

IsoDEC – A program for calculating diffraction elastic constants

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web address: <http://www.ncnr.nist.gov/programs/crystallography/software/downloads.html>

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1 Introduction

IsoDEC calculates diffraction elastic constants (DEC) for isotropic aggregates and for aggregates with preferred orientation. The functionality for materials or aggregates with preferred orientation requires the availability of the crystallite orientation distribution function (ODF) which must be supplied by the user, typically as output from popla [1] or MTEX [2]. MTEX is now the recommended ODF inversion software because of superior graphics of active maintenance. Byproducts of IsoDEC's functionality are several other useful features such as using the ODF to calculate anisotropic bulk elastic constants, pole figures (in popla format) and ODF intensities. The latter is useful in calculating mixture ratios of overlapped reflections of different (hkl). Another useful feature is the calculator function which allows to calculate macroscopic stress from lattice strain even for different (hkl) and vice versa (lattice strain from stress). IsoDEC can run on Linux machines using Wine.

2 Isotropic calculations


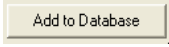
The start page is the “Isotropic” tab which allows the calculation of isotropic constants s_1 and $\frac{1}{2}s_2$. They are used in the equation

$$\varepsilon_{\varphi\psi} = \frac{1}{2}s_2(hkl) \left[\begin{array}{l} (\sigma_{11}\cos^2\varphi + \sigma_{22}\sin^2\varphi + \sigma_{12}\sin 2\varphi)\sin^2\psi + \\ (\sigma_{13}\cos\varphi + \sigma_{23}\sin\varphi)\sin 2\psi + \sigma_{33}\cos^2\psi \end{array} \right] + s_1(hkl)(\sigma_{11} + \sigma_{22} + \sigma_{33}) \quad (1)$$

Under “Compound” one can select a material from a database (pfcryst.dat) included in IsoDEC.zip. This loads the single crystal elastic constants, crystal symmetry, lattice parameters (important for non-cubic materials) and the (isotropic) bulk elastic constants E, nu, K, G, only two of which are independent. Then fill in values for H, K, L and click “Calc DEC” and you are done. The calculation is based on the Kröner model [3,7,10].

3 Entering a new material

If the elastic constants C_{ij} are not in the database then new values can be entered and stored in pfcryst.dat (pfcryst.dat is a textfile and can be edited). This is done using these steps:

- Enter a name in the “Compound” field
- Chose the crystal symmetry from the drop box.
- Enter the single crystal elastic constants
- On the top left corner, click 
- Enter the unit cell parameters. Particularly calculations for non-orthogonal unit cells rely on correct unit cell parameters!
- Optional: Enter a literature reference.
- Click 

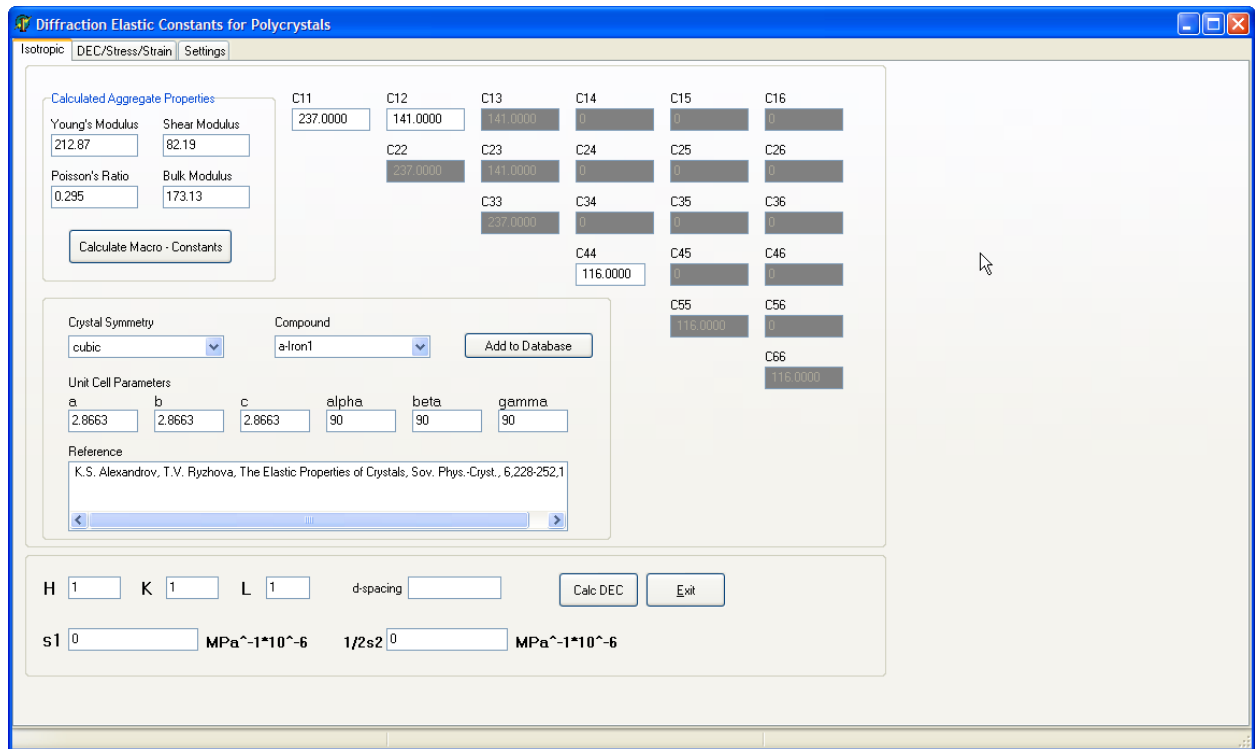
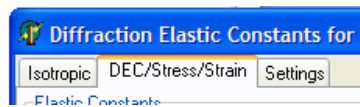


Figure 1: Screenshot of IsoDEC after startup.

3.1 Calculations in the isotropic case

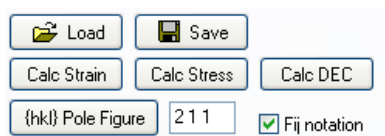
If texture is not an issue, and the more familiar notation of $S_1(hkl)$ and $\frac{1}{2}S_2(hkl)$ is preferred,

then one can, in the tab 'DEC/Stress/Strain'



, switch to this notation

by unchecking 'Fij notation' here:



In the strictly isotropic case (NO ODF or ☐ Use ODF for calculations deactivated, spherical grains for Kröner models), switching between the two has no bearing on the result (stress calculated). However, a switch to a different notation requires that the DEC are re-calculated.

4 Calculation of stress factors F_{ij} for materials with preferred orientation

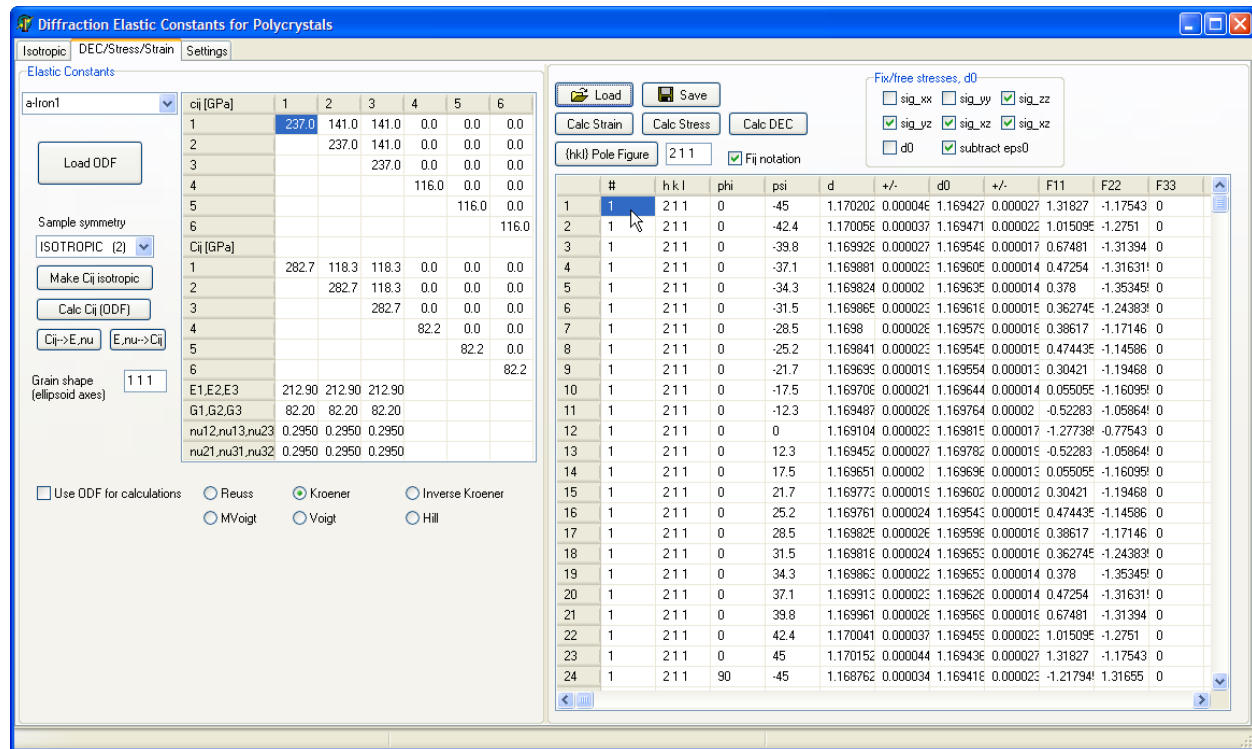


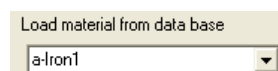
Figure 3. Calculating the anisotropic stress factors.

In materials with preferred orientation equation (1) can no longer be used because s_1 and $\frac{1}{2}s_2$ become dependent on ϕ and ψ . The relationship between lattice strain and macro-stress is now

$$\varepsilon(\varphi, \psi, hkl) = \frac{\partial \varepsilon(\varphi, \psi, hkl)}{\partial \bar{\sigma}_{ij}} \bar{\sigma}_{ij} = F_{ij}(\varphi, \psi, hkl) \bar{\sigma}_{ij} \quad (2)$$

The calculation of the F_{ij} is done in the following steps:

4.1 Load a set of materials constants



If this was done on the “Isotropic” page (see chapter 2) then proceed to

4.2 Load the orientation distribution function

Before loading the ODF make sure that the correct material and crystal symmetry has been selected. Then load the ODF (5x5x5 deg. mesh) by clicking

Load ODF

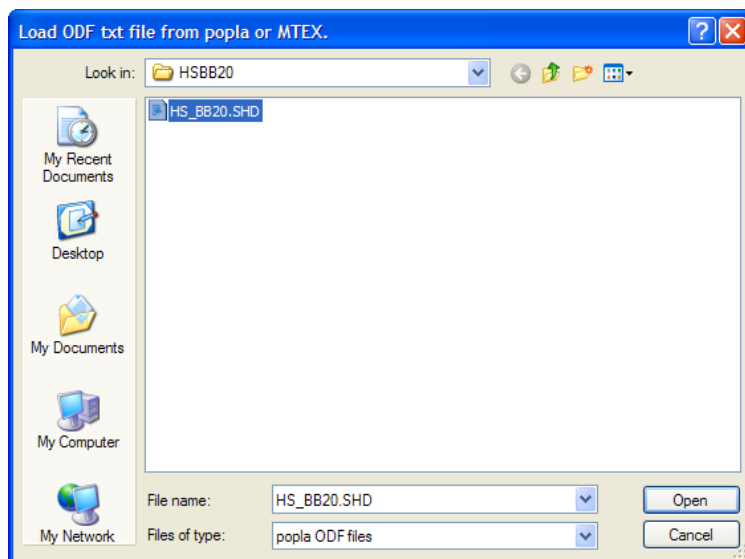
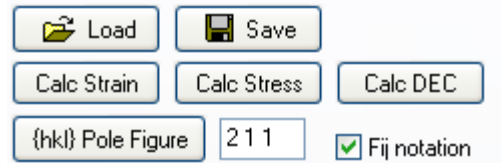


Figure 4. Choosing the correct file type for the ODF.

There are several examples of acceptable ODFs included, all of them generated by MTEX. PopLA files can be read but due to difficulties running popla (a DOS program) on my PC I no longer maintain active support. If you are not adept in using popla [1] or MTEX [2] then try to generate the ODF in a 4-column format (ϕ_1, Φ_1, ϕ_2 , ODF-value) with 5x5 deg. mesh for the interval $[0..2\pi; 0..\pi; 0..2\pi]$. This can then be easily modified to the format of MTEX output files (included). In the current version, two kinds of input are accepted:

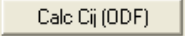
- a) Popla output files (*.SHD, *.SOD) in a 5x5x5 degree mesh, Bunge angles.
- b) MTEX output (typically with extension *.txt or *.MTX, also in a 5x5x5 mesh).

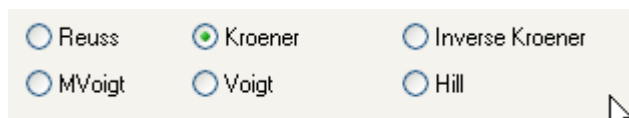
The symmetry of the ODF is important. The ODF is internally expanded to the full interval $[0..2\pi; 0..\pi; 0..2\pi]$, and for this to be done correctly the material/ crystal symmetry must be selected beforehand. Particularly MTEX has been known to change the ODF output format as new versions are released, and, if gone unnoticed, this can have consequences for the ODF expansion. In order to check that the ODF was read and expanded correctly it is advisable to



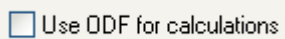
calculate a few pole figures with different combinations of (2 1 1) or (1 2 1). In the case of cubic, hexagonal or tetragonal crystal symmetry these pole figures should be identical with small variations possible due to the numerical integration involved.

4.3 Calculate the bulk constants

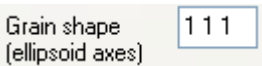
In many cases the degree of anisotropy in the bulk constants calculated using the ODF is quite small even for sharp textures. Nonetheless it should be done because it is simple enough by clicking . The grain interaction model used in this calculation is the one checked here:



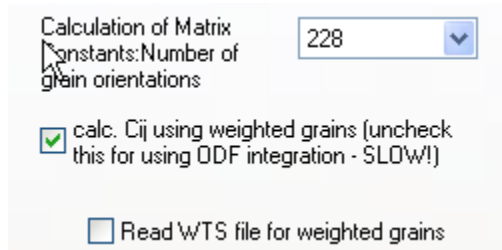
The models by Reuss, Voigt/MVoigt (in this context the same procedure is used) and Hill yield a weighted average with the weights calculated from the ODF. If no ODF was loaded, or the box



is unchecked then each orientation has the same weight, and the sample symmetry is isotropic. The same is true for the Kröner-type models except that a non-

spherical grain shape  will now produce orthorhombic sample symmetry even in the absence of preferred orientation. Also, the calculation is much more lengthy

because of operations on fourth-rank tensors performed for each grain orientation. The standard setting uses integration which has been much improved such that it can be used for subtler tests on grain shape effects. It is also possible to use a discrete set of random grain orientations generated from [12] for which the user can choose the number in the 'Settings' tab. More grains will approximate the polycrystal better but at the expense of a longer calculation:



For discrete grains, the equations used are

$$\text{Reuss:} \quad S_{ijkl}^{-1} = \left(\sum s_{ijkl}(g) f(g) / \sum f(g) \right)^{-1} \quad (3a)$$

$$\text{Voigt/mod. Voigt:} \quad C_{ijkl} = \sum c_{ijkl}(g) f(g) / \sum f(g) \quad (3b)$$

$$\text{Hill:} \quad C_{ijkl} = \frac{1}{2} (C_{ijkl}^{\text{Voigt}} + S_{ijkl}^{-1}) \quad (3c)$$

$$\text{Kröner:} \quad C_{ijkl} : \sum t(g) f(g) / \sum f(g) \rightarrow 0 \quad (3d)$$

$$\text{inverse Kröner:} \quad C_{ijkl} : \sum r(g) f(g) / \sum f(g) \rightarrow 0 \quad (3e)$$

$$r_{ijkl}(g) = c_{ijkl}(g) - C_{ijkl} + c_{ijmn}(g) u_{mnkl}(g) \quad (4a)$$

$$t_{ijkl}(g) = u_{ijmn}(g) S_{mnkl} \quad (4b)$$

$$u_{ijkl}(g) = -v_{ijmn}^{-1}(g) [c_{mnkl}(g) - C_{mnkl}] \quad (4c)$$

$$v_{ijkl}(g) = c_{ijkl}(g) - C_{ijkl} + C_{ijmn} w_{mnkl} \quad (4d)$$

The orientation g , in Bunge angles, is the rotation from the specimen reference frame to the crystal reference frame. The tensors given above are typically transformed in the inverse sense from the crystal frame to the specimen frame. For the integrations, the summations in (3a)-(3e) are replaced by the integral over the Euler angles (shown only for Voigt):

$$C_{ijkl}^V = \frac{\int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} c_{ijkl}(g^L) f(g^L) \sin \Phi d\varphi_1 d\Phi d\varphi_2}{\int_0^{2\pi} \int_0^{2\pi} \int_0^{2\pi} f(g^L) \sin \Phi d\varphi_1 d\Phi d\varphi_2} \quad (5)$$

Unchecking the first box means that the summation/average is replaced by a numerical integration in Euler space with the number of integration intervals given below

of integration intervals

20

.. This is usually very slow but may work better for very sharp textures.

In some case one has measured bulk constants such as (Young's modulus) $E \parallel \text{RD} = E1$, $E \parallel \text{TD} = E2$

E1,E2,E3	214.71	211.54	214.04
G1,G2,G3	81.10	79.70	81.50
nu12,nu13,nu23	0.2991	0.2872	0.2978
nu21,nu31,nu32	0.2946	0.2863	0.3013

and so on. In this case they can be entered here

E,nu,G → Cij

components of the bulk tensor C_{ij} by clicking . If one plays around with this and ends up with unreasonable values it is always possible to “go back” to the isotropic bulk tensor

by clicking . Note that the anisotropic Poisson's ratios are defined as follows

Make Cij isotropic

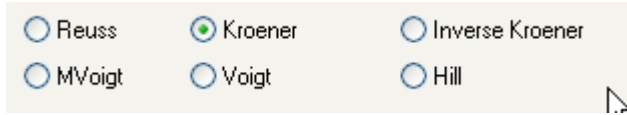
$$\text{uniaxial stress } \sigma_{11}: \quad \nu_{12} = -\epsilon_{22}/\epsilon_{11} \quad \nu_{13} = -\epsilon_{33}/\epsilon_{11}$$

$$\text{uniaxial stress } \sigma_{22}: \quad \nu_{21} = -\epsilon_{11}/\epsilon_{22} \quad \nu_{23} = -\epsilon_{33}/\epsilon_{22}$$

$$\text{uniaxial stress } \sigma_{33}: \quad \nu_{31} = -\epsilon_{11}/\epsilon_{33} \quad \nu_{32} = -\epsilon_{22}/\epsilon_{33}$$

The shear moduli are defined as $G_1 = C_{44}$; $G_{12} = C_{55}$; $G_3 = C_{66}$;

4.3.1 Select grain interaction model



These models lend themselves to use with preferred orientation. The models due to Reuss [4,9], modified Voigt [11], Hill [5,8,9] (Hill denotes the Reuss/Voigt average), Kröner [3,7,10] and the inverse Kröner [6] produce distinctive results due to the different assumptions of grain-interaction (or lack thereof as in the case of Hill and Reuss). Very simplified they can be written as follows:

$$\text{Reuss:} \quad F_{kl}(\varphi, \psi, hkl) = \overline{m_i m_j s_{ijkl}(g)} \quad (6)$$

$$\text{mod. Voigt:} \quad F_{kl} = m_i m_j \left[\int_0^{2\pi} c(g^L) f(g^L) d\lambda \bigg/ \int_0^{2\pi} f(g^L) d\lambda \right]_{ijkl}^{-1} \quad (7)$$

$$\text{Hill:} \quad F_{kl}(\varphi, \psi, hkl) = \frac{1}{2} m_i m_j \left(\overline{s_{ijkl}(g)} + \langle c_{ijkl}(g) \rangle \right) \quad (8)$$

$$\text{Kröner:} \quad F_{kl}(\varphi, \psi, hkl) = \overline{m_i m_j q_{ijkl}(g)} \quad (9)$$

$$\text{inv. Kröner:} \quad F_{kl}(\varphi, \psi, hkl) = \overline{m_i m_j p_{ijkl}^{-1}(g)} \quad (10)$$

with $\mathbf{m} = (\cos \varphi \sin \psi \quad \sin \varphi \sin \psi \quad \cos \psi)$ and

$$\begin{aligned} p_{ijkl}(g) &= C_{ijkl} + r_{ijkl}(g) \\ q_{ij}(g) &= S_{ijkl} + t_{ijkl}(g) \end{aligned} \quad (11)$$

with r and t defined in equations (4a)-(4d). C, S are the bulk stiffnesses and compliances, $s(g)$ and $c(g)$ single crystal constants for the orientation g (g itself is given by (hkl) and φ, ψ), w^{-1} is the Eshelby-tensor. The overbar signifies a partial orientation average over the orientations

fiber $g(\mathbf{m} | \mathbf{h})$ with \mathbf{h} as the direction perpendicular to the lattice plane (hkl). The angular brackets denote the complete orientation average over all orientations not weighed by the ODF, thus making $\langle c_{ijkl}(g) \rangle$ isotropic. Note that notation such as v_{ijmm}^{-1} always refers to a component of the inverse fourth rank tensor v^{-1} .

The Voigt-model is included for completeness even though it is generally discarded because it is hkl- and texture independent.

4.3.2 Select grain shape parameters

Only the Kröner and inverse Kröner models are sensitive to grain matrix interaction, i.e. the elastic effects of non-spherical grains, elastically hard grains in a soft matrix (e.g. SiC in Al) or soft precipitates in a hard matrix. Only for these models does it make sense to enter grain

Grain shape
(ellipsoid axes)

1 1 1

shape parameters here: $[1\ 1\ 1]$ represents a spherical grain, $[1\ 1\ 100]$ would be a needle-like grain aligned with the ellipsoid axes in the ND direction, and $[4\ 2\ 1]$ would be an ellipsoidal grain as a result of rolling/stretching in the RD direction. The stress factors are sensitive to the grain shape and sensible values should be used.

5 Entering Data

Data can be cut (CTRL-x) or copied (CTRL-c) from the worksheet or pasted (CTRL-v) into it from EXCEL or other compatible spreadsheet software. Copy/paste from text files is also possible as long as columns are tab separated. Both the mouse and arrow keys while holding down the SHIFT key should work. One can also fill in values by selecting a range

	#	h k l	phi
1		= 1 1 1	
2			
3			
4			
5			

then typing =1 1 1 and press CTRL+Enter.

What data are needed depends on the task to be done.

5.1 Data needed for Stress Factor Calculation

	#	h k l	phi	psi	d	+/-
1		2 1 1	0	-45		
2		2 1 1	0	-42.4		
3		2 1 1	0	-39.8		
4		2 1 1	0	-37.1		
5		1 1 1	0	-34.3		
6		2 1 1	0	-31.5		
7		2 1 1	0	-28.5		
8		2 1 1	0	-25.2		

As shown here and in equation (2) only (h k l), ϕ , ψ are needed to calculate F_{11} , F_{11} , F_{22} , F_{33} , F_{12} , F_{13} , F_{23} . Also calculated in I(ODF) in the column 'I(ODF)'. The units for the F_{ij} are TPa^{-1}

5.1.1 What is I(ODF)?

If no ODF is loaded then $I(\text{ODF})=1$. If an ODF is loaded then $I(\text{ODF})$ is calculated from

$$I(\phi, \psi, hkl) = \int_0^{2\pi} f(g^L) d\lambda \quad (12)$$

If all grains were the same size then this number would be a measure for the number of grains having an orientation that, in the direction ϕ, ψ would contribute to the reflection (hkl). It therefore reflects the intensity variations over ϕ, ψ caused by texture. $I(\text{ODF})$ does not contain the multiplicity of (hkl)! As an example one can look at the (511)/(333) reflection in cubic face centered materials. Both have the same d-spacing and therefore the same 2θ but (511) has a multiplicity of 24 and (333) has a multiplicity of 8. In the presence of preferred orientation the mixture ratio – and therefore the effective stress factors – can vary quite a bit as shown in this example for a copper sample with a near ideal cube texture

h k l	phi	psi	F11	F22	F33	F23	F13	F12	I(ODF)
5 1 1	0	0	-3.361959	-3.376962	9.150393	0.000000	0.000000	-0.043435	108.81
1 1 1	0	0	-1.941333	-1.941333	6.294138	0.000000	0.000000	0.000000	56.27
5 1 1	45	54	0.935034	0.593829	0.882609	4.065604	4.278595	4.176677	177.11
1 1 1	45	54	0.753760	0.753760	0.903952	2.769171	2.769171	2.695093	873.13

As shown in this table the ratios of $I(\text{ODF})$ values for the two overlapped reflections can vary widely from about 2:1 at (0,0) to 1:5 at (45,54).

$$F_{ij}^{\text{eff}}(\phi = 0, \psi = 0) = \frac{F_{ij}(0,0,(511)) * 24 * I(0,0,(511)) + F_{ij}(0,0,(333)) * 8 * I(0,0,(333))}{24 * I(0,0,(511)) + 8 * I(0,0,(333))}$$

If stress or strain are to be calculated, and the user wants to make this correction, then the calculation of effective F_{ij} have to be done by the user, and the newly calculated effective F_{ij} copied into the appropriate fields.

5.2 Data needed for Stress Calculations

A stress calculation needs strains and stress factors (elastic constants). The strains are supplied in the form of d-spacings with uncertainties and unstressed d-spacings d_0 with their uncertainties as shown below. Results are given in MPa (stress).

	#	h k l	phi	psi	d	+/-	d0	+/-	F11	F22
1	1	2 1 1	0	0	1.169158	0.000022	1.169815	0.000017	-1.261550	-1.26
2	1	2 1 1	0	90	1.170223	0.000041	1.169427	0.000027	4.449450	-1.26
3	1	2 1 1	90	90	1.168847	0.000033	1.169418	0.000023	-1.261550	4.449450
4	2	2 1 1	0	0	1.169342	0.000021	1.169815	0.000017	-1.261550	-1.26
5	2	2 1 1	0	90	1.170075	0.000037	1.169427	0.000027	4.449450	-1.26
6	2	2 1 1	90	90	1.16904	0.000031	1.169418	0.000023	-1.261550	4.449450
7	3	2 1 1	0	0	1.16949	0.000021	1.169815	0.000017	-1.261550	-1.26
8	3	2 1 1	0	90	1.169889	0.000037	1.169427	0.000027	4.449450	-1.26
9	3	2 1 1	90	90	1.169179	0.000032	1.169418	0.000023	-1.261550	4.449450

The worksheet format allows to process large amounts of data simultaneously by providing a qualifier for grouping them appropriately. This is done in column1 “#” by giving all data the same number that belong “together” (i.e. that belong to the same stress). In the above example, strains were measured in three specimen locations, with three specimen orientations each.

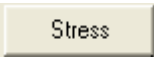
5.2.1 Fix/free parameters for stress fit

Fix/free stresses, d0
☐ sig_xx ☒ sig_zz ☒ sig_xz ☐ d0
☐ sig_yy ☒ sig_yz ☒ sig_xy ☐ subtract eps0

Checking a box means that this stress component or d_0 will be fixed parameters. In the previous example d-spacings/strains were measured in 3 directions , thus allowing to determine 3 stress tensor components, or 2 stresses and d_0 . Note that fixing a stress does not automatically mean the stress is fixed at zero! IsoDEC looks in the appropriate column for that stress and reads the value of that stress with a matching group qualifier (see columns 18+:

##	sig_xx	+/-	sig_yy	+/-	sig_zz	+/-	sig_yz	+/-	sig_xz	+/-	sig_xy
1	159.46	6.97	-46.58	5.94	0.00	0.00	0.00	0.00	0.00	0.00	0.00
2	109.75	6.37	-45.22	5.61	0.00	0.00	0.00	0.00	0.00	0.00	0.00
3	59.74	6.37	-46.57	5.73	0.00	0.00	0.00	0.00	0.00	0.00	0.00

With these values and now fixing Sig_yy and leaving both Sig_xx and d0 free then IsoDEC would fit (Sig_xx,d0) for group 1 (i.e. the first three values with sig_yy fixed to -46.58 MPa).

By clicking the stress button  the stress calculation is performed.

5.3 Strain/d-spacing Calculations

Much of chapter 5.2 applies here as well. Obviously stresses, elastic constants and values for phi and psi are needed here. One could do the steps described in chapter 5.2 and then simply fill in stress values for which strains are to be calculated:

##	sig_xx	+/-	sig_yy	+/-	sig_zz	+/-	sig_yz	+/-
1	500	0	0.00	0.00	0.00	0.00	0.00	0.00
2	350	0	0.00	0.00	0.00	0.00	0.00	0.00
3	100	0	0.00	0.00	0.00	0.00	0.00	0.00

The results are written in the column “d_calc”.

5.4 The eps0 correction

Fix/free stresses, d0

☐ sig_xx
 ☒ sig_zz
 ☒ sig_xz
 ☐ d0

☐ sig_yy
 ☒ sig_yz
 ☒ sig_xy
 ☐ subtract eps0

As suggested by “subtract eps0” this allows to provide a strain that is subtracted from measured d-spacings before a stress calculation. What is eps0? It could be intergranular strains or strains measured at zero stress or simply a correction curve reflecting instrumental effects or misalignments. The latter could be measured on a powder (no long range stress) or reference sample. However, if one uses d0-values that already contain intergranular strains then eps0 should not be based on the d0-values or otherwise the same effect will be subtracted twice!

6 Included Files

These files must be present in the same directory:

program executable:	Isodec.exe
help file	IsoDEC.pdf
elastic constants	pfcryst.dat
random grain orientations	random10416.wts, random1464.wts, random19860.wts, random228.wts, random33768.wts, random4572.wts, random64890.wts, random666.wts

ODFs, pole figures

The files under the ODF directory (ODFs: *.SHD, *.SOD, *.MTX) are intended for testing purposes. The ODFs can be read, and used for further calculations of bulk elastic constants, stress factors, ODF intensities, and pole figures. Files with the TSD extension contain measured d-spacings and stress factors and they can be imported directly into the worksheet and used for comparisons with known applied stresses.

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Publication Reference

Description of general capabilities:

T. Gnaupel-Herold, *IsoDEC: A software for calculating diffraction elastic constants*, J. Appl. Cryst. 45 (2012), 573-574

The Inverse Kröner model:

Gnäupel-Herold, T., Creuziger, A., Iadicola, M., A model for calculating diffraction elastic constants, (2012), J. Appl. Cryst. 45, 197-206

References

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