Identification of elastic constants of alloys with sheet and fibre textures
based on resonance measurements and finite element analysis

Jianbao Han\textsuperscript{a}, Albrecht Bertram\textsuperscript{a}, Jürgen Olschewski\textsuperscript{a}, Wolfgang Hermann\textsuperscript{b},
Hans-Georg Sockel\textsuperscript{b}

\textsuperscript{a}Bundesanstalt für Materialforschung und \textit{-prüfung}, BAM 1.31, Unter den Eichen 87, D-12205 Berlin, Germany
\textsuperscript{b}Institut für Werkstoffwissenschaften, Lehrstuhl 1, Universität Erlangen-Nürnberg, Martenstrasse 5,
D-91058 Erlangen, Germany

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Abstract

This paper presents a method for identifying the elastic constants of alloys of cubic crystal structure with sheet and fibre textures. It is based on conventional resonance measurements and finite element (FE) analysis. It includes a non-linear optimizer, an FE program for solving eigenvalue equations in which the exact stress-strain constitutive law for orthorhombic or hexagonal symmetry is considered, and a frequency assignment algorithm based on the orthogonality of natural modes. The identification strategy consists in the adjustment of the elastic constants in an optimization procedure by minimizing the differences between calculated and measured natural frequencies of several specimens. The determination of the elastic single-crystal constants from textured material measurements is also discussed. The results of four practical applications to Ni-based alloys demonstrate the efficiency and the economy of this method.

Keywords: Elasticity; Alloys; Finite element method; Fibres

1. Introduction

Future industrial gas turbines need to be operated at increasingly higher temperatures to improve the efficiency and to enhance power output. In order to meet the requirements for this application, turbine blades are manufactured from single crystal alloys or alloys with specific textures, such as directionally solidified (DS) alloys having fibre texture and directionally recrystallized (DR) alloys having sheet textures. With decreasing numbers of transverse grain boundaries, improved thermal fatigue resistance and creep strength of these materials are achieved, allowing higher stresses and temperatures in service [1]. Alloys with $\gamma'$-\{Ni$_3$(Al, Ti)\} precipitates, such as DS IN-738LC, DS IN-792, MAR-M 247 and DR MA 760, are of great interest [2].

For the design of statically and dynamically loaded blades, knowledge of the elastic moduli and of their variations with temperature and orientation is a fundamental requirement, especially for analyses of the vibrations, strength, fracture, or stability of structures. DS and DR alloys in general show a strong texture. DS alloys often show a {001} fibre texture, whereas in DR alloys a {100}/{110} sheet texture is found [2]. This causes strong variations in the elastic moduli with the orientation to the fibre axis or to the direction of recrystallization. The DR materials exhibit orthorhombic symmetry with nine independent elastic constants, and the DS materials exhibit hexagonal symmetry with five independent elastic constants. The present authors have proposed a method [3–5] for identifying the elastic constants and orientation of single crystal alloys based on resonance measurements and finite element (FE) analysis. It is a systematic extension of Förster’s [6] resonance method for anisotropic materials.

This paper presents an extension of this method described in [4] for identifying the elastic constants of alloys with sheet texture by resonance measurements and
FE analysis. The alloys with fibre texture are treated as a special case of those with sheet texture. The identification strategy consists in the adjustment of the elastic constants in an optimization procedure by minimizing the differences between calculated and measured natural frequencies of several specimens. The calculation of these frequencies is carried out by the FE code ADINA [7]. The principle of the resonance measurements has been described in [8]. In these measurements the applied temperature can be varied from 25 to 1200°C. Another way to determine the stiffness or the compliance of a textured alloy is their calculation from the elastic constants obtained by measurements on single crystals. Sometimes, however, it is impossible to obtain single crystals, e.g. from materials produced by sintering of powders. Therefore it is necessary to determine the elastic single-crystal constants from measurements on textured materials. In this paper, the determination of the elastic single-crystal constants from alloys of f.c.c. crystal structure with \( \langle 100 \rangle \) fibre texture is discussed. Four applications are given for the DR Ni-based alloy MA760 and also the DS alloys IN-738LC, IN-792 and MAR-M247.

2. Definition of elastic constants and orientation

The constitutive law which characterizes a linear elastic material subjected to small deformations may be written as

\[ \varepsilon = \mathbf{S} \sigma \]  

where \( \varepsilon \) is the elastic strain vector, \( \sigma \) is the stress vector, \( \mathbf{S} \) is the elastic compliance matrix.

For an orthorhombic material, Eq. (1) may be written in the following form:

\[
\begin{bmatrix}
\varepsilon_{11} \\
\varepsilon_{22} \\
\varepsilon_{33} \\
2\varepsilon_{33} \\
2\varepsilon_{13} \\
2\varepsilon_{12}
\end{bmatrix}
= \begin{bmatrix}
S_{11} & S_{12} & S_{13} & 0 & 0 & 0 \\
S_{22} & S_{23} & 0 & 0 & 0 & 0 \\
S_{33} & 0 & 0 & 0 & 0 & 0 \\
S_{44} & 0 & 0 & 0 & 0 & 0 \\
S_{55} & 0 & 0 & 0 & 0 & 0 \\
S_{66}
\end{bmatrix}
\begin{bmatrix}
\sigma_{11} \\
\sigma_{22} \\
\sigma_{33} \\
\sigma_{44} \\
\sigma_{55} \\
\sigma_{66}
\end{bmatrix}
\]  

(2)

The matrix \( \mathbf{S} \) is symmetrical and has nine independent components which are the nine independent elastic constants of the orthorhombic material. The structure of the matrix \( \mathbf{S} \) characterizes the orthorhombic anisotropy. It must be noted that the Eq. (2) refers to a principal axis coordinate system in the material. For an arbitrary specimen fixed-coordinate system in a cylindrical specimen consisting of an orthorhombic material, there are in general no components equal to zero in the compliance matrix, denoted by \( \mathbf{S}^* \). However, the components may be expressed by the nine independent constants shown in Eq. (2) and two Eulerian angles which describe the orientation of the specimen. This is illustrated in Fig. 1, where the Z axis is aligned with the recrystallization direction (RD), the Y axis with the transverse direction (TD) and the X axis with the normal direction (ND). The Y-Z plane corresponds to the \( \langle 100 \rangle \) plane, and \( \varphi_2 \) presents the angle between the specimen length direction and the recrystallization direction. For instance, the component \( S_{33}^* \) of the matrix \( \mathbf{S}^* \) is given by

\[
S_{33}^* = S_{11} \sin^4 \varphi_1 \sin^4 \varphi_2 + 2S_{12} \sin^2 \varphi_1 \cos^2 \varphi_1 \sin^4 \varphi_2 + 2S_{13} \sin^2 \varphi_1 \sin^2 \varphi_2 \cos^2 \varphi_2 + S_{22} \cos^4 \varphi_1 \sin^2 \varphi_2 + 2S_{23} \cos^2 \varphi_1 \sin^2 \varphi_2 \cos^2 \varphi_2 + S_{33} \cos^4 \varphi_2 + 4S_{44} \cos^2 \varphi_1 \sin^2 \varphi_2 \cos^2 \varphi_2 + 4S_{55} \sin^2 \varphi_1 \sin^2 \varphi_2 \cos^2 \varphi_2 + 4S_{66} \sin^2 \varphi_1 \cos^2 \varphi_2 \sin^2 \varphi_2
\]  

(3)

The nine independent elastic constants may be expressed in terms of traditional elastic moduli by three Young's moduli \( E_a, E_b \) and \( E_c \), three shear moduli \( G_{ab}, G_{ac} \) and \( G_{bc} \) and three Poisson's ratios \( \nu_{ab}, \nu_{ac} \) and \( \nu_{bc} \). They are defined with reference to a set of axes \( a, b, c \) which are aligned with the material's principal axes \( X, Y, Z \). The relations between the compliances \( S_{ij} \) and the moduli are as follows:

\[ E_a = 1/S_{11}, \quad E_b = 1/S_{22}, \quad E_c = 1/S_{33}, \quad G_{ab} = 1/S_{55}, \quad G_{ac} = 1/S_{44}, \quad G_{bc} = 1/S_{66}, \quad \nu_{ab} = -S_{12}/S_{22}, \quad \nu_{ac} = -S_{13}/S_{33}, \quad \nu_{bc} = -S_{23}/S_{33}. \]

From the condition of positive definiteness of the matrix \( \mathbf{S} \) in Eq. (2), the following relations must be fulfilled [7]:

\[ |\nu_{ij}| < \left( \frac{E_j}{E_i} \right)^{1/2}, \quad i, j = a, b, c \]

(4)

\[ \nu_{ab} \nu_{ac} \nu_{bc} < 0.5 \left( 1 - \nu_{ab}^2 \frac{E_a}{E_b} - \nu_{ac}^2 \frac{E_a}{E_c} - \nu_{bc}^2 \frac{E_b}{E_c} \right) < 0.5 \]

(5)
If the compliances \( S_j \) meet the constraints
\[
S_{22} = S_{11}, \quad S_{33} = S_{13}, \quad S_{55} = S_{44}, \quad S_{66} = 2(S_{11} - S_{12})
\]
then the matrix \( S \) is just the stress–strain constitutive compliance matrix of hexagonal materials, such as Ni-based DS alloys. In this case, the \( Z \) axis in Fig. 1 is aligned with the solidification direction of a DS alloy. The description of the orientation of a specimen needs only the polar angle \( \varphi_2 \). The azimuthal angle \( \varphi_1 \) is not necessary because of the transverse isotropy of the hexagonal materials. For this reason, the simulation of elastic properties of hexagonal materials may be treated as a special case of those of orthorhombic materials. The restrictions on the compliances \( S_j \) of a hexagonal material are
\[
S_{44} > 0, \quad S_{11} > |S_{13}|, \quad (S_{11} + S_{12})S_{33} > S_{13}
\]

3. Dependence of frequencies on orientation and elastic constants

For a cylindrical specimen of isotropic material which has only two independent elastic constants, analytical solutions have been worked out for the longitudinal, transverse and torsional vibration modes. The two constants (Young's modulus and shear modulus) can be calculated directly from these solutions [6]. However, this is not valid for the DR and DS alloys because of their anisotropy. As a result, the two frequencies of a transverse natural mode pair of a DS (or of a DR) alloy cylindrical specimen are not identical, if the polar angle \( \varphi_2 \) is not just equal to zero.

In our case, each of the specimens is modelled by isoparametric 20-node elements. The resulting eigenvalue equations are given by
\[
(-\omega_j^2 M + K)u_j = 0 \quad i = 1, 2, \ldots
\]
where \( \omega_j \) and \( u_j \) are the \( i \)th natural frequency and mode, \( M \) and \( K \) are the inertia and stiffness matrices of the FE model respectively. Fig. 2 shows the dependence of the first transverse and torsion natural frequencies of a cylindrical specimen of an orthorhombic material on \( \varphi_2 \) for different values of \( \varphi_1 \), and Fig. 3 the dependence of these frequencies on the constants \( E_a, E_b, E_c, G_{ab}, G_{ac} \) and \( G_{bc} \). A similar analysis of the
dependence of the natural frequencies of a cylindrical specimen of a hexagonal material on orientation and elastic constants was given in [9]. Figs. 2 and 3 show that, for a reliable identification of the nine elastic constants, at least three specimens are needed, the orientations of which lie near \((q_1 = 0^\circ, q_2 = 0^\circ)\), \((q_1 = 0^\circ, q_2 = 90^\circ)\) and \((q_1 = 90^\circ, q_2 = 90^\circ)\) respectively. A great advantage of the use of the above-proposed three specimens is that the experimental errors of orientations have relatively small influence on the natural frequencies because the lowest gradient occurs near these three orientations.

4. Optimization procedure

The strategy of the identification consists in the adjustment of the nine elastic constants \(E_{ab}, E_{c}, G_{ab}, G_{ac}, G_{bc}, v_{ab}, v_{ac}\) and \(v_{bc}\) for an orthorhombic material or of the five elastic constants \(E_{ab}, E_{c}, G_{ab}, G_{ac}\) and \(v_{ac}\) for a hexagonal material by an optimization procedure which minimizes the differences between the measured and calculated natural frequencies of several specimens. The object function of the optimizer is the square sum of these differences. The calculation of the natural frequencies of these specimens is done by solving Eq. (8) by the FE code ADINA. In every iteration step of the optimization procedure, the calculated frequencies for different modes must be assigned to the measured frequencies. This is carried out by using the orthogonality of natural modes. The details about the frequency assignment are given in [3]. The optimizer used here is from MINPACK [10]. It uses a modified Levenberg–Marquardt algorithm. The convergence is controlled by three parameters which measure the relative errors desired in the object function and in the approximation solutions as well as the orthogonality desired between the object function vector and the columns of the Jacobian matrix.

5. Application

The method has been used to identify the elastic constants of several Ni-based, Fe-based and Ti-based superalloys. Ni-based superalloys can exhibit several textures including \{100\}/\{110\} sheet texture and \{001\} fibre texture. The identified elastic constants of four textured Ni-based alloys of f.c.c. crystal structure are reported in the following. One of them is a DR polycrystal. The other three are DS materials.

In the first example, results are given for the DR Ni-based superalloy MA760 which exhibits a \{100\}/\{110\} sheet texture causing a macroscopic orthorhombic symmetry in the elastic behaviour with nine independent constants. Three specimens of the superalloy with different orientations with respect to the RD were used for the identification. The chosen orientations of these specimens were exactly those which were recommended in the preceding section. They were measured by the Laue back-reflection X-ray technique. The starting values for the variables are rather rough estimations. The identified constants at room temperature are presented in Table 1. In Table 2 a comparison between the measured and calculated natural frequencies is shown. The algebraic average and variance of the deviations are equal to 0.014% and 0.729% respectively.

The other three examples concern the DS superalloys IN-738LC, IN-792 and MAR-M 247 which exhibit a \{001\} fibre texture causing a macroscopic hexagonal symmetry in the elastic behaviour with five independent constants. For each of the three DS superalloys, at least three specimens are used for the identification of the elastic constants in the optimization procedure. The convergence for the three materials was very stable. Table 3 presents the results for DS IN-738LC. In Tables 4 and 5 the results for DS IN-792 and DS MAR-M 247 are listed. These data refer to room temperature. Table 6 shows a comparison between the measured and calculated natural frequencies of three specimens of DS MAR-M 247. The algebraic average and the variance of the deviations are equal to 0.153% and 0.631% respectively. The two values of the deviations between the measured and calculated frequencies for the specimens of DS IN-738LC and DS IN-792 have the same order as that of DS MAR-M 247. The smallness of the averages and the variances of the deviations in Tables 2 and 6 show the efficiency of the method and the good agreement between the calculated and measured natural frequencies.

A DS Ni-based alloy consists of many columnar grains which can be considered as single crystals. The single-crystal grains have an f.c.c. crystal structure and exhibit a cubic symmetry of the elastic behaviour with three independent constants. It is useful to determine these three constants from the five elastic constants of the DS alloy. For this the following are assumed.

1. In the plane normal to the direction of solidification there is a sufficient number of single-crystal columnar grains.

2. All the columnar grains are parallel to the direction of solidification.

3. These columnar grains are randomly oriented in the transverse direction, so that the DS alloy has an ideal transverse isotropy.

Under these assumptions it is easy to prove that the three single-crystal constants can be determined from
Table 1
Identified elastic constants for directionally recrystallized MA760

<table>
<thead>
<tr>
<th></th>
<th>$S_{11}$</th>
<th>$S_{12}$</th>
<th>$S_{13}$</th>
<th>$S_{44}$</th>
<th>$S_{15}$</th>
<th>$S_{66}$</th>
<th>$S_{16}$</th>
<th>$S_{56}$</th>
<th>$S_{33}$</th>
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<tr>
<td></td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
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<td>7.539</td>
<td>4.207</td>
<td>4.555</td>
<td>22.75</td>
<td>7.767</td>
<td>9.377</td>
<td>-0.150</td>
<td>-0.075</td>
<td>-0.065</td>
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<table>
<thead>
<tr>
<th>$E_a$</th>
<th>$E_b$</th>
<th>$E_c$</th>
<th>$G_{ab}$</th>
<th>$G_{ac}$</th>
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<th>$\nu_{ac}$</th>
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<td>(GPa)</td>
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<td>(GPa)</td>
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<td>(GPa)</td>
<td>(GPa)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>132.6</td>
<td>237.7</td>
<td>219.5</td>
<td>43.95</td>
<td>128.7</td>
<td>106.6</td>
<td>0.036</td>
<td>0.016</td>
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Table 2
Comparison of measured and calculated frequencies for directionally recrystallized MA760 where the deviation is the relative deviation between the measured and calculated frequencies

<table>
<thead>
<tr>
<th>Mode type</th>
<th>Frequency (Hz)</th>
<th>Specimen 1, $\varphi_1 = 0^\circ$, $\varphi_2 = 0^\circ$</th>
<th>Specimen 2, $\varphi_2 = 0^\circ$, $\varphi_2 = 90^\circ$</th>
<th>Specimen 3, $\varphi_1 = 90^\circ$, $\varphi_2 = 90^\circ$</th>
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</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Measured</td>
<td>Calculated</td>
<td>Deviation (%)</td>
</tr>
<tr>
<td>Transverse</td>
<td>7012</td>
<td>7013</td>
<td>0.028</td>
<td>7701</td>
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<td>Transverse</td>
<td>7084</td>
<td>7074</td>
<td>0.135</td>
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<td>Transverse</td>
<td>18514</td>
<td>18509</td>
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<td>Transverse</td>
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<td>Transverse</td>
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<td>36287</td>
<td>0.161</td>
<td>38520</td>
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<tr>
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<tr>
<td>Transverse</td>
<td>73941</td>
<td>73863</td>
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<tr>
<td>Longitudinal</td>
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<td>49624</td>
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<td>52105</td>
</tr>
<tr>
<td>Torsional</td>
<td>27184</td>
<td>27120</td>
<td>0.235</td>
<td>26715</td>
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<td>54058</td>
<td>54319</td>
<td>0.484</td>
<td>53173</td>
</tr>
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<td>Torsional</td>
<td>81910</td>
<td>81694</td>
<td>0.263</td>
<td>80341</td>
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Table 3
Identified elastic constants for directionally solidified IN 738LC

<table>
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<tr>
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<th>$S_{11}$</th>
<th>$S_{12}$</th>
<th>$S_{13}$</th>
<th>$S_{33}$</th>
<th>$S_{44}$</th>
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<tbody>
<tr>
<td></td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
<td>(10$^{-12}$ Pa$^{-1}$)</td>
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<td></td>
<td>5.920</td>
<td>-1.043</td>
<td>-3.182</td>
<td>8.249</td>
<td>8.161</td>
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<table>
<thead>
<tr>
<th>$E_a$</th>
<th>$E_b$</th>
<th>$E_{ac}$</th>
<th>$G_{ac}$</th>
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<tr>
<td>(GPa)</td>
<td>(GPa)</td>
<td>(GPa)</td>
<td>(GPa)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>168.9</td>
<td>121.2</td>
<td>71.81</td>
<td>122.5</td>
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</table>

the elastic properties in the solidification direction of the DS alloy. Table 7 shows the elastic single-crystal constants of the DS alloys IN-738LC, IN-792 and MAR-M 247. From Table 7 it can be found that there is no great difference between these elastic single-crystal constants of the three DS Ni-based alloys, in particular for the shear moduli.

It is well known that the lowest natural frequencies of a vibrating system can be calculated by a suitable FE model with any desired accuracy, if the number of these frequencies is much smaller than the number of degrees of freedom of the model. In our case, the number of the lowest natural frequencies of a specimen used in the procedure is not more than 10, and the
number of degrees of freedom of the FE model is 600. Moreover, the measured natural frequencies of these specimens arise from their free vibration. The suspension wires and suspension position have a very small influence on the measuring precision of the frequencies. Damping effects can be neglected, because the strains of the specimen are very small. For these reasons the resonance measurements can be regarded as free from disturbing influences. In this case, it can be supposed that the deviations between the measured and calculated natural frequencies are primarily due to the uncertainty of the identified constants. The good
agreement between the measured and calculated natural frequencies shown in Tables 2 and 6 allows us to conclude that the identified constants can be regarded as a good approximation for the exact constants.

6. Conclusions

The presented method enables us to identify the elastic constants of materials which exhibit sheet and fibre textures. The stress-strain constitutive compliance matrix of hexagonal materials may be treated as a special case of the orthorhombic materials. In principle, there are no limitations to the specimen shape and the specimen orientation, as long as the measurement of an accurate and complete resonance spectrum in a certain frequency range is possible. In the case of the hexagonal or orthorhombic symmetry of the elastic behaviour, reliable convergence of the identification procedure was ensured by the use of the four measured transverse pairs and three measured torsional natural frequencies of at least three specimens. Knowledge of the longitudinal natural frequencies is not necessary. Simultaneous use of the measured natural frequencies of several specimens is helpful for a stable convergence of the procedure. The successful identification of the constants shown in Tables 1, 3–5 and 7 are attributed to the suitable optimizer, the very good approximation of the natural frequencies by the FE code ADINA and the reliable frequency assignment scheme in every iteration. The practical application demonstrates the efficiency and economy of the procedure.

References


