

DETERMINATION OF SINGLE CRYSTAL ELASTIC CONSTANTS FROM
DS- AND DR-NI-BASED SUPERALLOYS BY A NEW REGRESSION METHOD
BETWEEN 20°C AND 1200°C

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Abstract

For the quantitative description of the elastic behaviour of a textured polycrystalline material the elastic constants of the single crystal and the orientation distribution function (ODF) are needed. The new regression method developed in this work allows the determination of single crystal elastic constants from directionally solidified (DS) or directionally recrystallized (DR) Ni-based superalloys. This method therefore provides the single crystal elastic constants even when only DS- or DR-materials with significantly different elastic moduli for different directions are available. The method is based on the measured elastic properties in different directions with regard to the direction of growth or recrystallization. These properties are obtained by the resonance method between 20°C and 1200°C. The evaluation of these data by the new J-regression method and the results for some alloys are presented and discussed.

Introduction

The quantitative description of the elastic behaviour of a textured polycrystalline material requires knowledge of the elastic constants of the corresponding single crystal and the orientation distribution function (ODF). Bunge [1], Zuidema et al. [2], Bayerlein et al. [3], and Bayerlein [4] have demonstrated that the elastic moduli of textured materials can be calculated with high accuracy by the Voigt-Reuss-Hill method [5-7]. The ODF can be determined experimentally by different methods depending on the grain size of the material. Problems can arise in obtaining the elastic constants of the single crystal if the latter is difficult to grow, expensive or cannot be prepared at all as in the case of ODS-alloys. In all these cases one must determine the elastic constants of the single crystal from measurements on textured polycrystalline material.

This determination is only possible if the polycrystalline material exhibits elastic properties which depend on the direction in the material. These properties must be measured in several directions. From such experimental results the elastic constants of the single crystal can be calculated if one refers to a concept which connects the properties of the textured polycrystalline and the monocrystalline material.

Using the concept of Hill [7] the elastic properties of textured materials can be calculated. A detailed description of this calculation procedure has been published recently [3]. Based on this concept it is possible to determine the elastic constants of the single crystal from the measured elastic properties of the corresponding textured material. The application of this method has limitations. The amount of calculations required can be tediously high and the results can exhibit relatively large errors even if the measured properties are determined with only small errors [4].

These problems provided the motivation for the development of a new empirical evaluation method which is named J-regression method.

New empirical evaluation method (J-regression method)

The new calculation method is based formally on the following relations between the elastic properties and the orientation parameter J for a single crystal of cubic crystal structure

$$E^{-1} = S'_{11}(J) = S_{11} - 2J(S_{11} - S_{12} - S_{44}/2) \quad (1)$$

$$G^{-1} = S'_{44}(J) = S_{44} + 4J(S_{11} - S_{12} - S_{44}/2) \quad (2)$$

in which the orientation parameter J is given by

$$J = \sin^2\theta \cos^2\theta + \frac{1}{8}\sin^4\theta(1 - \cos 4\varphi). \quad (3)$$

The S'_{ij} depend on the orientation of the considered axis in the crystal lattice which is determined by the two angles θ and φ . The constants S_{11} , S_{44} , and S_{12} characterize the elastic behaviour of a single crystal of cubic crystal structure.

In the formal adaptation of these relations to textured materials a parameter $J(\Delta)$ is introduced in such a way that the following relations

$$E(\Delta)^{-1} = S_{11} - 2 S J_e(\Delta) \quad (4)$$

$$G(\Delta)^{-1} (1-\kappa)^{-1} = S_{44} + 4 S J_g(\Delta) \quad (5)$$

are fulfilled. In the equations (4) and (5) the abbreviation $S = S_{11} - S_{12} - S_{44}/2$ is introduced and the direction-dependent coupling factor κ must be included in order to take into account a coupling of the translational and the torsional vibration modes of long and slender specimens [4]. Δ denotes the angle between a special direction of the texture, for instance the rolling direction or the direction of recrystallization, and the direction of the measurement in a plane determined by the special direction and the long transverse direction.

For the determination of $J_e(\Delta)$ and $J_g(\Delta)$ (the index e refers to E and g refers to G) the values $E(\Delta)$ and $G(\Delta)$ are calculated as free Hill's moduli for the existing texture and with approximately assumed elastic constants S_{11} , S_{12} , S_{44} of the single crystal [3]. These values of $E(\Delta)$ and $G(\Delta)$ are inserted into the eqns. (4) and (5). After this calculation of J_e and J_g the calculated values of $E(\Delta)$ and $G(\Delta)$ in the equations (4) and (5) are replaced by the measured moduli. A linear regression with respect to J_e and J_g leads to the constants S_{11} , S_{12} , and S_{44} of the single crystal. Using these constants of the single crystal, improved values of J_e and J_g can be determined as described. A second calculation procedure is often not necessary. In order to check the results, the Hill's moduli are calculated with the obtained elastic constants of the single crystal and compared with the corresponding measured values.

Materials

The described method has been applied successfully to the Ni-based superalloys IN 738 LC DS and MA 760 DR.

The elemental compositions of these alloys are given in Table I.

Table I Elemental compositions of IN 738 LC and MA 760 in wt.%

Alloy	C	Al	Co	Cr	Mo	Nb	Ta	Ti	W	Fe	Y ₂ O ₃	Ni
IN 738 LC	0.105	3.36	8.58	16.0	1.81	0.89	1.9	3.42	2.67	0.13	-	balance
MA 760	0.044	5.92	-	19.4	1.93	-	-	-	3.36	1.21	1.04	balance

MA 760 is an ODS alloy with γ' -precipitates. It was extruded and directionally annealed. The material was produced by Wiggins Alloys (U.K.) and supplied by ABB (Baden, Switzerland). The material was obtained in form of rectangular plates with dimensions 32x95x105 mm³. The mean grain diameter was 2.8mm, the grain length about 150mm. Cylindrical specimens of about 4.5mm in diameter and 40-50 mm in length were machined from the plate. The angle between the specimen axis and the extrusion direction was varied between 0° and 90° in steps of 15° (see Fig.1).

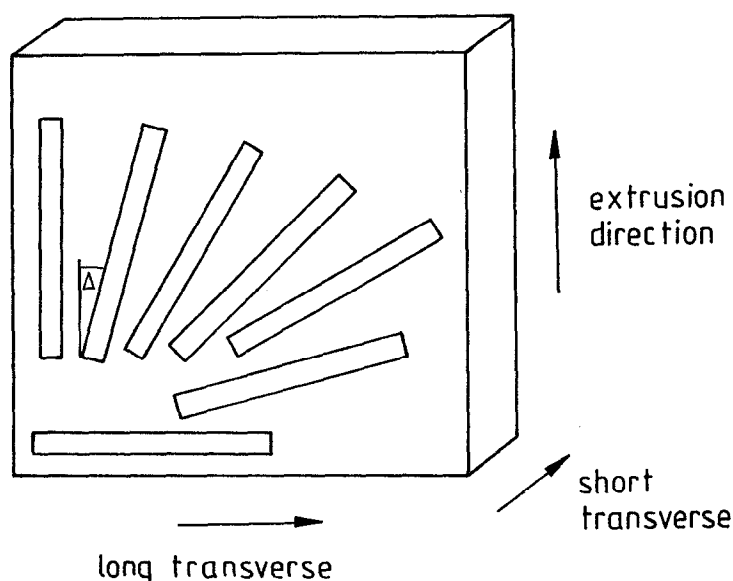


Figure 1 - Definition of the angle Δ between the direction of measurement in the sample axis and the extrusion direction in the as-received plate.

The γ' -precipitation hardened alloy IN 738 LC was available in form of a directionally solidified turbine blade. It was supplied by Siemens AG (KWU, Mühlheim, F.R.G.). The mean grain diameter was 4mm, the grain length larger than 100mm. The preparation of the specimens was carried out in the same way as described for MA 760, instead of the extrusion direction the direction of solidification was used in this case.

Experimental techniques

The elastic moduli were determined by using a dynamic resonance technique [8]. The measurements were carried out under vacuum between 25°C and 1150°C. The temperature was controlled by a Pt/PtRh-thermocouple located 1 mm away from the middle of the specimen. A schematic plot of the system used to determine the resonance frequencies is shown in Fig.2. From the resonance frequencies of bending and torsion the Young's modulus $E(T)$ and the shear modulus $G(T)$ were calculated for a given temperature T by means of the following theoretical relations [8]:

$$E(T) = 1.26193 \rho(T) l(T)^4 a(T)^{-2} f_b(T)^2 K_1 \quad (6)$$

$$G(T) = 4 \rho(T) l(T)^2 f_t(T)^2 K_2 \quad (7)$$

where $\rho(T)$ is the density, $l(T)$ the length and $a(T)$ the diameter of the specimen. The temperature dependence of these quantities is described by the coefficient of linear thermal expansion α . $f_b(T)$ denotes the fundamental resonance frequency in ben-

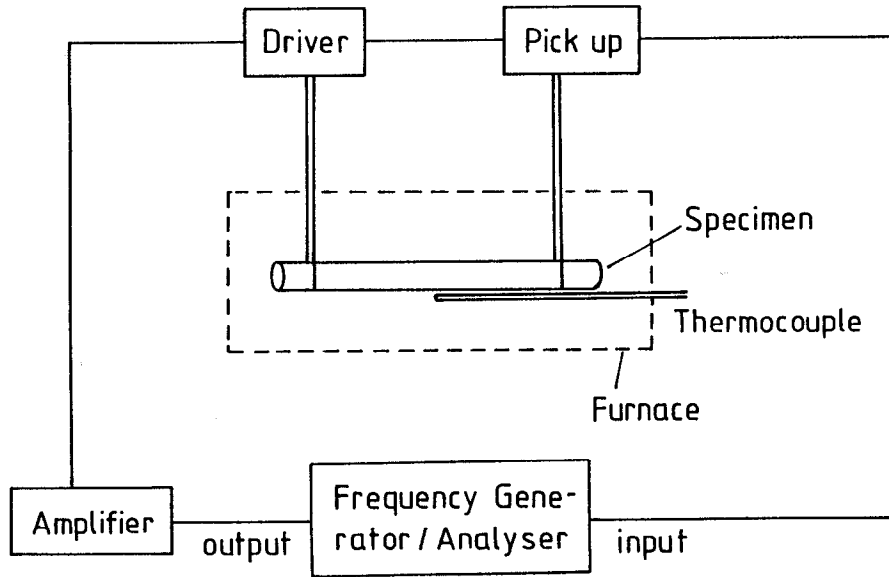


Figure 2 - Schematic representation of the experimental equipment for the determination of the resonance frequencies.

-ding and K_1 a correction term which takes into account the shear and the rotatory inertia [8]. $f_t(T)$ is the resonance frequency in torsion and K_2 a correction term which depends on the dimensions of the specimen [9], for a cylindrical specimen $K_2=1$. The uncertainty of E and G at 25°C is about 0.8%, at 1000°C about 1.5%, including all errors of the quantities in eqn. (6) and eqn.(7).

Because of the large grain diameter in both alloys the texture was determined by evaluating the orientations of 50 single grains by the Laue method. The ODF was calculated by the method of Bunge [1] from the orientations of the single grains and their corresponding volume fractions.

Results and discussion

The described investigation of the texture of the materials leads to the following results. The directionally recrystallized MA 760 exhibits a strongly developed {100} <110> texture. In the directionally solidified IN 738 LC a <100>-fibre texture is ob-

served, also strongly developed. It can be described quantitatively by a volume fraction of 93% occupied by grains with $\langle 100 \rangle$ -directions parallel to the fibre axis. The remaining volume fraction of 7% is occupied by randomly orientated grains. These evaluated textures were used in the mentioned calculations.

The experimentally determined $E(\Delta)^{-1}$ and $G(\Delta)^{-1}$ of the textured materials are plotted versus the calculated $J_e(\Delta)$ and $J_g(\Delta)$ respectively. An example of the obtained dependences is shown in Fig.3 for MA 760 at 25°C. The plotted properties exhibit a good linear dependence on $J_e(\Delta)$ or $J_g(\Delta)$ respectively. The evaluations of S_{11} and S_{44} by $J_e(\Delta)$ -, $J_g(\Delta)$ -regression according to eqns. (4) and (5) result in $S_{11} = 8.85 \cdot 10^{-12}/\text{Pa}$ and $S_{44} = 7.48 \cdot 10^{-12}/\text{Pa}$ at 25°C.

The complete evaluation of the experimental data for MA 760 and IN 738 LC leads to the values of S_{11} , S_{44} and S_{12} for different temperatures between 25°C and 1092°C (1142°C for IN 738 LC). These results are listed in Table II for MA 760 and in Table III for IN 738 LC.

The examinations of the accuracy of the evaluated single crystal constants S_{11} , S_{44} , and S_{12} had to be verified in different ways for the two alloys.

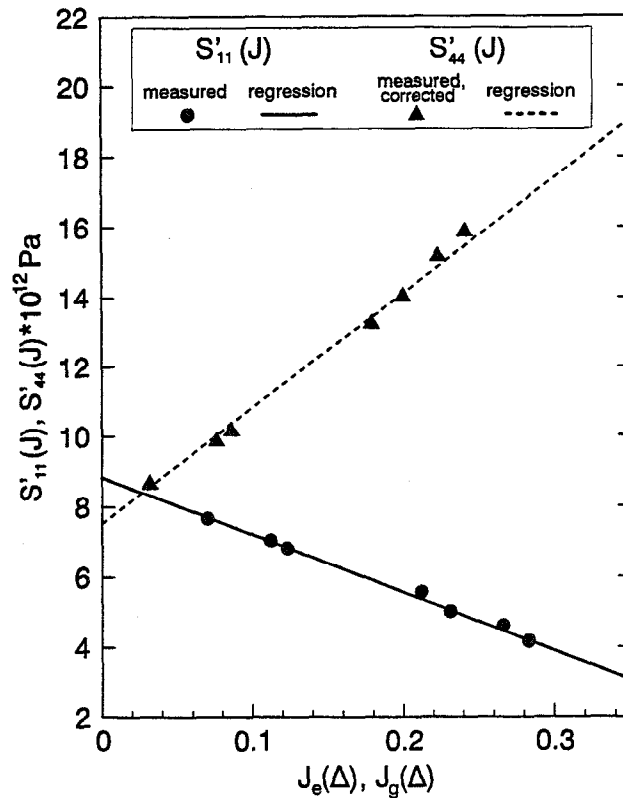


Figure 3 - Experimental values of $E(\Delta)^{-1}$ and $G(\Delta)^{-1}$ as a function of $J_e(\Delta)$ and $J_g(\Delta)$ for MA 760 at 25°C

Table II MA 760, S_{ij} obtained from measurements on directionally solidified material by the new J-regression method, S_{ij} in $10^{-12}/\text{Pa}$, temperature T in $^{\circ}\text{C}$

T [$^{\circ}\text{C}$]	S_{11}	S_{12}	S_{44}
25	8.85	-3.13	7.48
220	9.31	-3.41	7.92
420	9.87	-3.65	8.40
615	10.67	-3.95	8.85
800	11.94	-4.53	9.57
898	13.08	-5.07	10.23
992	15.24	-6.06	11.24
1092	18.73	-7.48	12.14

Table III IN 738 LC, comparison of S_{ij} obtained from measurements on single crystals and on directionally solidified material (<100>-fibre texture), in the second case the new J-regression method has been applied, SC: single crystal, J-R: J-regression, S_{ij} in $10^{-12}/\text{Pa}$, temperature T in $^{\circ}\text{C}$

T [$^{\circ}\text{C}$]	S_{11} (SC)	S_{11} (J-R)	S_{12} (SC)	S_{12} (J-R)	S_{44} (SC)	S_{44} (J-R)
25	7.97	8.20	-3.23	-3.20	7.87	7.55
220	8.48	8.76	-3.47	-3.54	8.28	8.03
420	9.09	9.30	-3.62	-3.81	8.67	8.50
615	9.83	10.01	-4.01	-4.09	9.19	9.01
800	10.72	11.08	-4.46	-4.60	9.92	9.69
898	11.45	11.92	-4.76	-5.07	10.53	10.19
992	12.99	13.40	-5.48	-5.86	11.16	10.95
1092	15.29	16.23	-6.70	-7.05	12.08	11.67
1142	17.55	18.33	-7.59	-7.97	12.95	12.31

For MA 760 no monocrystalline specimens with differently chosen orientations could be made available. From the used directionally recrystallized material one single crystal with $\langle 110 \rangle$ specimen axis could be prepared. This sample and in addition three samples parallel to the short transverse direction which had not been used in the evaluation of the S_{ij} were taken for the mentioned purpose.

Figure 4 presents measured and calculated elastic properties as a function of temperature for both specimens. In the calculations the evaluated single crystal constants S_{ij} and the ODF or the orientation have been used. Measured and calculated data exhibit very good agreement, the deviation is in the range of some percent. This result documents the high accuracy of the determined single crystal constants S_{ij} .

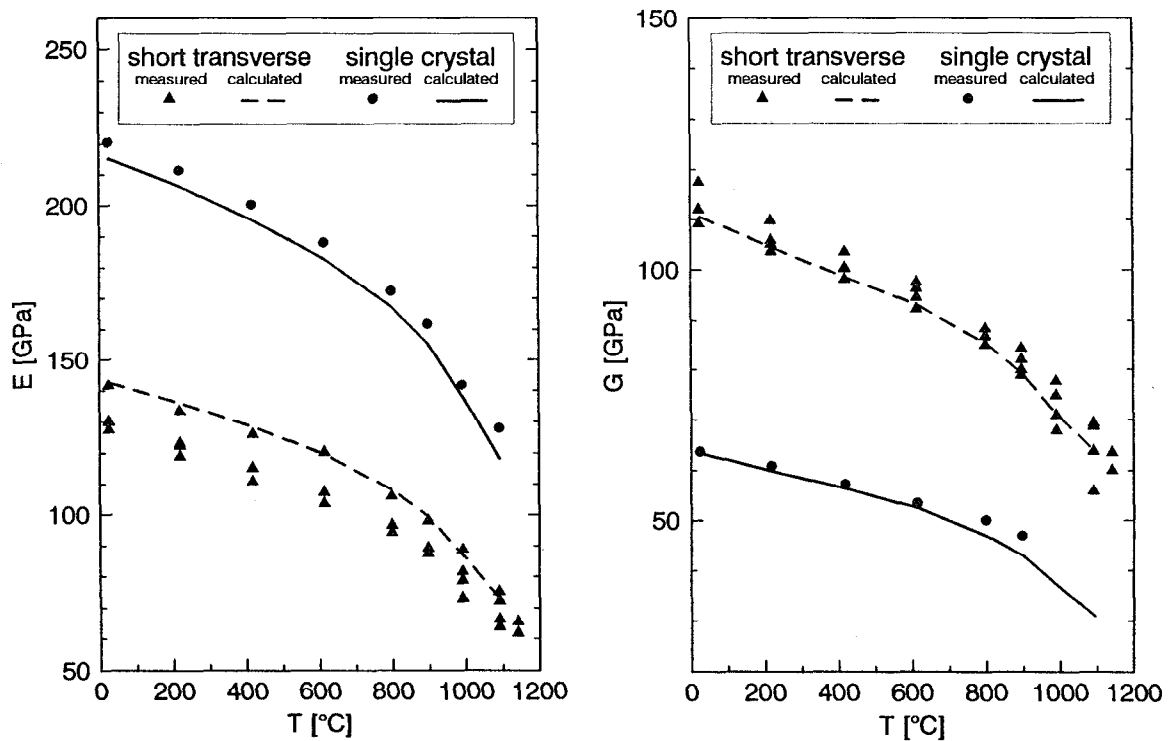


Figure 4 - MA 760, comparison of calculated and measured moduli for a single crystal and for three samples parallel to the short transverse direction in the DS-material

Single crystals of IN 738 LC are available. Measurements of the elastic properties for specimens of different orientations and an evaluation according to the eqns. (1) and (2) allow the determination of the single crystal constants S_{ij} . These data are included for comparison with the data from the new J-regression method in Table III. The comparison of the constants S_{ij} of different independent origin shows good agreement between them. The deviations lie in the range of 5% percent. Also this result confirms the good accuracy of the S_{ij} values from the new J-regression method.

Conclusions

The newly developed J-regression method allows the determination of single crystal constants S_{ij} for materials with cubic crystal lattices from measurements on directionally solidified or directionally recrystallized materials. It requires measurements of the elastic properties on specimens prepared with their axes at different angles to the direction of solidification or recrystallization.

Experiences with this method for different materials show that a strong direction dependence of the elastic properties in the textured materials is a fundamental requirement for a successful application of the new method.

The application of the new method and the results for MA 760 and IN 738 LC demonstrate convincingly the efficiency and the usefulness of the newly developed J-regression method.

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References

1. H.-J. Bunge, Mathematische Methoden der Texturanalyse (Berlin: Akademie Verlag, 1969).
2. J. Zuidema, O. Loopstra, and T.M. van Soest, "The (pseudo) isotropic Young's modulus and Poisson's ratio of anisotropic rolled sheets", Z. Metallk., 74 (1983), 643-651.
3. U. Bayerlein and H.G. Sockel, "Measurements and calculations of the elastic moduli of ODS and cast Ni-based superalloys", Mat. Sci. Eng. A141 (1991), 179-187.
4. U. Bayerlein, "Zur Ermittlung der Textur- und Gefügeabhängigkeit der elastischen Eigenschaften sowie der Einkristallkonstanten von Superlegierungen bei höheren Temperaturen" (Fortschritt-Berichte VDI Reihe 5 Nr.236, Düsseldorf: VDI-Verlag, 1991).
5. W. Voigt, Lehrbuch der Kristallphysik (Leipzig: Teubner, 1928).

6. A. Reuss, "Berechnung der Fließgrenze von Mischkristallen auf Grund der Plastizitätsbedingungen für Einkristalle", Z. angew. Math. Mech., 9 (1929), 49-58.
7. R. Hill, "The elastic behaviour of a crystalline aggregate", Proc. Phys. Soc., A65 (1952), 349-354.
8. J. Spinner and W.E. Teft, "A method for determining mechanical resonance frequencies and for calculating elastic moduli from these frequencies", Proc. ASTM 61 (1961) 1229-1238.
9. G. Pickett, "Equations for computing elastic constants from flexural and torsional resonant frequencies of vibration of prisms and cylinders", Proc. ASTM 45 (1945), 846-865.