Diffraction enhancement of symmetry and modular structures

A. Umayahara[1,2], B. Souvignier[1], M. Nespolo[2]

[1]*Radboud University, Faculty of Science, Mathematics and Computing Science, Institute for Mathematics, Astrophysics and Particle Physics. Postbus 9010, 6500 GL Nijmegen, The Netherlands.*
[2]*Université de Lorraine, CNRS, CRM2, Nancy, France*

akihiro.umayahara@univ-lorraine.fr

Diffraction enhancement of symmetry (DES) is a phenomenon by which the space-group symmetry suggested by the diffraction pattern of a crystal is higher than the space-group symmetry of the structure that has produced it [1-5]. The most well-known example is that of Friedel's law, which is however realized only when resonant scattering is not taken into account. In modular structures, DES does occur also when considering resonant scattering. We address this phenomenon in monoarchetypal modular structures [6]. The condition for DES to occur is that both the module and the vector set (set of all interatomic vectors) [7] are invariant under an isometry that is not a symmetry operation for the structure. Only τ-isometries [8], *i.e.* isometries that do not reverse the polarity of the stacking vectors, can lead to DES once resonant scattering is taken into account. The example of SiC polytypes, where the phenomenon has been confirmed experimentally, is studied in detail. The SiC layer has symmetry *p*6*mm* (diperiodic group); the stacking of SiC layer leads to many polytypes, rapidly increasing in number with the number of layers defining the period along to stacking direction. These polytypes can occur in four types of space group: $F43m$, $R3m$ $P6_3mc$ and $P31m$. If the vector set exhibits hexagonal symmetry, than the space group of the polytype can be either of type $P6_3mc$ or of type $P31m$. In both cases, the diffraction pattern shows hexagonal symmetry although in the latter case the structural symmetry is only trigonal: DES is thus observed. The number of polytypes showing DES increases rapidly with the number of layers, but the fraction of these polytypes with respect to the total number of polytypes decreases. These conclusions apply as well to all modular structures built by layers of the same symmetry, like ZnS.

[1] Iwasaki, H. (1972). On the Diffraction Enhancement of Symmetry. Acta Cryst. A28, 253-260.

[2] Perez-Mato, J. M. and Iglesias, J.E. (1974). *Acta Cryst*. **A33**, 466-474.

[3] Sadanaga, R. and Ohsumi, K. (1975). *Proc. Japan Acad*. **51**, 179-183.

[4] Sadanaga, R. and Ohsumi, K. (1979). *Acta Cryst*. **A35**, 115-122.

[5] Iglesias, J. E. (1979). *Z. Kristallogr*. **150**, 279-285.

[6] Ferraris, G.. Makovicky E. and Merlino, S. (2008). *Crystallography of Modular Materials*. Oxford: Oxford University Press, 384 pp..

[7] Buerger, M. J. (1950). *Acta Cryst*. **3**, 87-97.

[8] Dornberger-Schiff, K. and Grell-Niemann H. (1961). *Acta Cryst*. **14**, 167-177.

Keywords: Diffraction enhancement of symmetry; modular structures; silicon carbide