Phase heritage: deciphering evidence of pre-existing phases via inherited crystallographic orientations

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Introduction: The concept of 'phase heritage' (e.g., Timms et al., 2017a) involves microstructural recognition of the former presence of a phase that has since transformed to another via evidence encoded in crystallographic orientations. Phase heritage relies on the phenomenon that newly grown (daughter) phases nucleate with particular crystallographic orientation relationships with the preceding (parent) phase. This phenomenon is common for displacive (i.e., shear or martensitic) transformations, well documented in the metals and ceramics literature, but is relatively uncommon in geosciences. This presentation outlines the concepts behind this approach, showcases results from software for automated analysis of EBSD data, and illustrates examples of polymorphic and dissociation phase transformations in the $ZrSiO_4$-ZrO_2-SiO_2 system, which has particularly useful applications for 'extreme thermobarometry' in impact environments (Timms et al., 2017a).

Theoretical considerations: The crystal symmetry of parent and daughter phases and the nature of the orientation relationship between them determine the maximum number of permissible symmetrically equivalent variants of the daughter from a single parent (Cayron et al., 2006). This means that a microstructure comprising daughter grains that have completely transformed from a parent grain define a specific pattern of crystallographic orientations. The number of variants can be predicted from the order of the parent point group divided by the order of the intersection group (i.e., the group of orientation symmetries common to parent and daughter crystals). The number of operators is given by the rotation/misorientation angle/axis relationships between the daughter and parent crystals. Therefore, if the symmetry operators for the phase transformation are known, then the phase transformations can be reverse-engineered to not only recognise the former presence of a parent phase but also to derive its unique crystallographic orientation(s). In this way, the entire microstructure of parent grains can be completely reconstructed from daughters that have inherited their crystallographic orientations. In fact, different orientation relationships can be tested using software ARPGE to find the best one for the parent reconstruction (Cayron, 2007, Cayron et al., 2010). Several generations of phase transformations via multiple, symmetrically equivalent nuclei orientations can generate complex patterns of daughter orientations. Reconstruction of parent grains from a two-stage transformation history requires knowledge of the orientation relationships for both phase transformations (e.g., Cayron, et al., 2010). Subsequent reversion from daughter to parent phases follows the reverse orientation relationships. An equal probability of the nucleation of neoblasts in symmetrically equivalent orientations can still result in a bias in the proportions of final orientations.

Thermal dissociation of zircon to ZrO_2 polymorphs: Glassy impact melt rock from the Mistastin Lake impact structure, Canada, shows that entrained zircon ($ZrSiO_4$) grains have dissociated to ZrO_2 + SiO_2 forming reaction rims of twinned vermicular baddeleyite (monoclinic ZrO_2 stable at low-T) with interstitial silicate glass (Timms et al., 2017b).

Automated analysis of EBSD map data using ARPGE successfully reconstructs grandparent grains of cubic polymorph of ZrO_2 from baddeleyite with complex twinning, indicating a two-stage transformation involving an intermediate tetragonal ZrO_2 stage. The former presence of cubic ZrO_2 in this sample required melt temperatures in excess of 2370°C, which represents the hottest naturally-achieved temperature recorded by any rock at the Earth's surface (Timms et al., 2017b).

High-pressure polymorphic phase transformations zircon-reidite-zircon: Granular-textured zircon from a variety of impact melt rocks preserve crystallites with approximately orthogonal crystallographic orientation clusters (Timms et al., 2017a; Cavosie et al., 2016; 2018). This distribution is readily explained by partial transformation of pre-existing zircon to the high-pressure $ZrSiO_4$ polymorph reidite, which occurs via up to eight symmetrically equivalent variants, arranged into two groups of four that are broadly orthogonal to one another (Erickson et al., 2017). A random selection of transformation orientations followed by random selection for the reversion to zircon statistically favours the original host zircon orientation, which is consistent with observations. This process of generating granular zircon required shock metamorphism >30 GPa to produce reidite followed by reversion to zircon via the formation of a granular texture upon release from shock pressures and waste heating (Timms et al., 2017a). Granular-texture zircon with this type of encoded microstructure has been termed FRIGN zircons (Former Reidite In Granular Neoblasts) (Cavosie et al., in review), useful for deciphering P-T history where back-transformations are complete and other evidence of pre-existing high-pressure phases have been destroyed (e.g., Cavosie et al., 2016; 2018, in press).

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