ISODEC: software for calculating diffraction elastic constants

Thomas Gnäupel-Herold

Materials Science and Engineering, University of Maryland, Building 090, Room 2135, College Park, MD 20742, USA, and Center for Neutron Research, NIST, 100 Bureau Drive, Stop 6102, Gaithersburg, MD 20899-6102, USA. Correspondence e-mail: tg-h@nist.gov

A program is introduced that calculates diffraction elastic constants for the Reuss, modified Voigt, Hill, Kröner and inverse Kröner models. For materials with preferred orientation it uses the orientation distribution function (ODF) to calculate the anisotropic stress factors. The ODF is read in text format as output from the freely available texture programs *popLA* and *MTEX*. The software also calculates the orientation-dependent mixing ratios of intensities of overlapped reflections, anisotropic bulk constants, and stress from lattice strain and *vice versa*.

1. Introduction

Diffraction elastic constants (DECs) are necessary to convert orientation- and (*hkl*)-dependent lattice strains into macroscopic stress. The proliferation of diffractometer hardware capable of measuring *d* spacings for different specimen orientations has led to a widespread use of diffraction-based stress measurements. For textured materials this widening of the field has not been accompanied by equal advances in the interpretation of the measured lattice strains, particularly with respect to the DECs used in the conversion of lattice strain to stress. A survey of the literature shows that preferred orientation is often disregarded, which fact is due in no small part to the considerable requirements for appropriately addressing the effects of preferred orientation: (i) pole figures have to be measured; (ii) the crystallite orientation distribution function (ODF) has to be determined from these pole figures; and (iii) the DECs have to be calculated using the ODF. If the diffractometer hardware allows it, then pole figures can be measured easily. The calculation of the ODF can be done with the freely available software packages *popLA* (Kallend *et al.*, 1991) and *MTEX* (Hielscher & Schaeben, 2008). The *ISODEC* software introduced here is intended to address the calculation of directionally dependent DECs using the ODF as generated by *popLA* or *MTEX*.

2. Program code

The program consists of a single executable file that was compiled from more than 15 000 lines of code using *Turbo Delphi* for Windows operating systems. The use of other operating systems is possible through Windows emulators, among which *Wine* (x86 Linux) and *Darwine* (MacOS X) have been tested successfully. The program was written by and is maintained by the author. The downloadable package (http://www.ncnr.nist.gov/programs/crystallography/software/isodec/IsoDEC.zip) contains a help file, a database of single-crystal elastic constants, and several ODFs in text format that are readable by *ISODEC* for use in further calculations of DECs, pole figures, anisotropic bulk constants and ODF intensities for given specimen directions. Also included are several worksheet example files that contain sample orientations, measured *d* spacings, and the stress factors calculated from the *d* spacings and the known applied stresses.

The details of the stress factor measurements are described by Gnäupel-Herold *et al.* (2012).

3. Functions and features

The main function of *ISODEC* is the calculation of anisotropic stress factors or DECs for materials with preferred orientation. Other features that are by-products of the main functionality are the calculation of the following: isotropic DECs, pole figures, anisotropic bulk constants from the ODF and ODF intensities for given specimen directions. These last are useful for completely overlapped reflections of two or more (*hkl*), where the relative intensity fractions of the individual (*hkl*) vary with the specimen direction owing to preferred orientation. Other useful functions are the calculation of macroscopic stress from *d* spacings (lattice strain) as measured by diffraction and *vice versa*. These calculations are done in a spreadsheet within *ISODEC* that can import and save formatted data (examples are included). The worksheet also has basic copy and paste functionality to allow interchange of data from and to common spreadsheet software (*e.g. EXCEL*). Very large data sets can be treated this way.

There are several models implemented for DEC calculations: the Reuss model (Reuss, 1929; Möller & Martin, 1939), the Hill model (Hill, 1952; Reuss, 1929; Voigt, 1928), the modified Voigt model, the Kröner model (Kröner, 1958; Bollenrath *et al.*, 1967; Behnken & Hauk, 1986) and the inverse Kröner model (Kröner, 1958; Gnäupel-Herold *et al.*, 2012). This list includes only those models that are sufficiently general, *i.e.* models that at least include all crystal symmetries, all specimen symmetries and possible stress states. All models have to lend themselves to the effects of preferred orientation, which is included in the calculations by reading the ODF in text format. If not present in the full interval for the three Euler angles at input, then the ODF is internally expanded to $[0 \dots 2\pi; \; 0 \dots \pi; \; 0 \dots 2\pi]$ in Bunge (1982) angles and made quasi-continuous from the discrete table format of the input by means of trilinear interpolation. This allows the calculation of pole figures and, as required by DEC calculations, the calculation of Euler angles and ODF intensities for arbitrary orientation fibres through Euler space.

The aforementioned models can also be used in the calculation of bulk elastic constants with or without using the ODF. Additional

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microstructure information can be included in the Kröner-type models through grain-axis parameters which assume ellipsoidal grain shape and the alignment of the ellipsoid axes with the principal specimen axes.

4. Availability

The program home page and download link can be found at http://www.ncnr.nist.gov/programs/crystallography/software/isodec/. The download is a single compressed archive that contains the executable, the documentation, a database of elastic constants and a number of ODF files that can be read into *ISODEC* for further calculations. Also included are several data sets with measured *d* spacings/stress factors, together with pole figures and ODFs, to allow an all-round comparison between measured and calculated (using *ISODEC*) stress factors.

5. Disclaimer

Certain commercial firms and trade names are identified in this report in order to specify aspects of the experimental procedure adequately. Such identification is not intended to imply recommendation or endorsement by the National Institute of Standards and Technology, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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