A Software Program for Calculating Diffraction Elastic Constants of Textured Materials

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Diffraction based stress analysis depends critically on the use of the correct diffraction elastic constants. 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, i.e. to determine the orientation distribution function (ODF), and the lack of any software tool to perform calculations of anisotropic diffraction elastic constants. The latter involves calculations of considerable complexity, especially when based on Kröner/Eshelby type grain-matrix interaction models. In order to address the need for such a tool a software was developed that, for any crystal and specimen symmetry, calculates the orientation and (hkl) dependent stress factors using the ODF, the single crystal elastic constants and the bulk elastic constants as input. 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. The bulk elastic constants can be calculated as well if the ODF was supplied. Evidently the ODF is crucial. It needs to be supplied in textual form, i.e. using the output from freely available tools such as popla and MTEX.