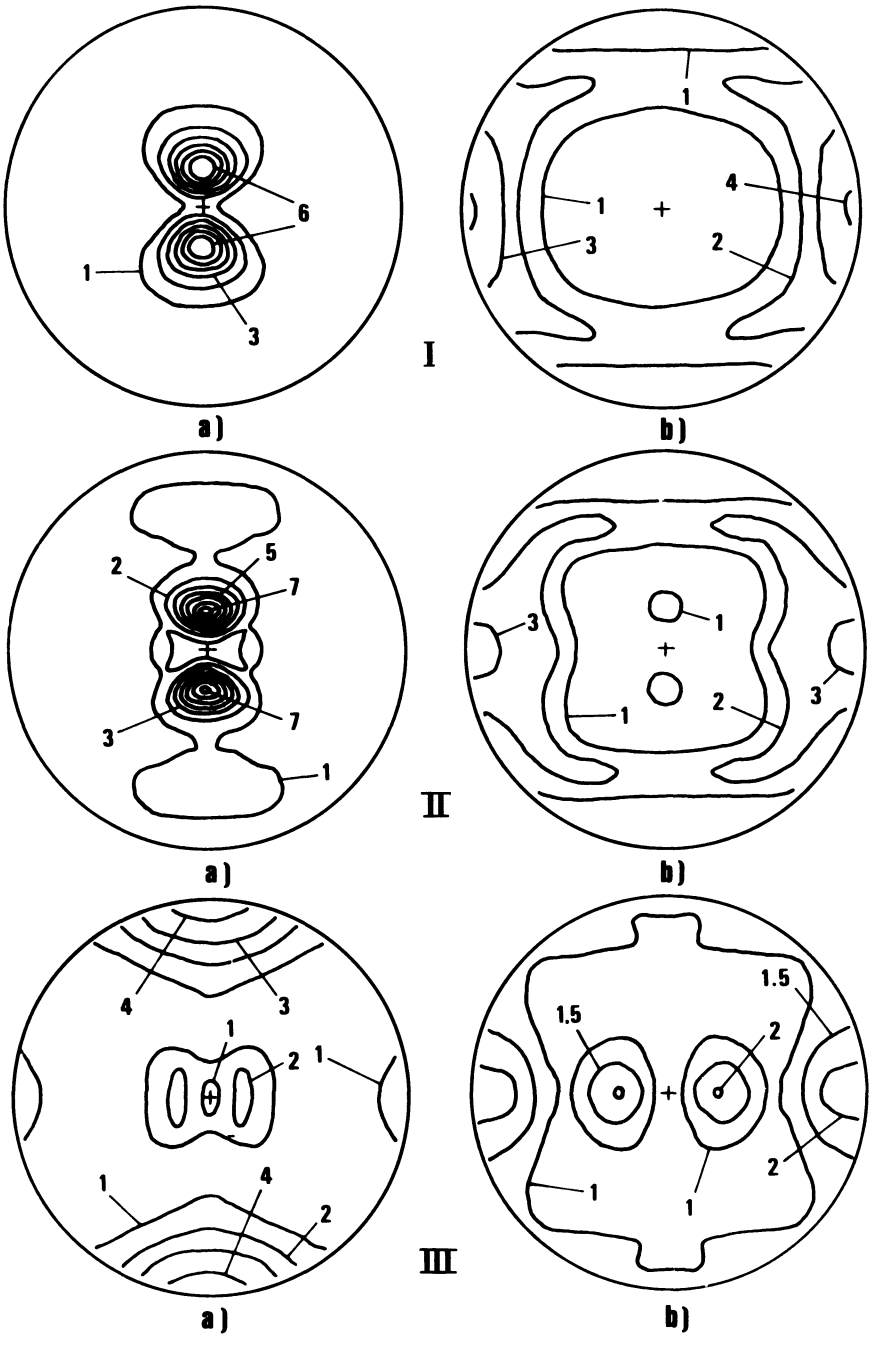

Figure 1 : (00.2) (a) and (10.0) (b) pole figures of samples I, II, III.

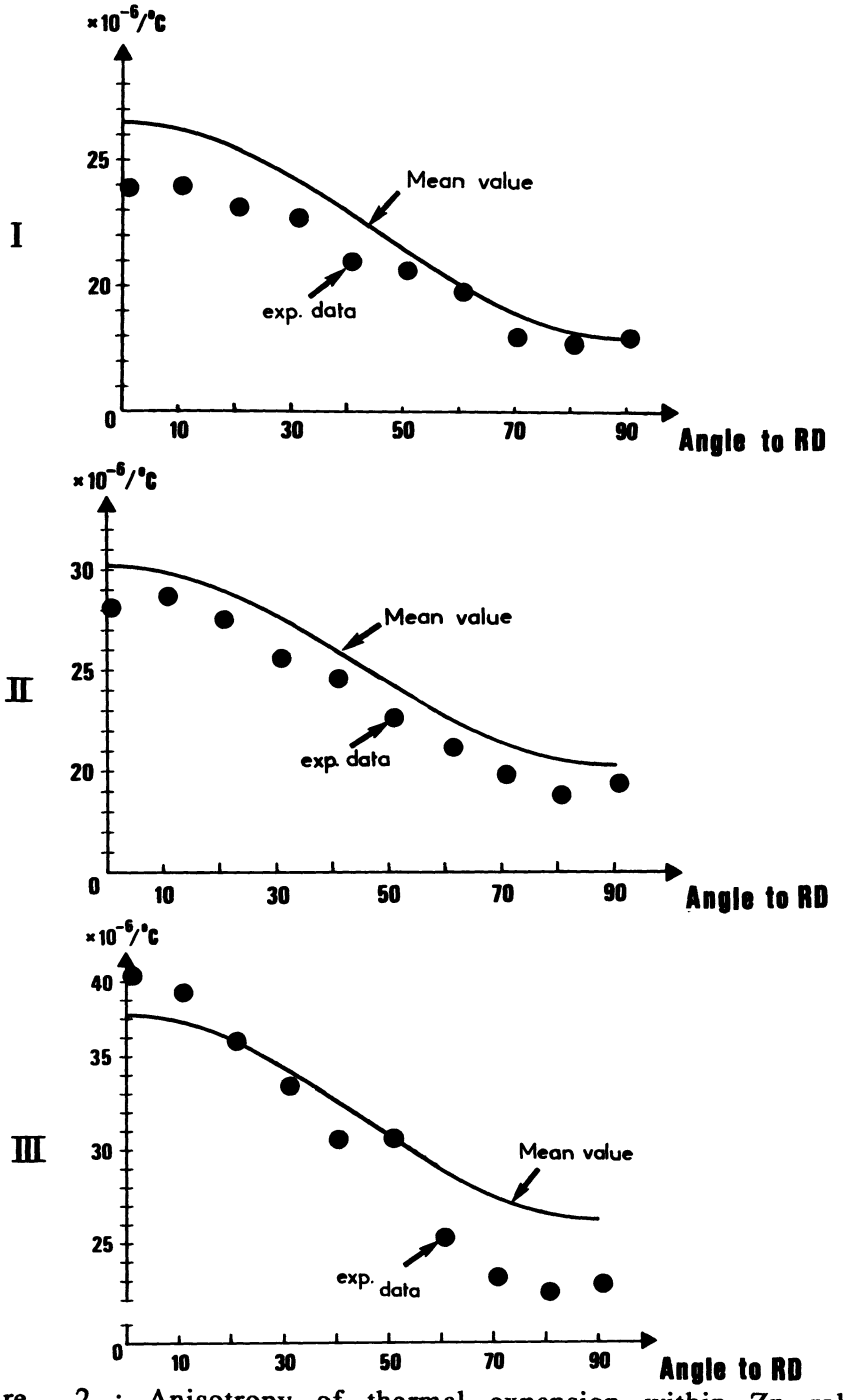

Figure 2 : Anisotropy of thermal expansion within Zn rolled samples I, II, III.

● experimental

— calculated by averaging

experimental and the calculated thermal expansions in different directions within the plane of the sheet for each sample. On the whole the calculated behaviour has the same aspect as the real one. Nevertheless, the previsions are always overestimated but remain compatible with the cumulated experimental errors of the texture determination and the thermal expansion measurements. As a matter of fact the largest difference hardly reaches 10 per cent.

Self consistent approach

We also checked the possibility of improving the thermal expansion previsions by taking the grain interactions into account statistically. To this purpose each grain is considered as an inclusion embedded in a homogeneous equivalent medium of the same properties as the real polycrystal. This problem has been treated in elasticity by different authors /8, 9, 10, 11/ and in thermal expansion as well /10, 12/.

These works have been adapted in the LM2P for studies of different textured hexagonal materials and the corresponding codes has been developed /13/.

The results of such a prevision are given in figure 3 for sample 2. In that prevision the grain shape has been taken into account. The prevision slightly deviates from the mean value prevision but remains in the experimental error margin.

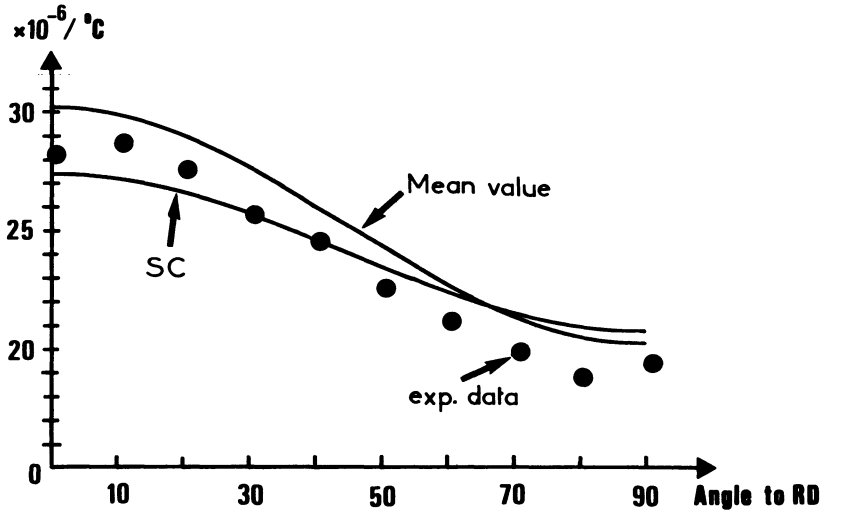

Figure 3 : Thermal expansion anisotropy within Zn rolled sheet II comparison between the experimental and the predicted data by averaging and by self consistent approach.

IV. Conclusion

In this investigation where different samples of different textures have been studied the mean value is sufficiently relevant to estimate the behaviour of the polycrystalline aggregate. In the case of hexagonal materials the complete calculation requires few coefficients of the ODF series expansion. In that case it is even possible to perform that type of prevision directly from only the complete pole figure of the c axis. The results given by a self consistent modelling differ only very slightly from the results obtained by the mean value modelling, at price of a complicated and time consuming program code.

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