

CALCULATION OF X-RAY STRESS FACTORS ON THE BASIS OF SO(3) VECTOR PARAMETRIZATION

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In the presence of texture, the concept of X-ray Elastic Constants (XEC) is inapplicable and the X-ray Stress Factors (XSF) connecting average strain and stress have to be used [1]. The conventional XSF calculation procedure involves the transformations of the fourth- and the second- rank tensors comprising the rotations related to different coordinate systems. The resulting expressions are quite bulky and obscure for the analytical investigation. In our work, we derive the explicit formulas for XSF in a compact form by decomposing the fourth-rank tensor into irreducible SO(3) representations and using the Fedorov's vector parameterization for SO(3) group [2]. The expressing of the fourth-rank tensor in terms of SO(3) irreducible representations makes possible the following effective simplifications: (i) separation of the isotropic and anisotropic parts of the compliance tensor for an arbitrary crystal symmetry, (ii) use of a single matrix in the space of irreducible representations instead of multiplication of four transformation matrices for each fourth-rank tensor index. The Fedorov's vector parameterization for SO(3) provides a smart composition law for successive rotation transformations, which is obscure in the case of the traditional parameterization by Euler angles. The use of new approach delivers a transparent expression for XSF for arbitrary crystal symmetry and simplifies essentially the algorithm for the numerical calculations.

[1] M. Leoni, U. Welzel, P. Lamparter, E.J. Mittemeijer and J.-D. Kamminga, *Philos. Mag. A*, **81**, 597-623 (2001)

[2] F. I. Fedorov, *The Lorenz Group*, 2-nd ed, Moscow: URSS (in Russian), 2003.