

### Development of the CrystalScope suite (John Wheeler's software used to quantify various aspects of EBSD data): specific use of Weighted Burgers Vector method

As some historical background, the software suite was initiated in 1998 to perform basic tasks and has developed from there. The WBV method was implemented beginning in the early 2000s, first presented at an HKL User Group meeting in 2004 and first published in 2009. Below is a list of papers using the method. Three Laue groups are not yet implemented but it will be straightforward to do this if required.

| Crystal system | Laue group | Phase                                     | Weighted Burgers Vector study | Reference                         |
|----------------|------------|---|-------------------------------|-----------------------------------|
| Cubic          | m3m        | Periclase                                 | example                       | [1]                               |
| Cubic          | m3         |   |                               | -                                 |
| Hexagonal      | 6/mmm      | Mg<br>Ti<br>Ice<br>Ice<br>Ice             | example                       | [1],<br>[4]<br>[6]<br>[7]<br>[15] |
| Hexagonal      | 6/m        |   |                               | -                                 |
| Trigonal       | -3m        | Quartz<br>Quartz<br>Calcite               | example                       | [1]<br>[2]<br>[12]                |
| Trigonal       | -3         |   |                               | -                                 |
| Tetragonal     | 4/mmm      | Zircon<br>Zircon<br>Zircon                |                               | [3]<br>[5]<br>[9]                 |
| Tetragonal     | 4/m        |   |                               | -                                 |
| Orthorhombic   | mmm        | Olivine<br>Olivine<br>Olivine<br>Olivine  |                               | [10]<br>[13]<br>[16]<br>[17]      |
| Monoclinic     | 2/m        | Titanite                                  |                               | [11]                              |
| Triclinic      | -1         | Plagioclase<br>Plagioclase<br>Plagioclase |                               | [8], [14]<br>[16]<br>[17]         |

*Last update: February 2024*

## References using John Wheeler's Crystalscape software: specific use of Weighted Burgers Vector method (in date order)

1. Wheeler, J., E. Mariani, S. Piazzolo, D.J. Prior, P. Trimby, and M.R. Drury, *The weighted Burgers vector: a new quantity for constraining dislocation densities and types using Electron Backscatter Diffraction on 2D sections through crystalline materials*. Journal of Microscopy, 2009. **233**(3): p. 482-494.
2. Billia, M.A., N.E. Timms, V.G. Toy, R.D. Hart, and D.J. Prior, *Grain boundary dissolution porosity in quartzofeldspathic ultramylonites: Implications for permeability enhancement and weakening of mid-crustal shear zones*. Journal Of Structural Geology, 2013. **53**: p. 2-14.
3. MacDonald, J.M., J. Wheeler, S.L. Harley, E. Mariani, K.M. Goodenough, Q.G. Crowley, and D. Tatham, *Lattice distortion in a zircon population and its effects on trace element mobility and U–Th–Pb isotope systematics: examples from the Lewisian Gneiss Complex, northwest Scotland*. Contributions To Mineralogy And Petrology, 2013. **166**: p. 21-41.
4. Trimby, P.W., Y. Cao, Z. Chen, S. Han, K.J. Hemker, J. Lian, X. Liao, P. Rottmann, S. Samudrala, J. Sun, J.T. Wang, J. Wheeler, and J.M. Cairney, *Characterizing deformed ultrafine-grained and nanocrystalline materials using transmission Kikuchi diffraction in a scanning electron microscope*. Acta Materialia, 2014. **62**: p. 69-80.
5. Kovaleva, E., U. Klotzli, G. Habler, and J. Wheeler, *Planar microstructures in zircon from paleo-seismic zones*. American Mineralogist, 2015.
6. Piazzolo, S., M. Montagnat, F. Grennerat, H. Moulinec, and J. Wheeler, *Effect of local stress heterogeneities on dislocation fields: Examples from transient creep in polycrystalline ice*. Acta Materialia, 2015. **90**: p. 303-309.
7. Chauve, T., M. Montagnat, S. Piazzolo, B. Journaux, J. Wheeler, F. Barou, D. Mainprice, and A. Tommasi, *Non-basal dislocations should be accounted for in simulating ice mass flow*. Earth And Planetary Science Letters, 2017. **473**: p. 247-255.
8. Kendrick, J.E., Y. Lavallee, E. Mariani, D.B. Dingwell, J. Wheeler, and N.R. Varley, *Crystal plasticity as a strain marker of the viscous-brittle transition in magmas*. Nature Communications, 2017. **8**(1): p. Art. No. 1926.
9. Kovaleva, E., U. Klotzli, J. Wheeler, and G. Habler, *Mechanisms of strain accommodation in plastically-deformed zircon under simple shear deformation conditions during amphibolite-facies metamorphism*. Journal Of Structural Geology, 2018. **107**: p. 12-24.
10. Tielke, J.A., J. Mecklenburgh, E. Mariani, and J. Wheeler, *The influence of water on the strength of olivine dislocation slip systems*. Journal Of Geophysical Research: Solid Earth, 2019. **124**: p. 6542-6559.
11. Timms, N.E., M.A. Pearce, T.M. Erickson, A.J. Cavosie, A. Rae, J. Wheeler, A. Wittman, F. Ferriere, M.H. Poelchau, N. Tomioka, G.S. Collins, S.P.S. Gulick, C. Rasmussen, J.V. Morgan, and I.-I.E. Scientists, *New shock microstructures in titanite (CaTiSiO<sub>5</sub>) from the peak ring of the Chicxulub impact structure, Mexico*. Contributions To Mineralogy And Petrology, 2019.
12. Mcnamara, D.D., A. Lister, D.J. Prior, A. Scully, J. Gardner, and J. Wheeler. *Microanalysis of Calcite Scaling in a Fractured Geothermal System*. 2020.
13. Wieser, P., M. Edmonds, J. Maclennan, and J. Wheeler, *The Record of Magma Storage under Kīlauea Volcano preserved in Distorted Olivine Crystals*. Nature Communications, 2020.
14. Gardner, J., J. Wheeler, and E. Mariani, *Interactions between deformation and dissolution-precipitation reactions in feldspar at greenschist facies*. Lithos, 2021. **396-397**.
15. Fan, S., J. Wheeler, D.J. Prior, M. Negrini, A.J. Cross, T.F. Hager, D.L. Goldsby, and D. Wallis, *Using misorientation and weighted Burgers vector statistics to understand intragranular boundary development and grain boundary formation at high temperatures*. Journal of Geophysical Research - Solid Earth, 2022. **127**(8): p. 26 pages.
16. Gardner, J., D. Wallis, L.N. Hansen, and J. Wheeler, *Weighted Burgers Vector analysis of orientation fields from high-angular resolution electron backscatter diffraction*. Ultramicroscopy, 2024. **257**: p. 113893.

17. Wheeler, J., S. Piazzolo, D.J. Prior, P.W. Trimby, and J.A. Tielke, *Using crystal lattice distortion data for geological investigations: the Weighted Burgers Vector method*. Journal of Structural Geology, 2024. **179**: p. 105040.