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An ODF-Analysis Program for Orthorhombic Crystal Symmetry and its Application to CuZnAl Shape-Memory-Alloys

No Jin Park and Hans Joachim Bunge
Department of Physical Metallurgy, TU Clausthal
Großer Bruch 23, D-3392 Clausthal-Zellerfeld, FRG

1 Introduction

In the last few years texture analysis was extended from basic metals, mainly with cubic and hexagonal structure, to materials such as intermetallic phases e.g. shape memory alloys, ceramics, e.g. HTc-superconductors or polymers. These materials often have lower crystal symmetries and more complex diffraction spectra with partially or totally overlapping diffraction peaks. Therefor, new methods of ODF calculation had to be developed taking these conditions into account. In the present work an ODF program for orthorhombic crystal and sample symmetry was developed which accepts incomplete and superposed pole figures. The program is based on the series expansion method. The positivity condition is taken into account by an iteration process. The program was applied to study texture development in a shape memory alloy in the CuZnAl system. In CuZnAl-alloys shape memory effects are observed in the vicinity of 14 % Zn and 6 % Al. The high temperature phase is b.c.c whereas the low-temperature phase is monoclinic. The monoclinic angle β deviates, however, only very little, i.e. 1.21^0 from 90^0. Hence, for a first investigation the symmetry can be considered to be orthorhombic.

2 Mathematical fundamentals

The orientation distribution function $f(g)$ of the crystallites of a polycrystalline material is defined by the volume fraction dV/V of crystals which have an orientation g within the range dg

$$f(g) = \frac{dV(g)/V}{dg} \quad ; \quad g = \{\varphi_1, \Phi, \varphi_2\} \tag{1}$$

The function $f(g)$ can be obtained from pole figure measurement followed by pole figure inversion (ODF-analysis)

$$P_{\mathbf{h}}(\mathbf{y}) = \frac{1}{2\pi} \int_{\mathbf{h}\|\mathbf{y}} f(g)\, d\psi \tag{2}$$

where $\mathbf{h}$ is the crystal direction and $\mathbf{y}$ is the sample direction.

To solve eq.2 for $f(g)$ with several given pole figures, $f(g)$ is expressed in terms of a series expansion

$$f(g) = \sum_{l=0}^{l_{max}} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} C_l^{\mu\nu} \cdot \tilde{T}_l^{\mu\nu}(g) \tag{3}$$

This leeds eq.2 to the following form

$$P_{\mathbf{h}}(\mathbf{y}) = \sum_{l=0}^{lmax} \sum_{\mu=1}^{M(l)} \sum_{\nu=1}^{N(l)} \frac{4\pi}{2l+1} C_l^{\mu\nu} \cdot \dot{k}_l^{*\mu}(\mathbf{h}) \cdot \dot{k}_l^{\nu}(\mathbf{y}) = R_{\mathbf{y}}(\mathbf{h}) \tag{4}$$

The pole figure $P_{\mathbf{h}}(\mathbf{y})$ is the distribution of a particular crystal direction $\mathbf{h}$ with respect to the sample coordinate system.
If, on the other hand, one keeps a particular sample direction $\mathbf{y}$ constant and takes the crystal direction $\mathbf{h}$ as variable then eq.4 describes the inverse pole figure, which indicates the frequencies with which different crystal directions occur in a specified sample direction.

The texture coefficients $C_l^{\mu\nu}$ can be determined from experimental pole figures by solving eq.4.
Due to the experimental conditions, however, the following complications must also be taken into account:

– The pole figures are being measured incompletely. In order to deal

with this difficulty it is useful to take the necessary positivity condition $P_{\mathbf{h}}(\mathbf{y}) \geq 0$ into account which must be fulfilled for all (hkl) including those which were not measured as pole figures.

– Pole figures with different (hkl) may be superposed at the same Bragg-angle θ. Hence, the measured pole figures

$$P_\theta(\mathbf{y}) = \sum_{i=1}^{I} q_i \cdot P_{\mathbf{h}_i}(\mathbf{y}) \tag{5}$$

are superpositions of the ones defined by eq.4. The superposition factors q_i are calculated by an iteration process in the pole figure inversion procedure.

– The coefficients $C_l^{\mu\nu}$ with odd l-values cannot be obtained from eq.4. The odd coefficients can, however, be obtained by using the necessary positivity of the function $f(g) \geq 0$ in a second iterative process.
This procedure is illustrated schematically in Fig.1.

3 Experimental Results

The alloy Cu-14.2 wt% Zn-5.6 wt% Al was melted in a medium frequency induction furnace and hot rolled at 750^0C in steps of 20% to a final thickness of 1 mm equivalent to 96% total rolling reduction. Thereby several intermeditate annealing treatments at 750^0C were necessary. After that the material was cooled down to room temperature whereby it transforms from b.c.c. to monoclinic.
The transformation temperatures were found to be

$$M_s = 115^0C, \quad M_f = 99^0C, \quad A_s = 119^0C, \quad A_f = 128^0C.$$

The lattice parameters of the monoclinic phase are

$$\mathrm{a} = 4.457 \text{ Å}, \quad \mathrm{b} = 5.326 \text{ Å}, \quad \mathrm{c} = 38.184 \text{ Å}, \quad \beta = 88.79^0$$

Samples for texture measurement were prepared from the middle of the sheet. Twelve incomplete pole figures were measured in steps of $\Delta\alpha = 5^0$, $\Delta\beta = 3.6^0$ up to $\alpha_{max} = 70^0$ using CoK_α-radiation. Six of

the twelve pole figures were superposed ones.
The measured pole figures (after normalization) are shown in Fig.2. The ODF was then calculated with $l_{max} = 22$. The mean absolute values of the coeffients $C_l^{\mu\nu}$ are given in Fig.3. They are compared with their probable errors which can be estimated along with the least-squares solution. The pole figures recalculated from the obtained ODF-coefficients are shown in Fig.4. One sees that they agree quite well with the experimental ones.
The complete ODF is shown in Fig.5. With a maximum value of 31.11 it represents a rather strong texture. The texture contains several orientation components, which are given in Table 1 along with their respective densities and approximate indices of rolling plane and rolling direction.
According to the orientation relationships between b.c.c. austenit and monoclinic martensit $[100]_M||\langle 110\rangle_A$, $[010]_M||\langle 100\rangle_A$, $[001]_M||\langle 504\rangle_A$, the major components are assumed to orginate from an orientation $\{001\}\langle 011\rangle$ of the high temperature b.c.c. phase as the strongest component of the b.c.c.-rolling textur. Finally, the inverse pole figures for the rolling (RD) and normal (ND) directions are shown in Fig.6. In these figures also the orientation components A – F (Tab.1) are indicated.

4 References

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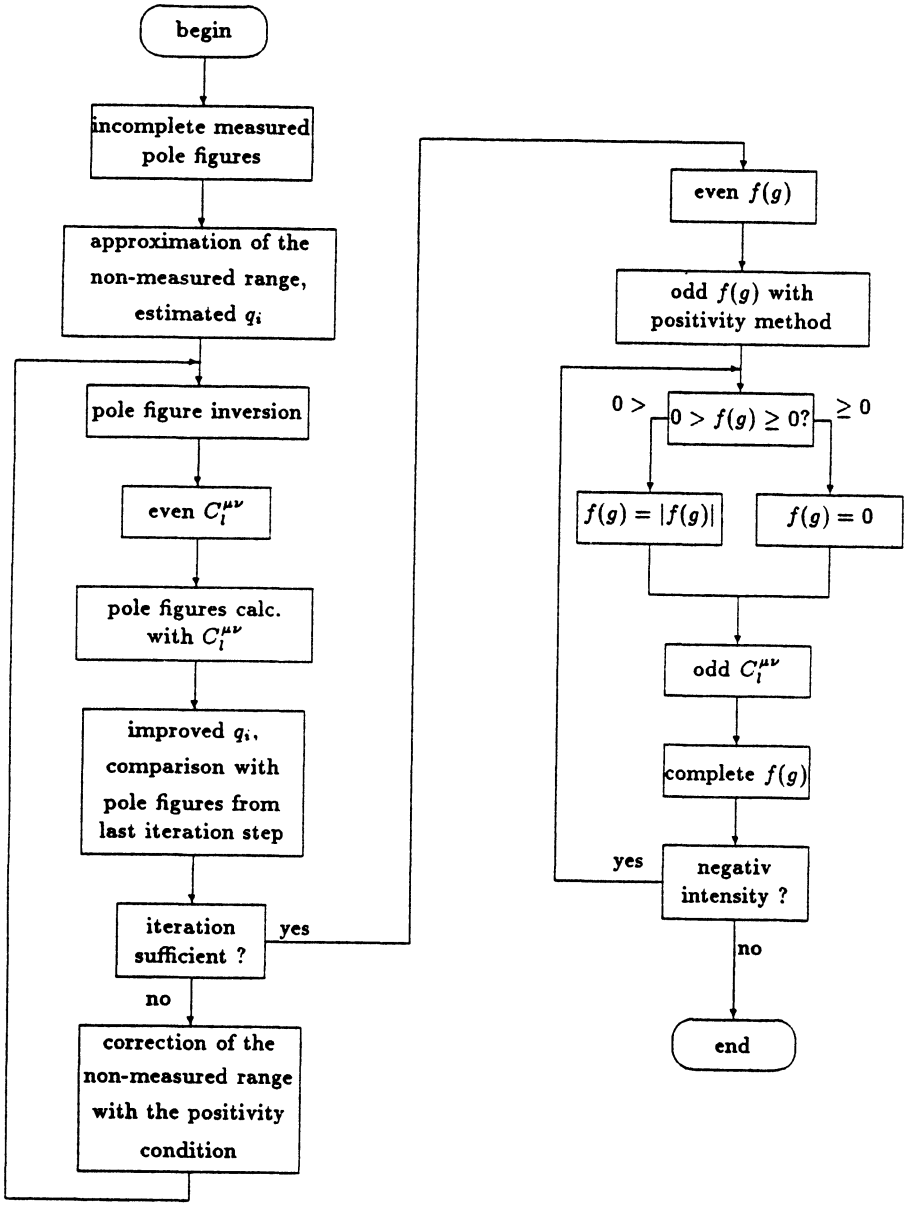

Fig.1 : Flow diagram for the calculation of the complete ODF from incomplete superposed pole figures

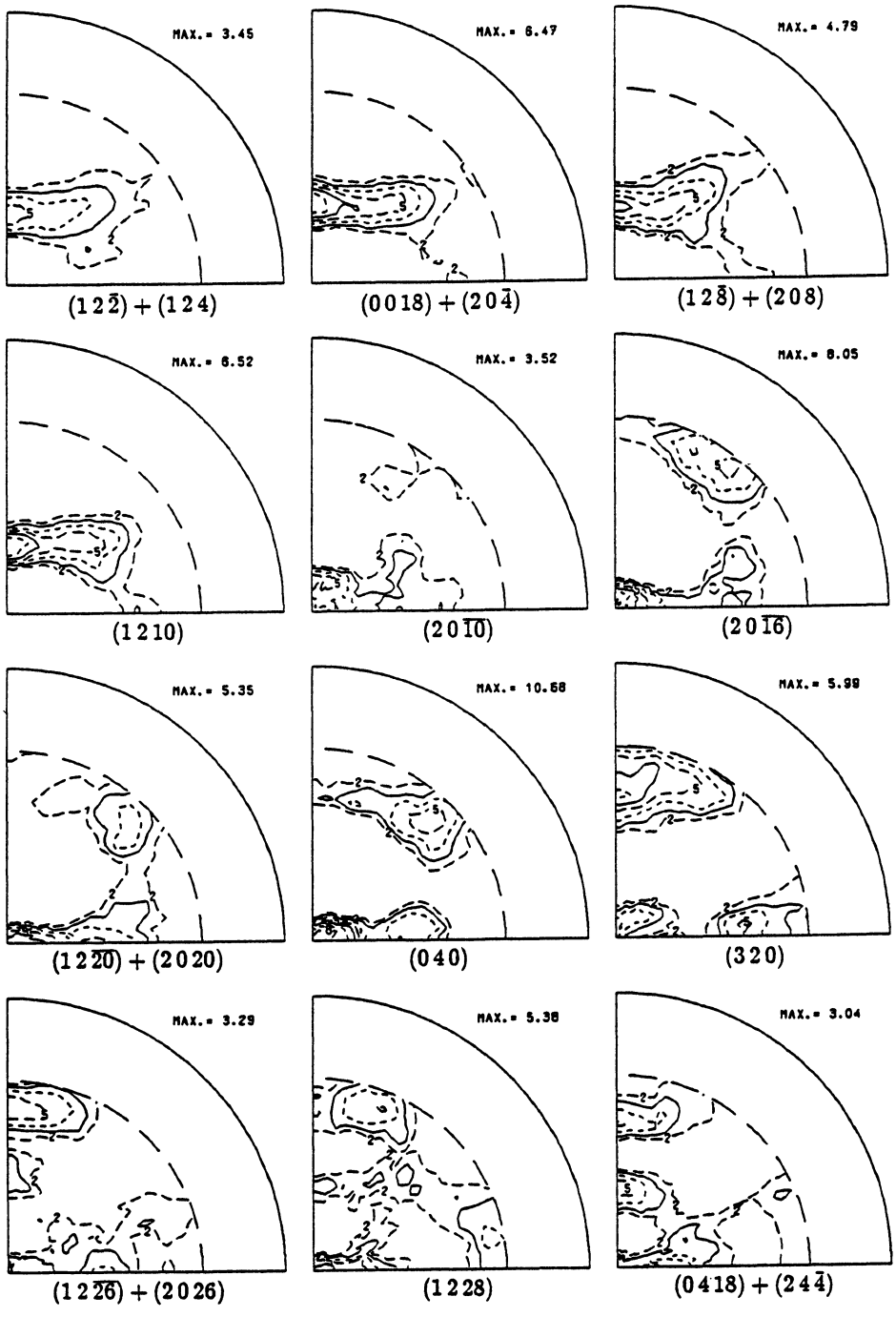

Fig.2 : Measured pole figures of an alloy Cu-14.2%Zn-5.6%Al after normalization

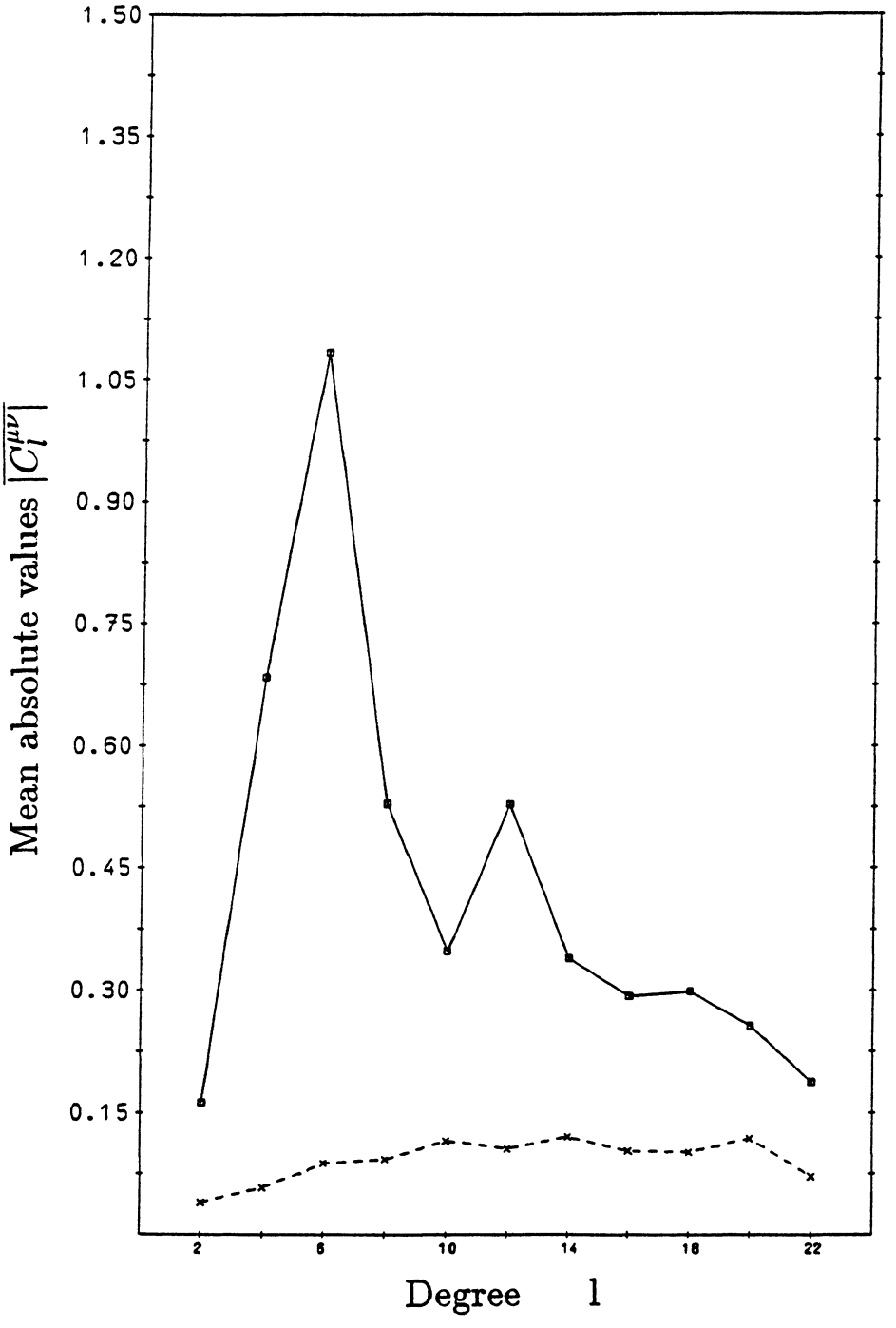

Fig.3 : Mean absolute values $\overline{|C_l^{\mu\nu}|}$ and their respective errors

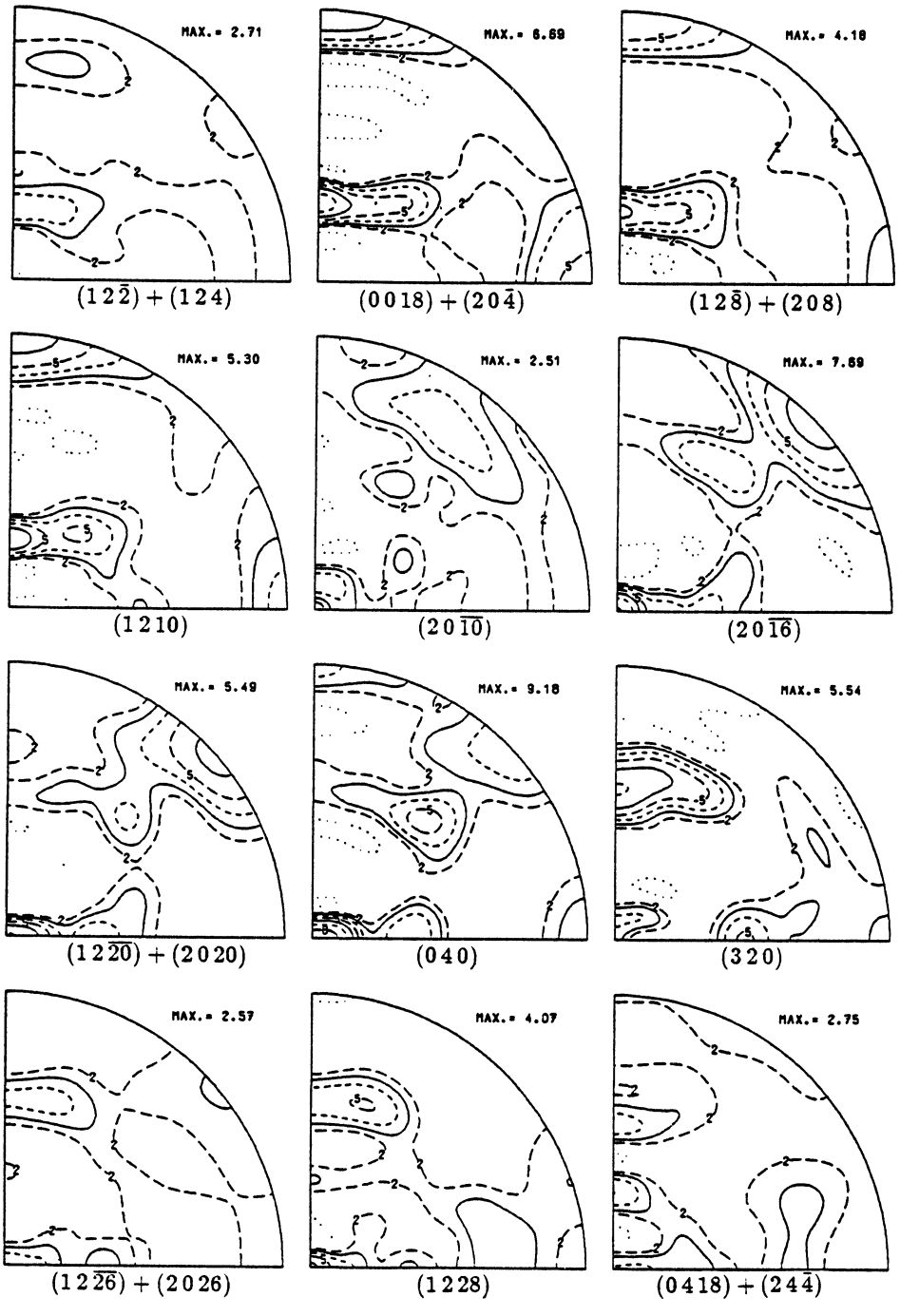

Fig.4 : Calculated pole figures of an alloy Cu-14.2%Zn-5.6%Al

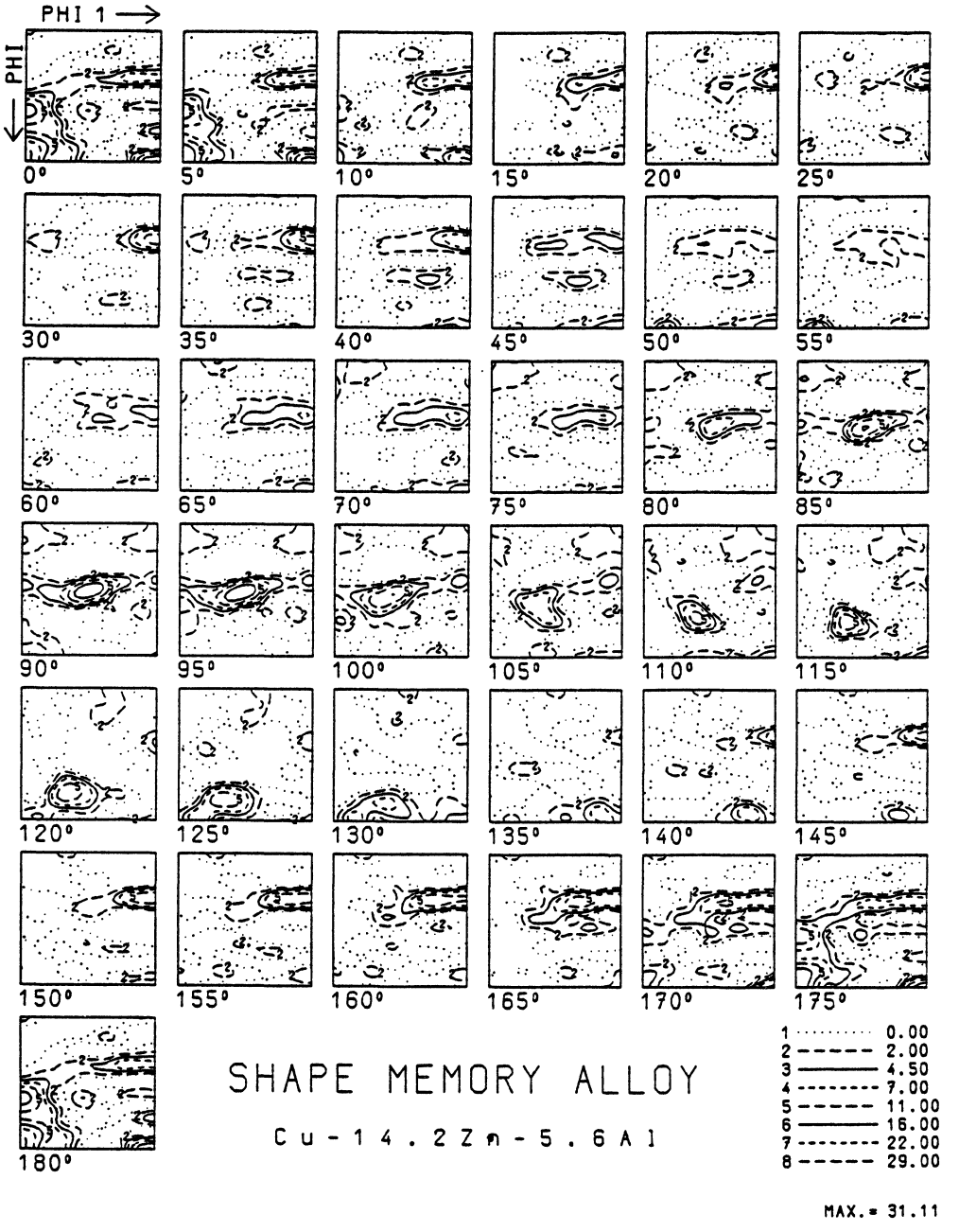

Fig.5 : ODF of hot rolled Cu-14.2%Zn-5.6%Al

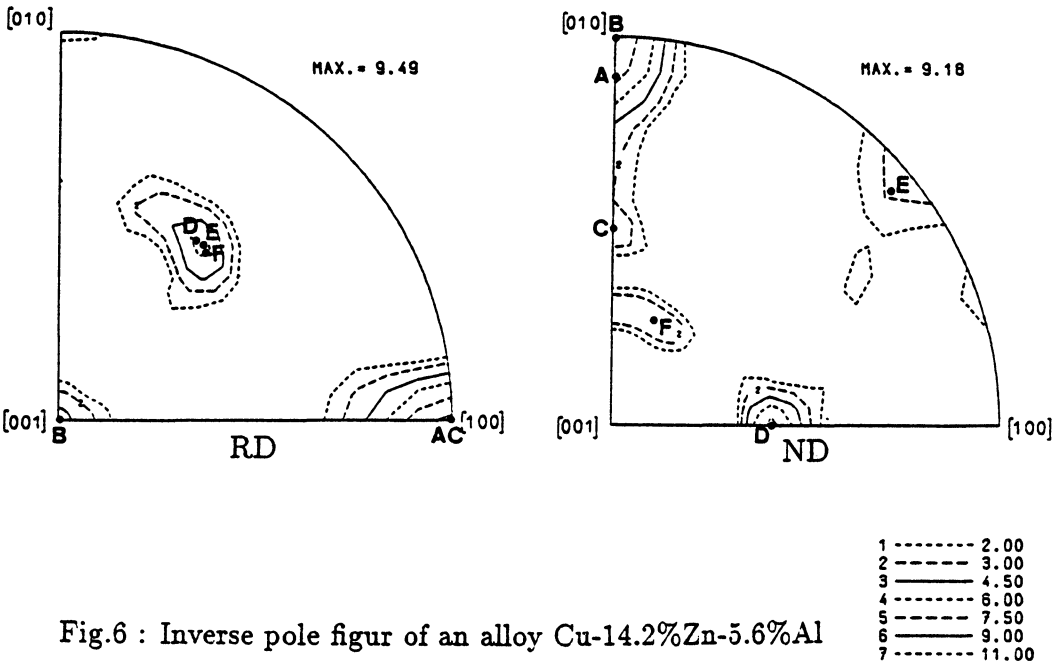

Fig.6 : Inverse pole figur of an alloy Cu-14.2%Zn-5.6%Al

Table 1: orientation components of 96% hot rolled CuZnAl-alloy

component	φ_1	Φ	φ_2	$(hkl)[uvw]$	$f(g)$
A	0°	82°	0°	(0 1 1)[1 0 0]	31.1
B	90°	90°	0°	(0 1 0)[0 0 1]	23.1
C	0°	54°	0°	(0 1 5)[1 0 0]	18.8
D	45°	45°	90°	(1 0 9)[9.10.$\bar{1}$]	21.6
E	30°	73°	120°	(10.$\bar{7}$.30)[10.10.$\bar{1}$]	14.9
F	68°	32°	160°	(1.$\bar{3}$.37)[10.$\bar{9}$.$\bar{1}$]	15.2