A software for diffraction stress factor calculations for textured materials

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(Received 8 February 2012; accepted 29 February 2012)

A software for the calculation of diffraction elastic constants (DEC) for materials both with and without preferred orientation was developed. All grain-interaction models that can use the crystallite orientation distribution function (ODF) are incorporated, including Kröner, Hill, inverse Kröner, and Reuss. The functions of the software include: reading the ODF in common textual formats, pole figure calculation, calculation of DEC for different (hkl,φ,ψ), calculation of anisotropic bulk constants from the ODF, calculation of macro-stress from lattice strain and vice versa, as well as mixture ratios of (hkl) of overlapped reflections in textured materials. © *International Centre for Diffraction Data*
[doi:10.1017/S0885715612000267]

Key words: diffraction, elastic constants, texture, strain, stress

I. INTRODUCTION

Diffraction-based stress analysis depends critically on the use of the correct diffraction elastic constants (DEC). A survey through the literature makes it abundantly clear that in the vast majority of cases in which lattice strain needed conversion to stress-preferred grain orientation (texture) is – justifiably or not – disregarded, and isotropic diffraction elastic constants were used. The main reasons for this apparent oversimplification are the added need to quantify the degree of preferred grain orientation through pole figure measurements, and the use of pole figures to determine the orientation distribution function (ODF). Even with the ODF, further calculations are hampered by the lack of freely available software tools to perform calculations of anisotropic diffraction elastic constants. The IsoDEC (Gnäupel-Herold, 2011) software program introduced here was developed to address this need.

II. FEATURES AND FUNCTIONALITY

The main purpose of IsoDEC is the calculation of the orientation and (hkl) dependent stress factors using the ODF (in the textual form as provided by the output of freely available texture packages), the single crystal elastic constants and the bulk elastic constants as input. The latter can be calculated from the ODF. The software can also be used to calculate stress from measured lattice strains using the thus determined stress factors or, in reverse, calculate lattice strains from a given stress tensor. Some of the implemented models for DEC calculations also allow including the grain shape, expressed as a general ellipsoid, into the calculation of the DEC.

Evidently the ODF is crucial. It needs to be supplied in textual form, i.e., using the output from popLA (Kallend *et al.*, 1991) or MTEX (Hielscher and Schaeben, 2008). The ODF is expected in a $5° \times 5° \times 5°$ equidistant spacing for the three Euler angles $\varphi_1 \Phi \varphi_2$ (Bunge notation). This tabular form is internally expanded to the full interval [$0 \ldots 2\pi$; $0 \ldots \pi$; $0 \ldots 2\pi$] and made quasi-continuous by means of trilinear interpolation. This allows the computation of pole figures (in popLA format) and orientation fibers (i.e., ODF values for a series of Euler angle combinations) through Euler space. Orientation fibers are a key element of DEC calculations that use the ODF. The models for DEC calculations are the Kröner model (Kröner, 1958; Bollenrath *et al.*, 1967; Behnken and Hauk, 1986), the Reuss model (Reuss, 1929; Möller & Martin, 1939), the Hill model (Voigt, 1928; Reuss, 1929; Hill, 1952), the inverse Kröner model (Kröner, 1958; Gnäupel-Herold, 2012), and the modified Voigt model (Murray and Noyan, 1999). The two Kröner-type models allow the user to devise complex elastic interactions: first, one can approximate multi-phase composites (e.g. elastically hard particles in a soft matrix such as SiC in Al) by using appropriate set of single crystal constants and bulk constants. Second, the effects of elongated or otherwise non-spherical grains can be included by changing the grain-shape parameters in IsoDEC.

Input and output in IsoDEC can be done through the spreadsheet that allows the import and export of text files with its content as well as basic copy and paste exchanges with common spreadsheet programs such as EXCEL. Large datasets consisting of d-spacings, their uncertainties, unstressed d-spacings with uncertainties, and measurement directions ($\varphi\psi$) can be treated this way. Stress tensor components and the unstressed d-spacing can be fixed or free parameters in the stress fit, depending on boundary/equilibrium conditions.

III. OPERABILITY

IsoDEC offers two visual interfaces: one for isotropic calculations and one for calculations that include preferred orientation. The interface for isotropic calculations is shown in Figure 1. The fewest possible steps for calculating the isotropic constants $s_1(hkl)$ and $\frac{1}{2}s_2(hkl)$ are loading a set of material constants from the drop-down list, entering the indices h, k, and l, and starting the calculation. Elastic constants that are not found in the database included can be entered manually, but must include the lattice parameters and, after entering the single crystal elastic constants, a calculation of the isotropic bulk constants (upper left).

For anisotropic calculations, the amount of information that has to be provided increases as shown in Figure 2.

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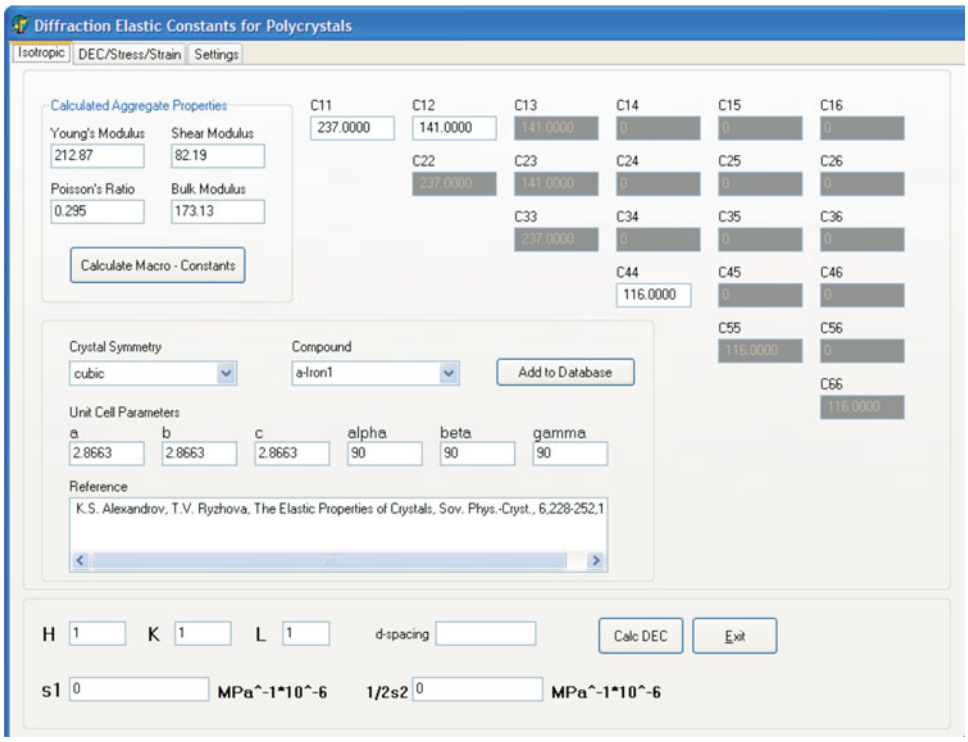

Figure 1. Screenshot of IsoDEC for isotropic calculations.

Generally the ODF has to be provided either in popLA format or in MTEX format ("Load ODF"). There is also the possibility of not using an ODF, and entering user values for the bulk constants, e.g. using a rotated single crystal constants tensor to simulate the effects of individual texture components on the stress factors. Of course, the anisotropic bulk constants can be calculated from the ODF, the average grain shape (as ellipsoid axis ratios) can be entered, and the model (Hill, Reuss, Kröner, inverse Kröner and Voigt/modified Voigt) can be chosen. The stress factors are calculated for the fields in which h, k, l, phi and psi are given. This step has to precede any stress or strain calculations that require the stress factors. A stress calculation needs the additional input of d-spacings, the d-uncertainties, the reference or unstressed d-spacing and their uncertainties, and a sorting qualifier (column 1 in the worksheet) that allows to group those data together that are to be used for the calculation of the same stress tensor (i.e., same location on the sample or similar). The reverse calculation d-spacing/strain from stress naturally requires stress values entered in their appropriate columns. The output of this calculation is in the column "d_calc", which means that if strain is desired one has to perform the explicit calculation $(d - d_0)/d_0$ oneself.

IV. PLATFORM AND AVAILABILITY

IsoDEC was written in Turbo Delphi for the Windows operating system. It can also be used under MacOS X+ and x86 linux if Windows emulator software is present. Both Darwine (MacOS X and Wine) have been tested successfully.

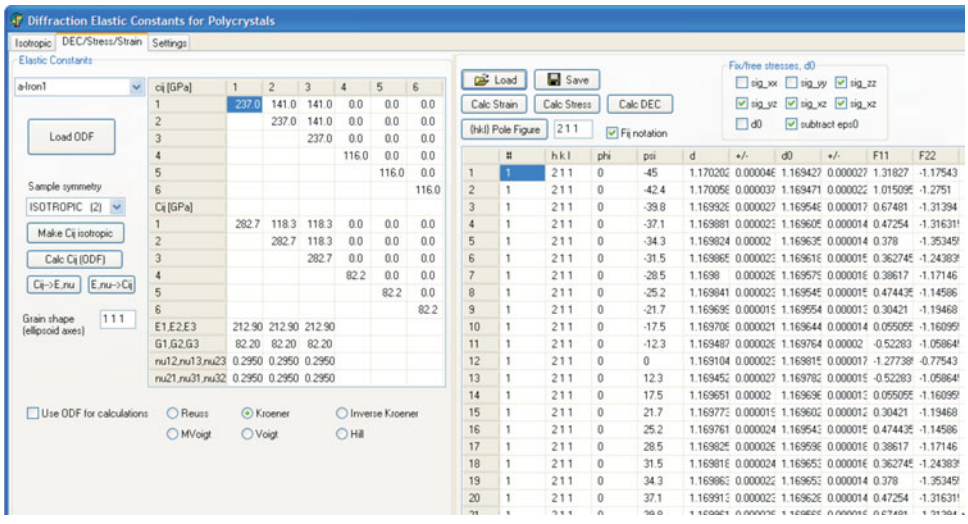

Figure 2. Interface for anisotropic calculations.

The installation package contains a help file, a database of single crystal elastic constants and several ODFs in textual form that are readable by IsoDEC for use in further calculations of DEC, pole figures, anisotropic bulk constants, and ODF intensities for given specimen directions. The program home page and the download link can be found at http://www.ncnr.nist.gov/programs/crystallography/software/isodec/.

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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