QCSP - a computer program for stereographic projection of quasicrystals

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Abstract: Whilst the stereographic projection is widely used for crystallographic analyses of conventional Bravias crystals, the stereogram approach is not generally applied to the case of quasicrystals. Although several software packages are available for the description of quasicrystals(Zhou *et al.*, 1994) (Weber, 1999), to our knowledge, there are no published calculations that enable the combination of conventional crystal structures and quasicrystal structure into the one stereographic projection. This is useful, for example, for exploring the orientation relationships between the two, such as when investigating precipitation or twinning in multiphase materials containing quasicrystals. This contribution is focussed on describing these calculations, providing a crystallographic bridge between the two types of structure, and so enabling stereographic projections of arbitrary quasicrystals (octagonal, decagonal, dodecagonal and icosahedral) together with those of conventional Bravais crystals. Our calculations can also be utilised for the interpretation and analysis of crystallographic information in atom probe tomography data acquired from quasicrystals. The 'crystallographic calculator' for the quasicrystals, and the complex index conversion between the Cartesan, Elser and Cahn indices for icosahedral quasicrystals is also provided (index conversion for 2D quasicrystals is under developing).
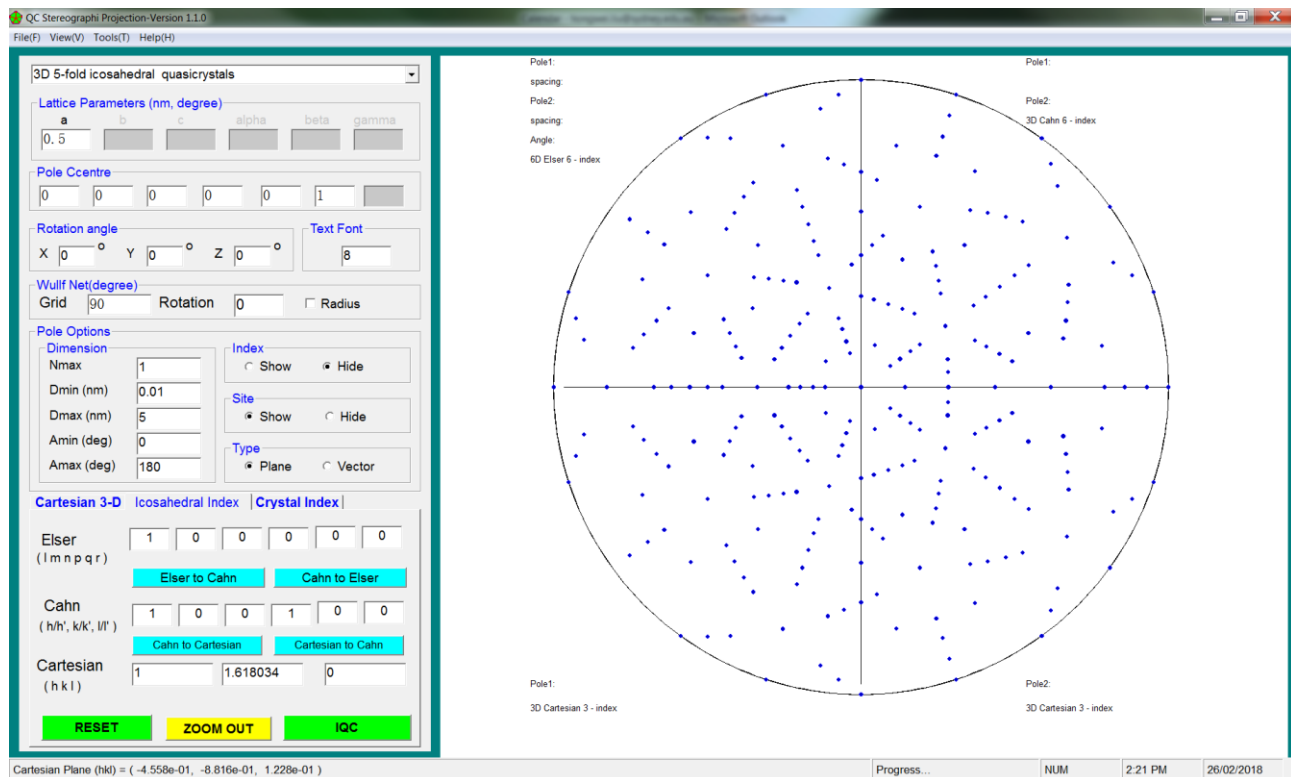
Figure abstract: A screenshot of The University of Sydney's Quasicrystal Stereographic Projection software user interface, showing a stereographic projection of five-fold symmetric axis of an icosahedral quasicrystal.

Acknowledgement

References:

Weber, S. (1999). *Journal of Applied Crystallography* **32**, 375-375.
Zhou, W., Wang, R., Gui, J., Zhao, J. & Jiang, J. (1994). *Journal of Applied Crystallography* **27**, 13-19.