

# Identification of elastic constants and orientation of single crystals by resonance measurements and FE analysis

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**Abstract:** This paper presents an optimization procedure that uses FE analysis to identify the elastic constants of single crystals at elevated temperatures and the crystal orientation of a specimen based on resonance measurements. First, the measured natural frequencies are assigned to those predicted by an FE model according to the orthogonality of the natural modes. Then, the constants and orientation are adjusted by minimizing the differences between the measured and calculated frequencies. The results for single crystals of the Ni-based superalloy SRR99 demonstrate the versatility and efficiency of the method.

**Key words:** anisotropy, elastic constant, optimization, resonance method, single crystal.

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## 1 INTRODUCTION

The development of single crystals of superalloys has led to superior thermo-mechanical properties compared to the conventional polycrystalline superalloys due to the absence of the grain boundaries, which provide paths for fast diffusion and oxidation. However, single crystals exhibit anisotropy in their properties. For design purposes the determination of the anisotropic elastic behaviour is fundamental, especially for vibrational analysis. The theoretical foundations of crystal elasticity have been well known for about a century [1, 2]. The main unsolved problem, however, is the determination of the elastic constants at high temperatures by suitable experiments. Static tests are difficult and costly because of anisotropic effects and high temperatures. An alternative approach is to use resonance measurements as proposed by F. Förster [3].

The experimental device is relatively simple. A specimen is hung between two loops of temperature resistant wire. One of them is excited under controlled frequencies, while the other leads to a pick-up for the measurement of the response. In this way, several lowest natural

frequencies of the specimen can be determined. By use of the measured frequencies the elastic constants are calculated from the analytic formulas which relate the constants to the frequencies. For anisotropic materials, however, in contrast to the case of isotropic ones, there are in general no analytic solutions for their free vibration. After introducing FEM for predicting the natural frequencies, the resonance method has been extended to a broad class of materials by Olschewski [4] and Bertram *et al.* [5].

This paper presents a systematic procedure for identifying the elastic constants of single crystals at elevated temperatures based on resonance measurements and FE analysis. Under certain conditions, the crystal orientation of a specimen can also be identified without further measurements. The basic idea of the procedure in the adjustment of the constants and of the orientation is to minimize the differences between the measured and calculated natural frequencies of one or several specimens. The calculation of the frequencies is carried out by FEM. The assignment of the calculated frequencies to the measured ones, the sensitivity analysis, the test of the measured frequencies particularly distorted by experimental errors, and the stability of the solution are

discussed in this paper. The uniqueness of the solution is discussed by examples. As a practical application, we consider single crystals of the f.c.c. nickel base superalloy SRR99 which has cubic symmetry. The constants up to 1200°C have been determined. Although only single crystals with cubic symmetry are considered in this study, the method and the code are applicable to materials of any other symmetries in the same way. To save space, the data of the specimens used in this paper are listed together in Appendix B.

## 2 ELASTIC BEHAVIOUR OF SINGLE CRYSTALS

Hooke's law relates the stress vector  $\sigma$  to the strain vector  $\varepsilon$

$$\sigma = C\varepsilon, \quad (1)$$

where  $C$  is the elasticity matrix. Equation (1) represents the constitutive relationship of elastically anisotropic single crystals. The matrix  $C$  has in general twenty-one independent components with respect to an arbitrarily selected coordinate system, but this number can be drastically reduced in the presence of material symmetries. For instance, the single crystals with cubic, hexagonal and orthorhombic symmetries have three, five, and nine independent elastic constants, respectively. If the selected coordinate system is aligned to the crystal axes, the matrix has the simplest form. The transformation of the matrix from this form to the general form in Equation (1) can be done by use of three Eulerian angles which describe the crystal orientation [4].

The aim of this paper is to identify the elastic constants of single crystals of superalloys and the three Eulerian angles of a specimen simultaneously by FE analysis.

## 3 INVERSE PROBLEM

For a specimen consisting of an anisotropic material, e.g. single crystals of superalloys, there are no general analytic solutions for its free vibration, even if it has the simplest shape: cylindrical. To determine the eigenvalues of the free vibration, one can model the specimen by FEM and solve the resulting eigenvalue problem using a suitable algorithm, if the elastic constants, the orientation and the geometrical data of the specimen are known.

In our case, however, we are dealing with the inverse problem: determination of the elastic constants and the crystal orientation by use of FE analysis and the measured natural frequencies. We set an initial value for the constants and the orientation, calculate the natural frequencies of one or several specimens by using FEM, and determine the differences between the measured and calculated frequencies. The values of the constants and the orientation are then adjusted by minimizing the differences. Mathematically this is achieved by nonlinear

optimization procedures such as gradient methods, e.g. the Levenberg-Marquardt algorithm. It allows the determination of the values of these unknowns so that the natural frequencies calculated by them are identical with the measured ones within given tolerant limitation. The eigenvalue problem of the specimens is solved by the FEM code ADINA [6]. The optimizer used here is from MINPACK [7]. An appropriate selection of the unknowns used for the procedure is helpful for stability and precision of the solution. Another important problem in this procedure is to assign the calculated frequencies to the measured ones in every iteration step. This is discussed in the following section. Figure 1 gives a schematic view of the optimization procedure.

### 3.1 Assignment of frequencies

In the iterative optimization shown in Figure 1 the values of the unknowns are improved in every step. Consequently, the order of the calculated frequencies of certain modes can vary with the changes of the values of the unknowns. In such a case the calculated frequencies must be assigned to the associated measured ones in every iteration step. This is achieved by following procedure.

It is well known that the natural modes  $u_i$  of a vibrating system are orthogonal with respect to the mass matrix  $M$ . The frequencies are assigned by the use of this orthogonality which can be formulated by

$$u_i^T \cdot M \cdot u_j = \delta_{ij}, \quad i, j = 1, 2, \dots, N, \quad (2)$$

where  $\delta_{ij}$  is the Kronecker delta, and  $N$  is the degree of freedom of the vibrating system.

The normalization scheme of  $u_i$  used in Equation (2) yields

$$u_i^T \cdot K \cdot u_i = \omega_i^2, \quad i = 1, 2, \dots, N, \quad (3)$$

where  $\omega_i$  is the  $i$ th natural frequency in radians per second. Initially, we have calculated a set of reference modes using an FE model of an isotropic specimen with similar geometry. These reference modes can be divided into three vibrational types: the transversal, torsional, and longitudinal ones. The frequencies of each type are also numbered in terms of their values. Two frequencies of transversal modes of the isotropic specimen are identical due to rotational symmetry. However, for an anisotropic specimen this does not hold. Each of the anisotropic modes can be represented as linear combinations of the reference modes with different weighted coefficients  $A_{ij}$ , which represent the coupling degrees of an anisotropic natural mode with the reference modes and are calculated by

$$A_{ij} = u_i^{aT} \cdot M \cdot u_j^r, \quad (4)$$

where  $u_i^a$  and  $M$  are the  $i$ th natural mode and the mass matrix of the anisotropic specimen, respectively, and  $u_j^r$  is the  $j$ th reference mode. The values of  $A_{ij}$  vary in the range [0, 1]. Figure 2, for instance, shows the coupling degree of a natural mode of an anisotropic specimen with

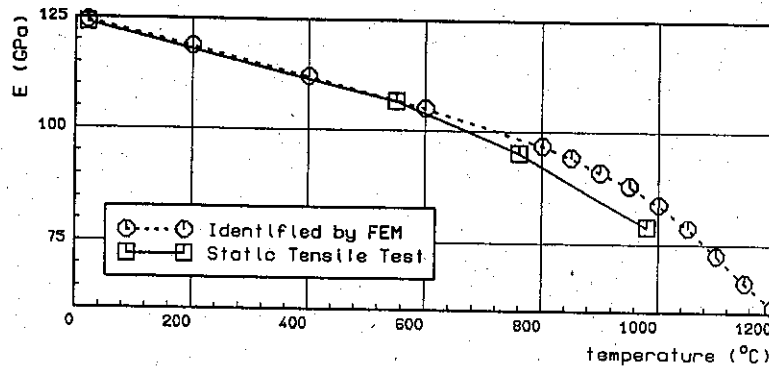


Figure 7 Determined constants of the single crystal SRR99.

one can see that there is a linear relationship between the frequencies and the constants  $c_i$ , if the influence of the constants on the natural modes is neglected. In terms of this linear relationship, one can conclude that the errors of the solution will also be statistically independent random variables of a Gaussian distribution  $N(0, \sigma_{c_i})$ , for which the standard deviations  $\sigma_{c_i}$  are calculated by

$$\sigma_{c_i}^2 = \left( \sum_{j=1}^q H_{ij}^2 f_j^2 \right) (\sigma_e^2 + \sigma_f^2), \quad (11)$$

where  $i = 1, 2, \dots, P$ , and  $H_{ij}$  form a coefficient matrix calculated by the FE model.

As a practical application, we consider the results for the single crystal of the f.c.c. nickel base superalloy SRR99, which has three independent elastic constants. The measured frequencies of three cylindrical specimens were used in the procedure. The constants up to 1200°C were determined by using three transversal pairs, two torsional and one longitudinal measured frequencies. At four temperatures, the constants of the three specimens were measured by static tensile test and averaged. The static measurements were carried out at BAM by K. Naseband. Table 1 presents the constants identified at 20°C and 600°C.

The results of  $E$  in the whole investigated temperature range are shown in Figure 7. Table 2 represents the measured and calculated natural frequencies of one specimen at room temperature. In Table 2 the three higher transversal and two torsional measured frequencies were not used in the optimization procedure, but the values of the corresponding frequencies predicted with the identified constants were also compatible with them. Among the fourteen frequencies listed in Table 2, the deviation of the first longitudinal natural frequency is 3.7 times higher than the maximum for the others. This means that, if all the other measured frequencies are of equal precision, the measured value of the longitudinal frequency is particularly strongly distorted by experimental error.

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 degree of freedom of the model. In our case, the number of the frequencies of a specimen used in the procedure is not more than 10, and the degree 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 very small influence on the measuring precision of the frequencies. Damping

Table 2 Comparison of the measured and calculated natural frequencies.

Mode type	Measured [kHz]	Calculated [kHz]	Deviation in %
transversal	5.822	5.782	0.68
transversal	5.839	5.802	0.62
transversal	15.34	15.24	0.59
transversal	15.54	15.44	0.60
transversal	28.38	28.22	0.48
transversal	29.17	29.01	0.54
transversal	43.36	43.35	0.01
transversal	60.51	60.50	0.03
transversal	63.48	63.41	0.12
torsional	22.26	22.35	0.39
torsional	46.47	46.44	0.07
torsional	67.97	68.25	0.40
torsional	90.35	90.91	0.62
longitudinal	33.79	32.94	2.50

effects can be neglected because of the very little strains of the specimen. For these reasons the resonance measurements can be regarded as free from distortion. In such a 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 Table 2 allows the conclusion that the identified constants can be regarded as a good approximation for the exact ones. The successful identification of the constants by our optimization procedure are attributed to the suitable optimizer, the very good approximation of the natural frequencies by FEM and the reliable assignment scheme in every iteration. The practical application demonstrates the efficiency and economy of the procedure.

## 5 CONCLUSION

The presented method enables us to identify the elastic constants of single crystals and the orientation of a specimen. In principle, there are no limitations to the crystal symmetry, 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 cubic symmetry, a reliable convergence of the identification procedure was ensured by the use of three measured transversal pairs and two measured torsional natural frequencies. The longitudinal natural frequencies are not necessary. The convergence is in general strongly influenced by the initial values. A theoretical proof of the uniqueness of the solution and a reliable error estimation are subjects of the further research.

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## APPENDIX A

$$E = (C_{11} + 2C_{12})(C_{11} - C_{12}) / (C_{11} + C_{12}),$$

$$G = C_{44}/2, \nu = C_{12} / (C_{11} + C_{12}), K = E / [3(1 - 2\nu)]$$

## APPENDIX B

- 1 Data of the cylindrical specimen for Figure 2  
 $L = 49.5 \text{ mm}, D = 5.0 \text{ mm}, \rho = 8.7 \text{ g/cm}^3,$   
 $E = 122.0 \text{ GPa}, G_0 = 131.0 \text{ GPa}, \nu = 0.365,$   
 $\varphi_1 = 25.0^\circ, \varphi_2 = 32.0^\circ$
- 2 Data of the cylindrical specimen for Figure 3  
 $L = 20.0 \text{ mm}, D = 2.0 \text{ mm}, \rho = 8.0 \text{ g/cm}^3,$   
 $E = 125.0 \text{ GPa}, \nu = 0.3$
- 3 Data of the cylindrical specimen for Figures 4 and 5  
 $L = 50.0 \text{ mm}, D = 7.0 \text{ mm}, \rho = 7.8 \text{ g/cm}^3,$   
 $E_0 = 125.0 \text{ GPa}, G_0 = 120.0 \text{ GPa}, K_0 = 208.0 \text{ GPa},$   
 $\text{tr.}[001] = 9878.0 \text{ Hz}, \text{to.}[001] = 39231.0 \text{ Hz},$   
 $\text{lo.}[001] = 39963.0 \text{ Hz}$
- 4 Data of the cylindrical specimen for Figure 6  
 $L = 50.0 \text{ mm}, D = 5.0 \text{ mm}, \rho = 7.8 \text{ g/cm}^3,$   
 $E_0 = 125.0 \text{ GPa}, G_0 = 120.0 \text{ GPa}, \nu = 0.4,$   
 $\varphi_{20} = 35.0^\circ$
- 5 Orientations of the three cylindrical specimens for Figure 7  

1:	$\varphi_1 = 39.3^\circ,$	$\varphi_2 = 50.0^\circ$
2:	$\varphi_1 = 5.5^\circ,$	$\varphi_2 = 39.5^\circ$
3:	$\varphi_1 = 24.8^\circ,$	$\varphi_2 = 28.5^\circ$



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