Electron backscatter diffraction analysis of zircon: A systematic assessment of match unit characteristics and pattern indexing optimization

STEVEN M. REDDY,¹,⁎ NICHOLAS E. TIMMS,¹ AND BRUCE M. EGLINGTON²

¹Department of Applied Geology, Curtin University of Technology, GPO Box U1987, Perth, WA 6845, Australia
²Saskatchewan Isotope Laboratory, Geological Sciences, University of Saskatchewan, 114 Science Place, Saskatoon, Saskatchewan S7N 5E2, Canada

ABSTRACT

Quantitative microstructural analysis of zircon using electron backscatter diffraction (EBSD) requires a comparison of empirically collected electron backscatter patterns with theoretical patterns or “match units” derived from known crystallographic parameters. There are 23 possible crystallographic data sets for zircon, and associated match units, derived from natural and synthetic zircon and from theoretical calculations over a range of pressures and different rare earth element (REE) compositions. A systematic assessment of these match units has been undertaken by EBSD analysis of each of four zircons from a range of geological environments combined with principal components analysis and self-organizing map networks. Comparison of the different match units shows a systematic relationship across all samples that are related to changes in unit-cell dimensions associated with pressure and compositional variations. Systematic variations in the data generated from 96 EBSD maps, each comprising 10,000 electron backscatter patterns, indicate that match units associated with increasing pressure or REE dopants yield poorer quality EBSD data. The match units from low-pressure, undoped, natural zircon consistently yield the best EBSD results and are recommended for natural zircon EBSD studies irrespective of the zircon source or U content. The results provide a clear strategy for optimizing the acquisition and analysis of EBSD data from zircon from both crustal and mantle sources. In addition, the developed approach to match unit analysis may be applied to all other crystalline materials, potentially optimizing EBSD analyses from a range of materials.

Keywords: EBSD, microstructure, zircon, reflector file, match unit, REE, pressure, rare earth element

INTRODUCTION

The mineral zircon (ZrSiO₄) is widely used by the earth science community to provide geochemical and temporal constraints on a range of important geological processes. The justifications for its widespread use are its ability to incorporate a wide range of elements into its lattice (e.g., the radioactive element, U) and its ability to retain compositional information to temperatures approaching 1000 °C. Despite the successful application of zircon geochemical and geochronological data to various disciplines, recent studies have documented that zircon may deform by crystal plasticity within the Earth’s crust (Reddy et al. 2007). Studies linking quantitative microstructural and geochemical analysis of an Indian Ocean zircon illustrate that crystal plasticity of zircon may facilitate the geochemical modification of zircon rare earth elements (REE) at temperatures significantly below those suggested for volume diffusion (Reddy et al. 2006). In a similar study, U-Th variations have also been linked to deformation-related crystal plasticity in zircon (Timms et al. 2006). These findings have the potential to lead to the refinement of geochemical models and the development of new applications of zircon geochemical data to earth-science research. However, such applications require the quantitative and non-destructive microstructural analysis of zircon by electron backscatter diffraction (EBSD) to allow integration of orientation data with high-spatial resolution geochemical information.

Electron backscatter diffraction is a quantitative microstructural technique (e.g., Prior et al. 1999) that relies on a comparison of an empirically obtained electron diffraction pattern (EBSP) with a theoretically calculated reference diffraction pattern, often referred to as a “match unit,” to constrain the orientation of a crystalline material at the point at which the diffraction pattern is generated. Critical to the successful EBSD analysis of a material is the ability to generate theoretical match unit files that reliably represent the material being analyzed. However, the parameters used to generate match unit files, including unit-cell dimensions and atomic positions, may change with both intrinsic (e.g., composition) and extrinsic (e.g., pressure) factors.

Several different studies have constrained the crystallographic parameters of zircon over a range of chemical (REE) and pressure variations, such that there are currently 23 possible structural data sets, each of which allow the calculation of a different zircon match unit file (Table 1; Fig. 1). These 23 different sets...