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Modelling of the anisotropy of Young's modulus in polycrystals

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The crystallographic orientation distribution of cold rolled and recrystallized low-carbon deep drawing steel is quantitatively investigated by means of the series expansion method and the technique of model component fit. The results of both methods are utilized to describe the elastic properties of the inspected sheets. The application of the model components allows a very good approximation of the course of Young's modulus and corresponds to experimental results as well as to the predictions stemming from the series expansion method. In addition to the influence of peak-type texture components also the impact of complete and incomplete fibre-type texture components on the course of Young's modulus is inspected.

Modellierung der Anisotropie des Elastizitätsmoduls in Polykristallen. Die kristallographischen Orientierungsverteilungen von kaltgewalztem und rekristallisiertem niedriggekohltem Tiefziehstahl werden quantitativ mittels der Reihenentwicklungsmethode und der Modellanpassung untersucht. Die Ergebnisse beider Verfahren werden zur Modellierung der elastischen Eigenschaften der untersuchten Bleche herangezogen. Die Verwendung der Modellanpassung erlaubt eine sehr gute Beschreibung des Verlaufs des Elastizitätsmoduls und entspricht sowohl den experimentellen als auch den aus der Reihenentwicklung berechneten Ergebnissen. Zusätzlich zum Einfluß von Einzeltexturkomponenten wird auch die Auswirkung von vollständigen und unvollständigen Fasertexturkomponenten auf den Verlauf des Elastizitätsmoduls untersucht.

The crystallographic orientation distribution of the crystals within a polycrystalline aggregate which is hereafter referred to as crystallographic texture is of dominant relevance for numerous macroscopically directional properties of polycrystalline specimens. Whereas the impact of the texture on plastic anisotropy such as the deep drawing properties [1; 2], on local orientation inhomogeneities such as the ridging phenomenon in ferritic stainless steels [3; 4] and on the strength of steels [1] has already been subject to numerous examinations, its influence on the elastic properties of steels has not yet been treated accordingly [1; 5; 6].

The planar course of Young's modulus, which is of main importance for the directional elastic properties of polycrystalline samples, often reveals a considerable variation with respect to the rolling direction, **figure 1** [1; 5; 6]. Since the elastic anisotropy is inherent to every crystal unit cell the macroscopically detected elastic properties of a polycrystal represent an integration over the individual properties of all grains which are characterized by their orientation and size. The macroscopic elastic anisotropy of steels is thus strongly determined by the crystallographic texture. In the present work the elastic anisotropy of polycrystalline steels is computed from their corresponding crystallographic texture which is represented by the three-dimensional orientation distribution function (ODF), making use either of the series expansion method according to Bunge [7] or the method of decomposing a texture into superimposed Gauss-like scattering model functions according to Lücke et al. [8].

Determination of Young's modulus from the texture

The average property of a polycrystalline material may in a first approximation be tackled without regarding any interaction between neighbouring grains [1]:

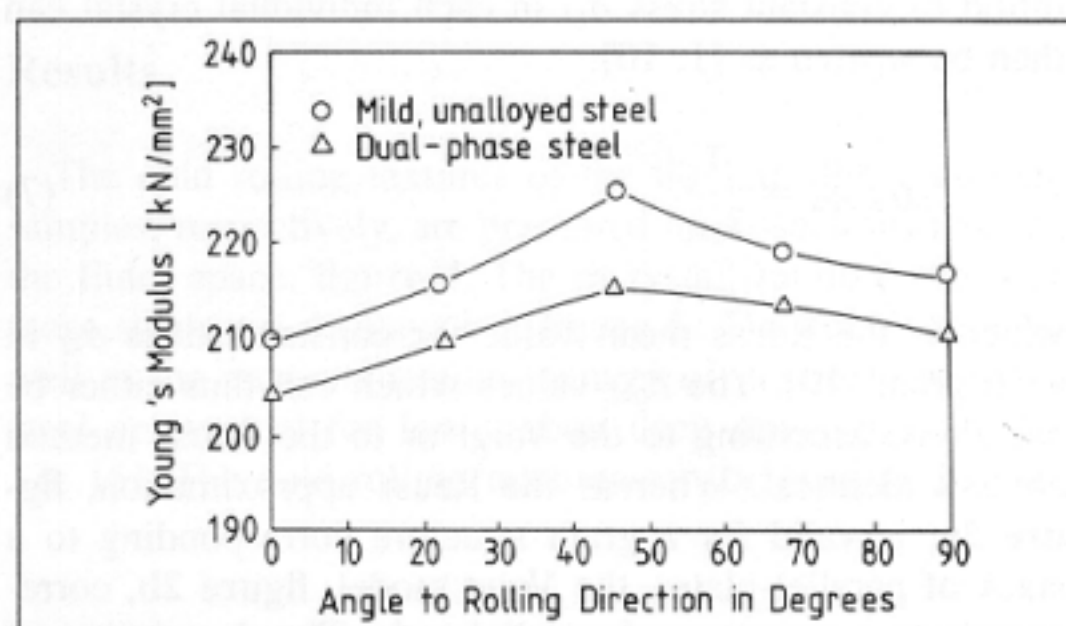


Figure 1. Experimentally detected course of Young's modulus in the sheet plane for two different steels, according to Lotter and Bleck [6]

$$\bar{E} = \oint E(g)f(g)dg \quad (1)$$

In this expression E is the individual elastic property depending on the orientation g and f the orientation density of the considered orientation g in the interval dg . Due to equation (1) Young's modulus can therefore be determined from the ODF, which is defined as follows [7]:

$$\frac{dV(g)}{V} = f(g)dg \quad (2)$$

where $dV(g)/V$ is the volume fraction of grains in the orientation interval dg . The averaged mean value as expressed by equation (1) does not regard any interaction between neighbouring grains nor does it take into consideration the influence of the grain shape. Hooke's generalized law which describes the elastic response of a material under an external load is usually given in the form:

$$\sigma_{ij} = \sum_{k,l} c_{ijkl} \epsilon_{kl} \quad (3)$$

where σ_{ij} is the stress tensor, ϵ_{kl} the strain tensor and c_{ijkl} the forth-rank tensor of the elastic constants. Hooke's law, written in the form of equation (3) assumes constant strain

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in each grain. According to equation (1) the averaged elastic constants can then be computed as follows:

$$\bar{c}_{ijkl,Voigt} = \oint c_{ijkl}(g)f(g)dg \quad (4)$$

In this expression $c_{ijkl,Voigt}$ is the Voigt-mean value for constant strain ε_{kl} [1; 9]. Equation (3) may be also written in the form:

$$\varepsilon_{ij} = \sum_{k,l} s_{ijkl} = \sigma_{kl}, \quad s_{ijkl} = \frac{1}{c_{ijkl}} \quad (5)$$

According to equation (1) the averaged value of s_{ijkl} then is:

$$\bar{s}_{ijkl,Voigt} = \oint s_{ijkl}(g)f(g)dg \quad (6)$$

The Reuss mean value of the elastic constants for the condition of constant stress σ_{kl} in each individual crystal can then be written as [1; 10]:

$$\bar{c}_{ijkl,Reuss} = \frac{1}{\bar{s}_{ijkl}} \quad (7)$$

which is the Reuss mean value for constant stress σ_{kl} in each grain [10]. The \bar{c}_{ijkl} values which can thus either be calculated according to the Voigt or to the Reuss method are not identical. Whereas the Reuss approximation, **figure 2a**, is valid for a grain structure corresponding to a stack of parallel plates, the Voigt model, **figure 2b**, corresponds to a structure of parallel rods. The description of an authentic equiaxed grain structure by simply averaging the mean value of the Voigt and Reuss approximation has been suggested by Hill [11], **figure 2c**:

$$\bar{c}_{ijkl,Hill} = \frac{1}{2}(\bar{c}_{ijkl,Voigt} + \bar{c}_{ijkl,Reuss}) \quad (8)$$

The Hill mean value is widely accepted to reveal better agreement with the experimentally achieved values when compared to the predictions stemming from the Voigt and Reuss approximations, respectively. The latter models are frequently applied for upper and lower bound estimations when an elongated grain morphology occurs parallel to the transverse (Reuss) or rolling (Voigt) direction (**figure 2**).

Experimental and evaluation methods

Table 1 shows the chemical composition of the examined steel. The hot rolled bar of this industrially processed steel was exposed to a heat treatment at 1023 K in order to precipitate the AlN and to obtain coarse grain boundary cementite as in high temperature coiled material. After this processing the steel was cold rolled homogeneously under

Table 1. Chemical composition of the examined steel (mass contents in %)

C	Mn	Al	N	P	S
0.035	0.225	0.042	0.003	0.023	0.013

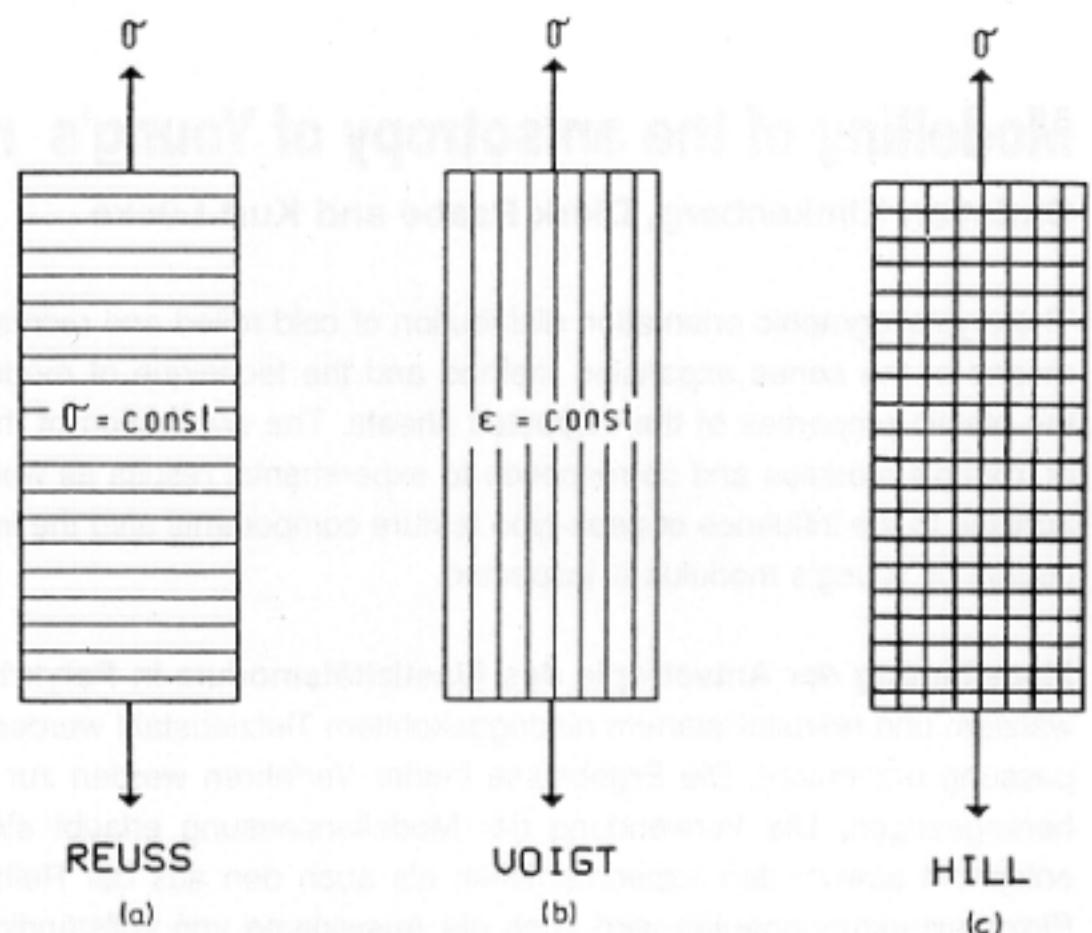


Figure 2. Schematic presentation [1] of the grain morphology accounting for the elastic models of Reuss [10], Voigt [9] and Hill [11]

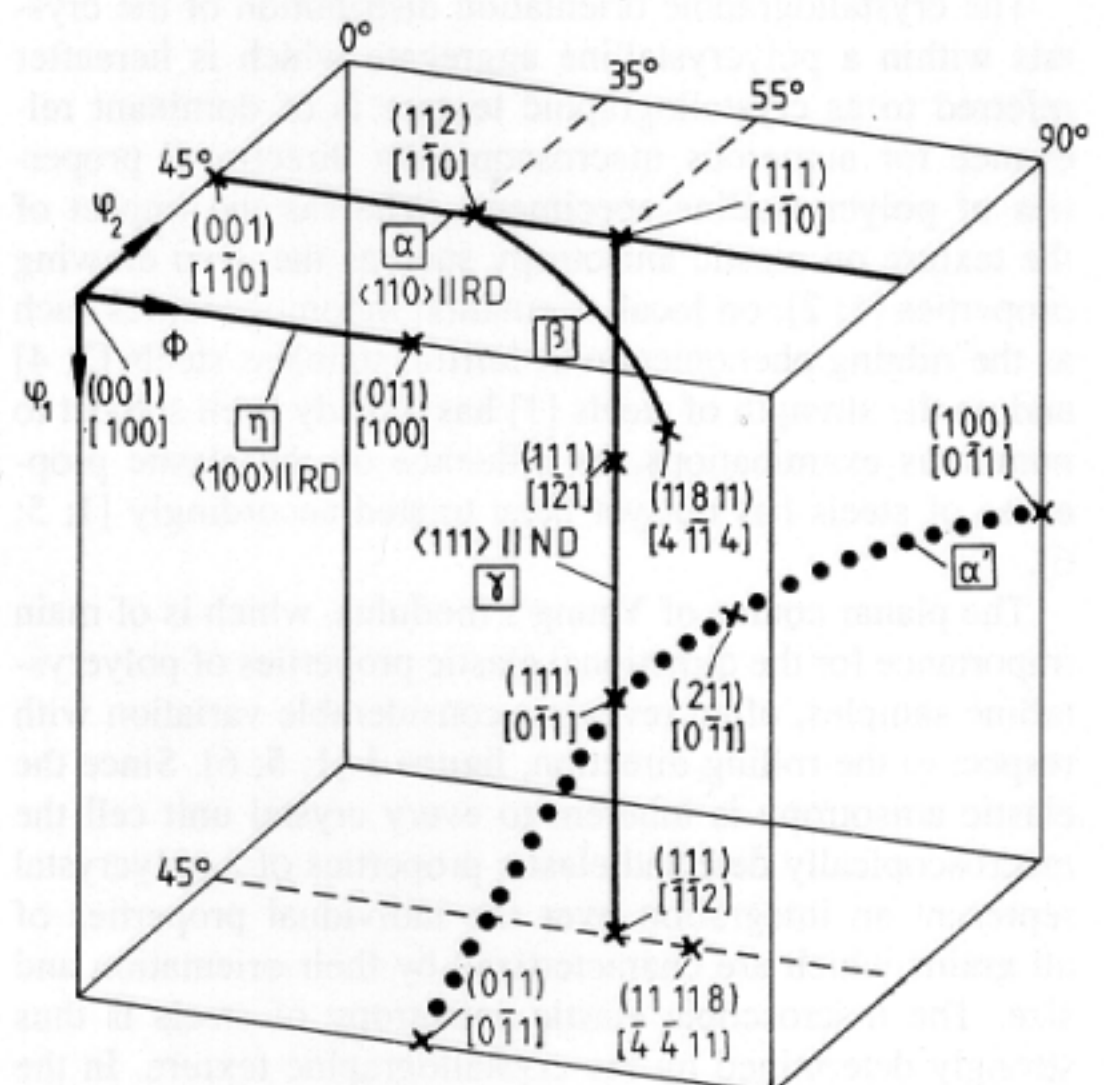


Figure 3. Orientation space showing the main texture components

oil lubrication to 80 and 90% thickness reduction, respectively. Subsequently the sheet was annealed in a salt bath at 973 K for 150 s. The heating rates were, according to the preceding degree of deformation, within the range 200 to 400 K/s. The cooling rates were within the range 9 to 15 K/s, which is comparable to the industrial conditions of compressed air cooling. The heating and cooling rates were determined by use of thermocouples, which were positioned upon the samples.

All textures were quantitatively examined by measuring the four incomplete pole figures $\{110\}$, $\{200\}$, $\{112\}$ and $\{103\}$ from an area of 14.24 mm² in the range of the pole distance angle α from 5 to 85° with MoK α 1 radiation in the back reflection mode [12]. Since the pole figures taken from polycrystalline aggregates represent two-dimensional projections of the three-dimensional texture its interpretation becomes ambiguous because of the superposition of the

considered types of poles, so that the ODF was computed by the series expansion method ($l_{max}=22$) [7]. In case of the cubic crystal symmetry of ferritic steels and the orthorhombic sample symmetry, defined by rolling, normal and transverse direction (RD, ND, TD) an orientation can then be expressed by the three Euler angles φ_1 , Φ , φ_2 in the reduced Euler space. For better comprehension an orientation is often accordingly characterized by the Miller notation $\{hkl\} \langle uvw \rangle$, where the first three indices $\{hkl\}$ describe the crystallographic plane parallel to the sheet surface whereas the second triplet $\langle uvw \rangle$ indicates the direction parallel to RD. The typical cold rolling and recrystallization textures of low carbon steels may be described by three texture fibres, i.e. first by the incomplete α -fibre which is characterized by $\langle 110 \rangle$ parallel to RD, second by the complete γ -fibre which comprises all crystals with a $\langle 111 \rangle$ direction parallel to ND and third by the complete η -fibre which includes all grains with a $\langle 100 \rangle$ direction parallel to RD, **figure 3**.

According to Lücke et al. [8] the volume fractions of the different texture components were determined by decomposing the ODFs into a number of superimposed isolated and fibre-type Gauss-like scattering model components. This method was originally developed for the correction of mathematical errors in the ODF proceeding from the absence of the odd coefficients in the harmonic series expansion. Especially in fcc metals which usually contain various isolated Gauss-type components this shortcoming led to considerable errors in the ODFs. Due to the higher symmetry of the fibre-type textures of bcc materials which contribute to the decreasing importance of the missing odd coefficients, until now only a few attempts have been ex-

Table 2. Volume fractions of individual texture components in the cold rolled and recrystallized state

sample condition	Volume fractions of texture components in %				
	α -fibre	γ -fibre	η -fibre	Σ others	background
80 % CR	41.6	26.6	-	29.7	2.1
80 % CR+RX	14.2	41.6	4.5	29.8	8.0
90 % CR	55.5	24.0	-	19.1	1.4
90 % CR+RX	1.9	55.8	1.3	41.2	1.7

CR cold rolled

RX recrystallized

cuted to analyze steel textures also by the method of component fit. In the present work, however, not only isolated but also complete and incomplete fibre-type texture components were tackled. The volume fractions of the individual texture components, which were detected in the investigated specimens, are given in **table 2**. Since the ODFs can thus be decomposed into a number of peak-type or fibre-type single components, the influence of these individual components on the macroscopic elastic behaviour of polycrystalline aggregates was quantitatively simulated.

Results

The cold rolling textures of the 80 and 90% deformed samples, respectively, are presented in φ_1 -sections through the Euler space, **figure 4**. The recrystallization textures of these steels are displayed in **figure 5**. The cold rolling as well as the recrystallization textures of the here examined steel are typical for low carbon deep drawing steels [2; 13...15]. The cold rolling textures can be described by an

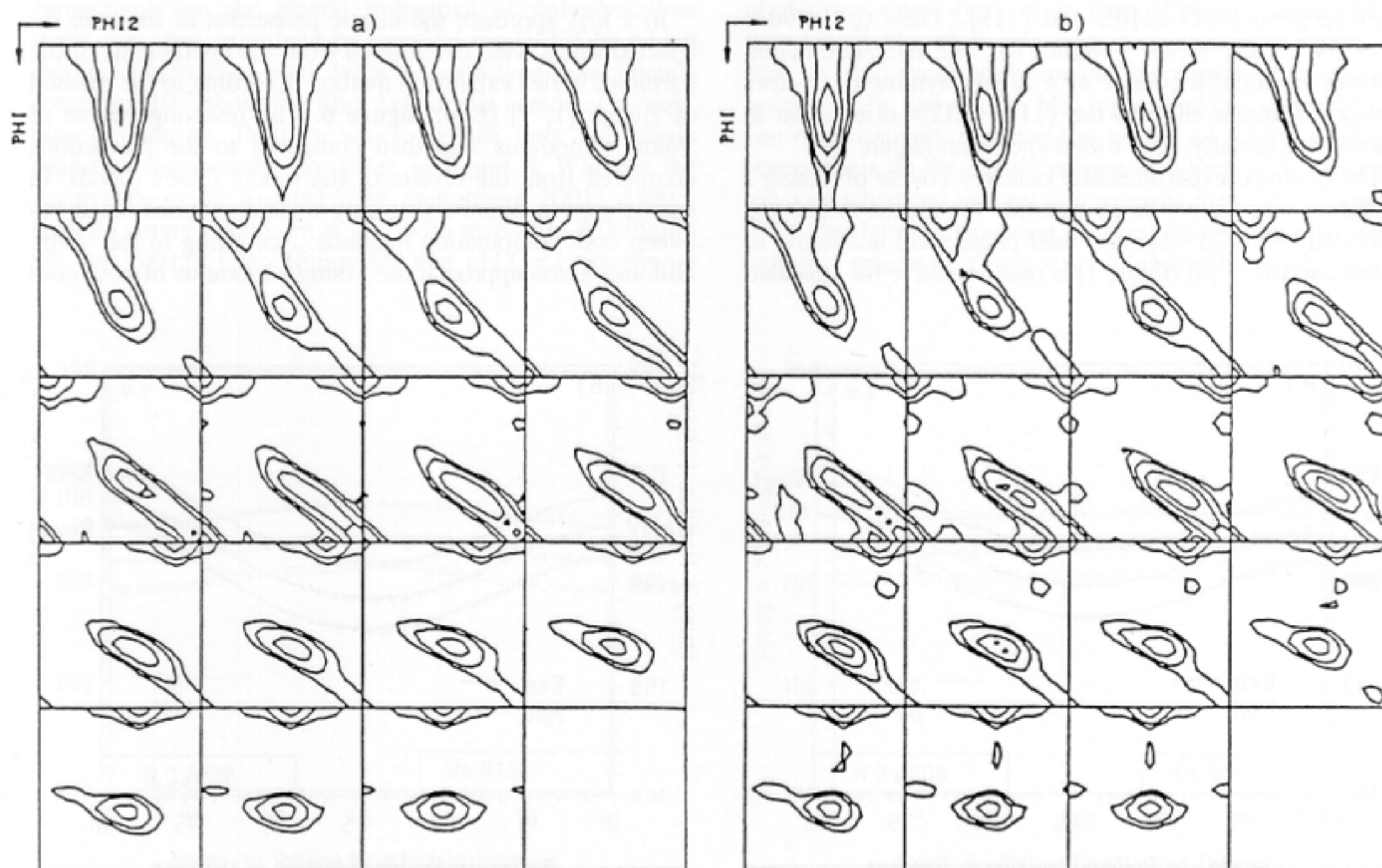


Figure 4. Cold rolling textures in φ_1 -sections, series expansion method, a) 80%, b) 90%; measurement of pole figures carried out in the center layers

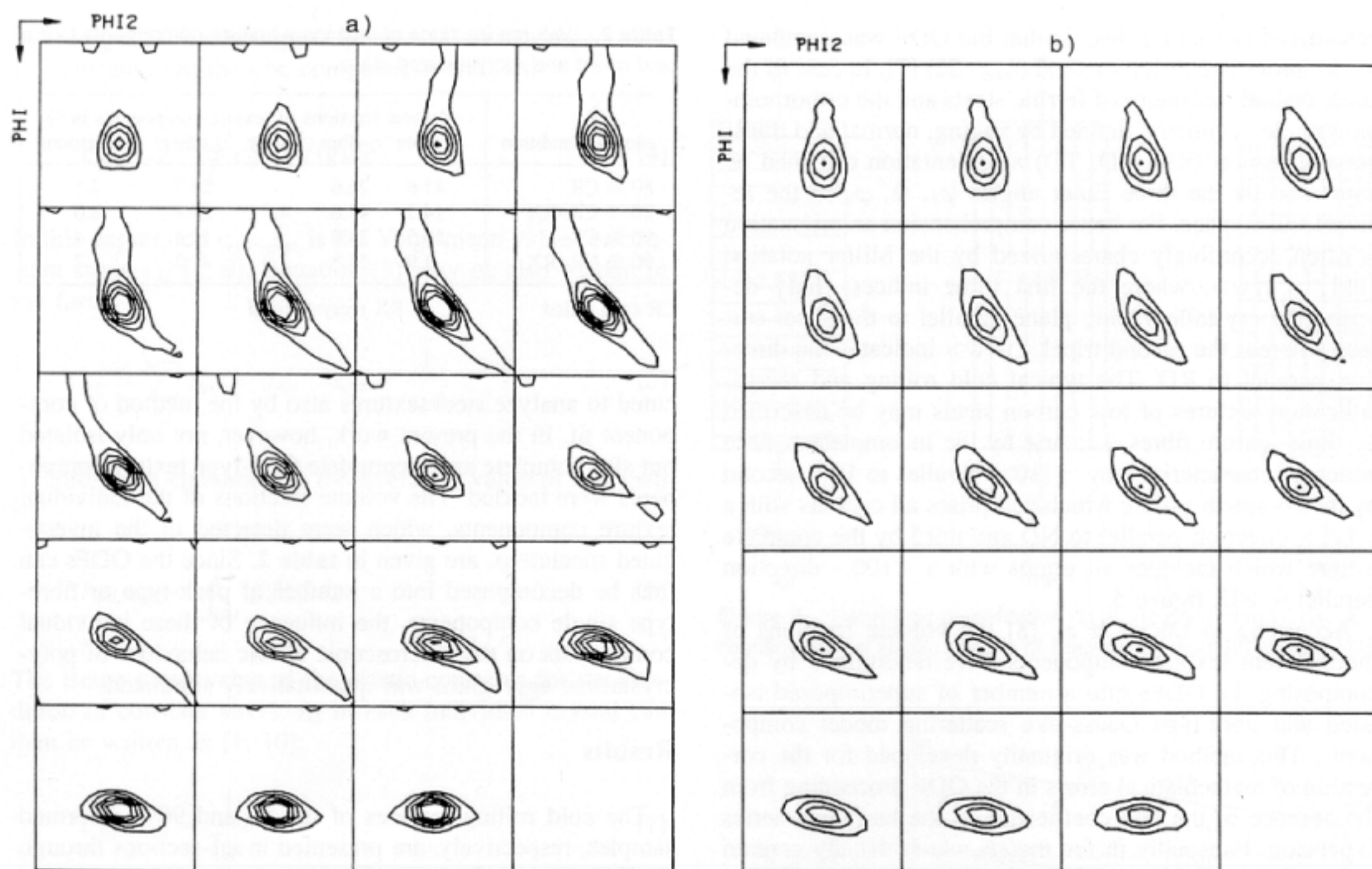


Figure 5. Recrystallization textures in φ_1 -sections, series expansion method, a) 80%, b) 90%; measurement of pole figures carried out in the center layers

incomplete α -fibre with main texture components within the range $\{001\}\langle 110 \rangle$ ($\varphi_1 = 0^\circ$, $\Phi = 0^\circ$, $\varphi_2 = 45^\circ$) to $\{111\}\langle 110 \rangle$ ($\varphi_1 = 0^\circ$, $\Phi = 54.7^\circ$, $\varphi_2 = 45^\circ$) and the complete $[\gamma]$ -fibre with dominant orientations between $\{111\}\langle 110 \rangle$ and $\{111\}\langle 112 \rangle$ ($\varphi_1 = 90^\circ$, $\Phi = 54.7^\circ$, $\varphi_2 = 45^\circ$) (figure 4). The recrystallization textures essentially consist of a highly symmetric γ -fibre with a maximum close to the $\{111\}\langle 112 \rangle$ orientation in case of the initially 90% rolled specimen (figure 5).

The depicted experimentally detected course of Young's modulus, here shown as an example for a cold rolled and recrystallized mild steel and dual phase steel according to Lotter and Bleck [6] (figure 1) is representative for annealed

steels and has accordingly been published by various workers [1; 5; 6]. The measurements are conventionally carried out by inducing bending oscillations and detecting the natural frequency of the samples.

In a first approach the elastic properties of the here inspected steels were determined from the coefficients of the harmonic series expansion method according to the method of Bunge [1; 7] (Exp), **figure 6**. The resulting course of Young's modulus was then compared to the predictions computed from the results of the model ODFs (Mod). In can be seen in figure 6 that only weak deviations occur between both computation methods. According to the Voigt, Hill and Reuss approach the Young's modulus of both cold

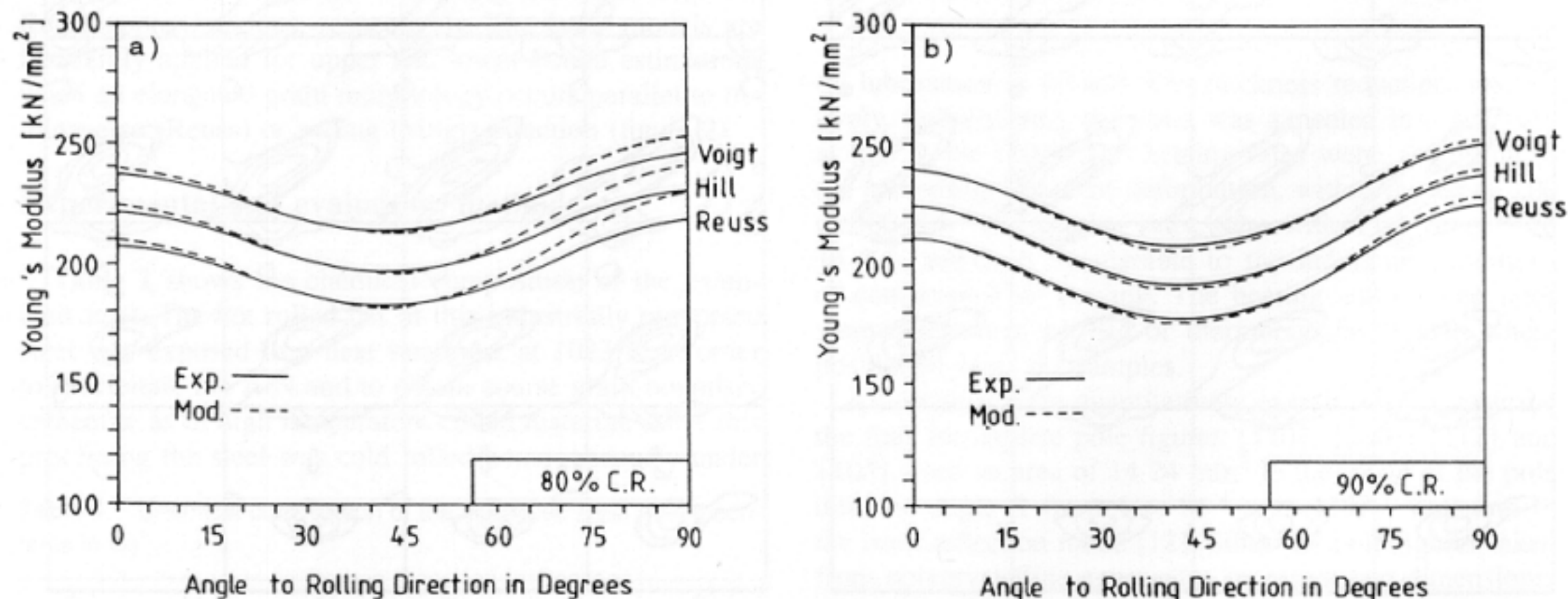


Figure 6. Young's modulus of the cold rolled sheets calculated from the coefficients of the series expansion method (Exp) and from model data (Mod). The corresponding model components are listed in table 2

rolled samples varies in the sheet plane with the angle between the inspected direction and RD, exhibiting a minimum at 45° (figure 6b). In both cases the maxima are positioned parallel to RD and TD. It becomes apparent that the Voigt approximation represents an upper bound estimation and the Reuss approximation a lower bound value. Both predicted curves reveal a deviation of about 15 kN/mm^2 with respect to the Hill approximation.

The recrystallized samples show a different course of the Young's modulus when compared to the cold rolled specimens, figure 7. After 80% cold reduction and subsequent annealing the variation of the Young's modulus shows a maximum at about 45° and minimum values parallel to RD and TD, i.e. altogether an inverse course when compared to the predictions for the 80% cold rolled sample (figure 6). As in the cold rolled material the values parallel to RD are slightly lower than those at TD. Recrystallization after 90% cold reduction leads to a nearly linear curve of the Young's modulus in the sheet plane revealing only a slight increase towards TD. The upper and lower values calculated according to the Voigt and Reuss approximations, respectively, again reveal a deviation of about 15 kN/mm^2 from the Hill mean value. Also the recrystallized samples show a very satisfying correspondence between the elastic data calculated from the experimental and modelled ODFs. The volume fractions which were applied to model the elastic curves are given for all inspected samples in table 2.

The excellent agreement between the values for the Young's modulus calculated either from the ODFs achieved from the series expansion method or those computed by component fit shows that the crystallographic texture may be described as superposition of several fibre-type and peak-type components.

In a second approach the impact of individual texture components on the elastic properties of polycrystalline steels was thus examined by creating model ODFs which merely consisted of well defined Gauss-type components, scattering 10° about the fibre axis or the center of a peak-type orientation. Textures which include only one single peak-type component, are given in figure 8. Whereas the occurrence of an isolated cube component $\{001\} \langle 100 \rangle$ leads to strong maximum at 45° with respect to RD (figure 8a), the $\{001\} \langle 110 \rangle$ (figure 8b) and $\{112\} \langle 110 \rangle$ (figure

8c) orientations both lead to a minimum at 45° and maxima parallel to RD and TD. The application of fibre-type components reveals the influence of a complete symmetric group of orientations, figure 9. The elastic modelling of a texture consisting only of an α -fibre leads to a course of Young's modulus which reveals considerable correspondence with that predicted by the isolated orientations of the $\{001\} \langle 110 \rangle$ and $\{112\} \langle 110 \rangle$ (figure 9a). The γ -fibre, on the other hand (figure 9b), shows a very symmetric course, i.e. no dependence on the angle versus RD. The assumption of a complete η -fibre, which is of relevance for the discussion of transformer steels bearing a strong Goss component, $\{110\} \langle 001 \rangle$, reveals a strong maximum close to 45° and a minimum parallel to RD (figure 9c).

Discussion

Although the elastic interactions of adjacent crystals have been neglected in the present investigation it is revealed that the experimentally detected elastic properties of polycrystals (figure 1), i.e. essentially the course of Young's modulus can be conveniently modelled by use of the coefficients of the harmonic series expansion of the corresponding crystallographic texture (figures 4-7). The predictions of the Voigt and Reuss approaches represent the upper and lower bounds of the current approximation, respectively. By use of these models the influence of the grain shape can be taken into account (figure 2). Although the basic correlation between the coefficients of the harmonic series expansion on the one hand and the elastic properties of the inspected sample on the other hand has already been thoroughly discussed by Bunge [1], Hu [5] and Lotter and Bleck [6], in the present work it was clearly revealed that an arbitrary orientation distribution can be decomposed into a small set of discrete single-type, or in case of ferritic steels, fibre-type Gauss like scattering texture components, which can then be used accordingly for the description of the macroscopic elastic anisotropy. Making use of this approach one can quantitatively describe the impact of arbitrary texture components on the elastic properties which, vice versa, allows an advanced progression towards materials design.

In the latter conception it was shown that the most isotropic course of Young's modulus is achieved in case of

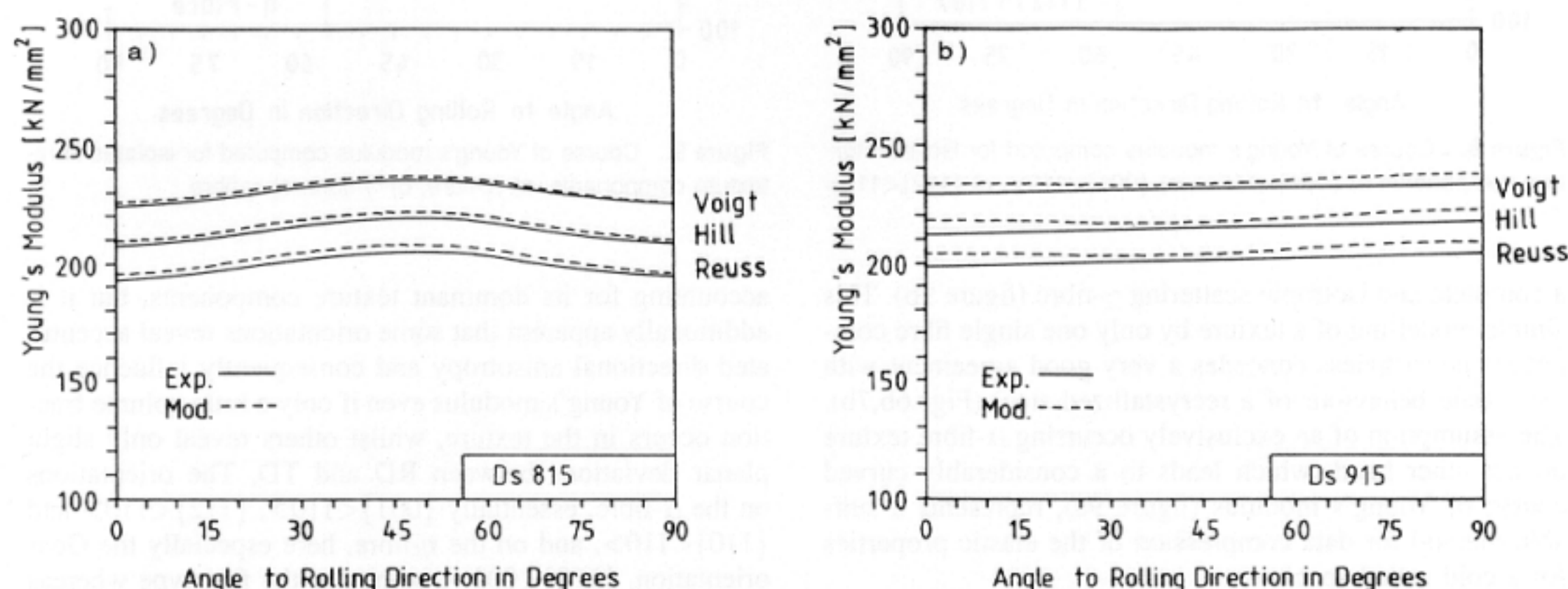


Figure 7. Young's modulus of the recrystallized sheets calculated from the coefficients of the series expansion method (Exp) and from model data (Mod), a) 80%, b) 90%. The corresponding model components are listed in table 2

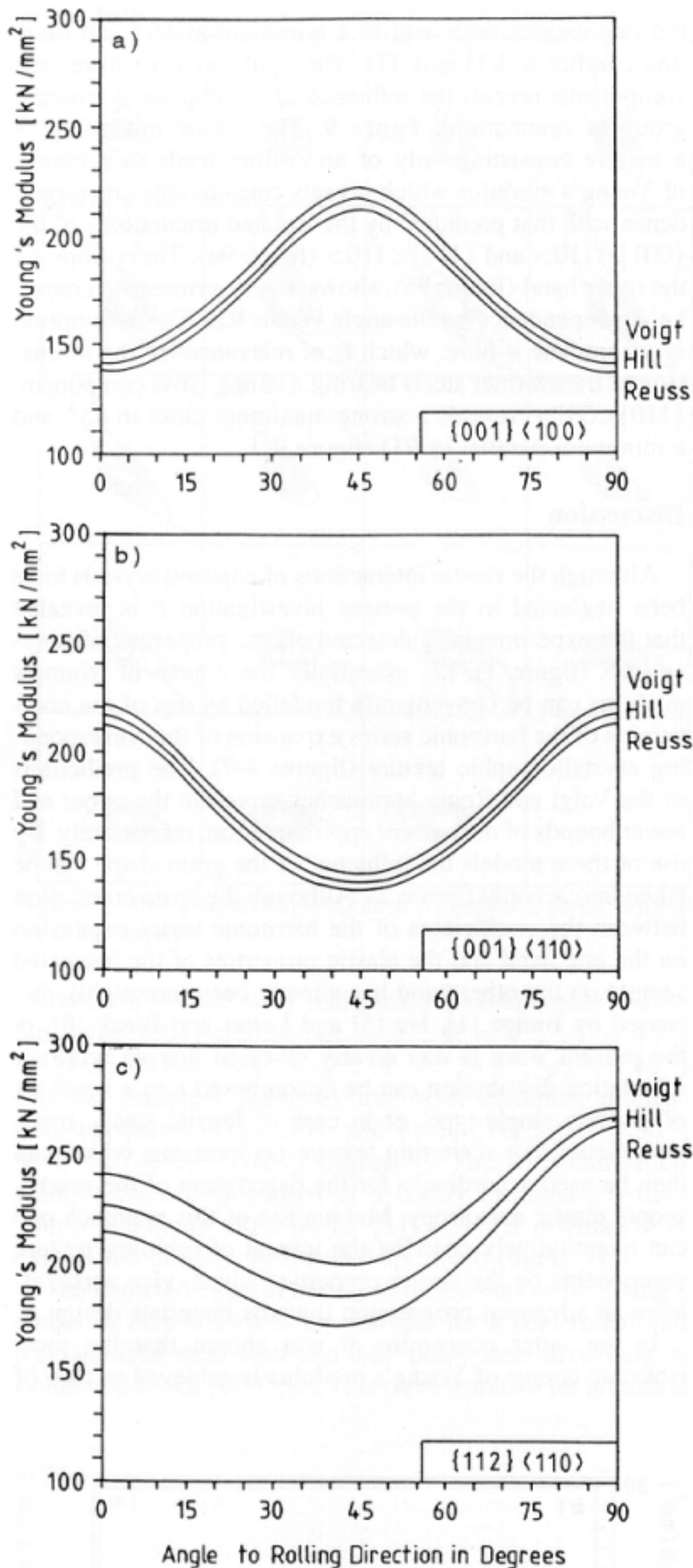


Figure 8. Course of Young's modulus computed for isolated texture components a) {001}<100>, b) {001}<110>, c) {112}<110>

a complete and isotropic scattering γ -fibre (figure 9b). This simple modelling of a texture by only one single fibre component nevertheless concedes a very good agreement with the elastic behaviour of a recrystallized steel (Figs.6b,7b). The assumption of an exclusively occurring α -fibre texture on the other hand, which leads to a considerably curved course of Young's modulus (figure 9a), represents a suitable method for data compression of the elastic properties for a cold rolled specimen.

It becomes, however, not only evident that the elastic response of a polycrystalline sample can be approximated by

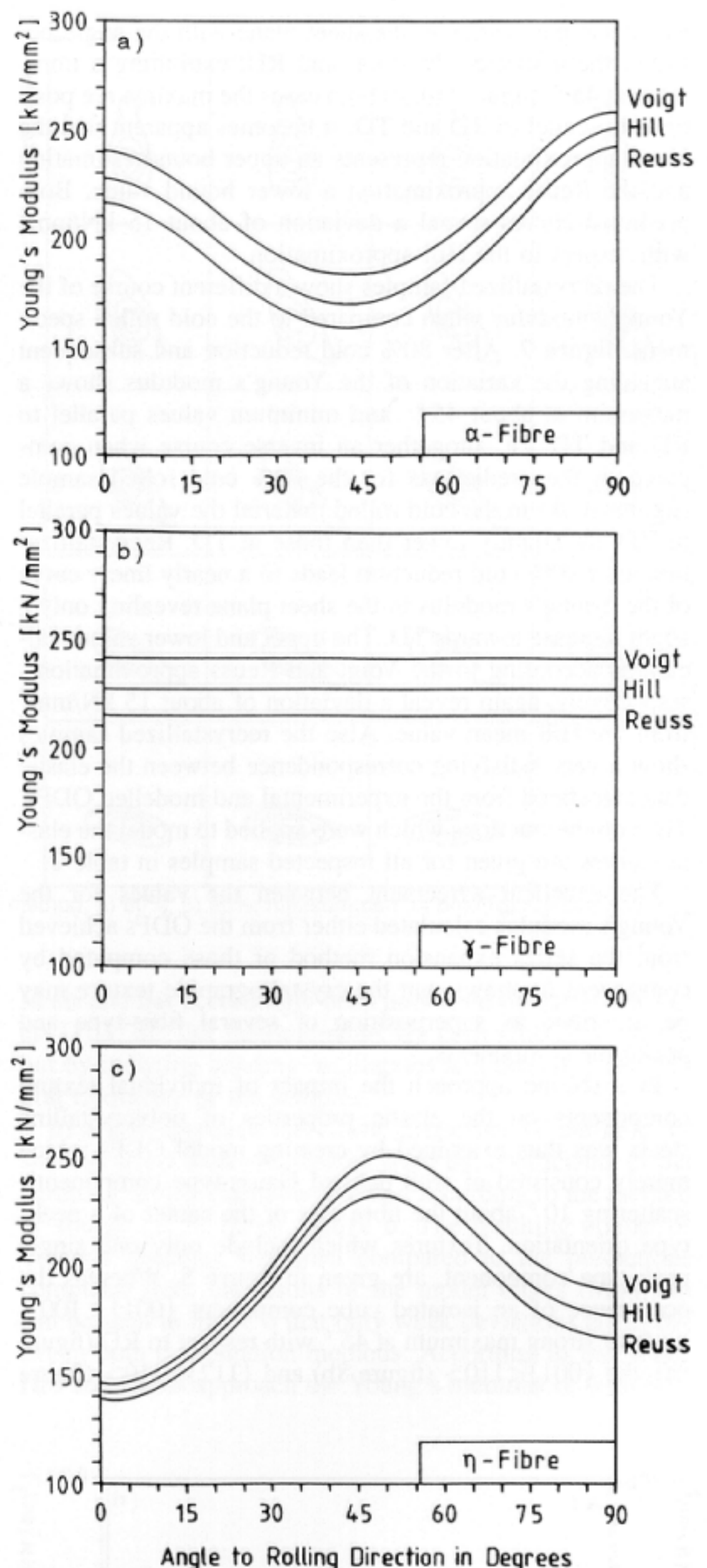


Figure 9. Course of Young's modulus computed for isolated fibre-texture components, a) α -fibre, b) γ -fibre, c) η -fibre

accounting for its dominant texture components, but it is additionally apparent that some orientations reveal accentuated directional anisotropy and consequently influence the course of Young's modulus even if only a little volume fraction occurs in the texture, whilst others reveal only slight planar deviations between RD and TD. The orientations on the α -fibre, essentially {001}<110>, {112}<110> and {110}<110>, and on the η -fibre, here especially the Goss orientation, {110}<001>, belong to the first type whereas the γ -fibre orientations conform to the second type of texture components.

Conclusions

The macroscopic elastic properties of a polycrystalline rolled and annealed low-carbon deep drawing steel was investigated by means of quantitative texture analysis. The results are in very good agreement with experimental findings. The obtained results, stemming from the harmonic series expansion of the texture, were additionally investigated by means of the ODF model analysis where the texture is decomposed into a small set of Gauss type model functions. It was shown that the computation of the elastic anisotropy on the basis of only a few isolated model components also concedes a very good approximation of the course of Young's modulus when compared to experimental data or to the results which were computed conventionally on the basis of the series the expansion coefficients.

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