DEFORMATION HISTORY RECONSTRUCTION USING RAMAN MICROSCOPY DATA OF SINGLE QUARTZ GRAINS. Á. Skultétí, T. M. Tóth, K. Fintor and F. Schubert. 1Department of Mineralogy, Geochemistry and Petrology, University of Szeged, H-6722 Szeged, Egyetem Street 2., skulteti.agi@gmail.com

Introduction: Quartz is among the most common minerals in the Earth’s crust, which is stable within a wide range of temperature and pressure conditions. This mineral is very sensitive to stress and, at different P-T conditions deforms in different ways following diverse deformation mechanisms resulting in grains with various microstructures.[1-3] As a consequence, in a quartz bearing rock each grain may provide information about the deformation history of the rock body itself. As ductile deformation processes are usually very slow in reaching equilibrium, thus each quartz grain appears a little bit elsewhere in the evolution, but they together may help to sketch the deformation history of the host rock body.

The study area is an active shear zone situated in Central Europe, in the South Transdanubian region of Hungary. Deep understanding of the present and past behavior of this tectonic zone is, nevertheless, crucial, because of several aspects. For example, it goes only a few km north of the low and intermediate level radioactive waste deposition place of Hungary and at several places, due to the intensive deformation, shear zone rocks behave as excellent fractured fluid reservoir. Our samples represent a newly bored geothermal well located inside the dislocation zone. This deep well brought drilling chips from around 2 km depth to the surface giving an exclusive possibility to investigate the shear zone underneath.

The aim of the work is to discriminate and characterize the microstructurally different quartz grains by using only traditional optical methods and Raman spectroscopy. Further on, the other purpose is to work out a method allows reconstruction the deformation history of the shear zone using only the tiny quartz chips.

Samples and Methods: The investigated drilling chip samples came from the Szentlőrinc-1 deep drilling, the studied interval was 1600-1820 m. The drilling chip collection includes just a few, small rock grains not available for any traditional petrographic evaluation. More than 80% of the material consists of tiny (<1 mm) single quartz grains.

Firstly during the microstructural analysis around 500 quartz grains were studied, than on 13 selected quartz grains Raman microspectroscopy was performed. The Raman spectra were evaluated by PeakFit v4.12 software, the determined spectral variables were the peak position, amplitude, full width at half maximum (FWHM), full width at base (FW base), integrated area and standard deviation of the bands of interest. For the resulted data discriminant function analysis were executed, the aim of the calculations was to find those functions of the original spectral parameters that separate diverse quartz groups the best.

Results: The 500 single quartz grains studied under the microscope have various microstructures. Three of them can be defined as microstructurally extreme; grains with undulose extinction (type 0: T0) (Fig. 1a), grains with subgrains (type 1: T1) (Fig. 1b) and grains consisting of small, undeformed recrystallized grains (type 2: T2) (Fig. 1c)[4].

Beside the quartz grains, which belong to any of the above groups, there are numerous grains with heterogeneous microstructure too. These exhibit simultaneously more extreme textures within a single grain (transitional grains) (Fig. 1d).

![Figure 1. Characteristic quartz grain types in the analyzed samples. (a) Quartz grain with undulose extinction (type 0: T0), (b) quartz grain with subgrains (type 1: T1), (c) quartz grains with small recrystallized grains (type 2: T2) and (d) transitional quartz grain with heterogeneous microstructure.][4]

In the first step of the Raman spectroscopic investigation the three representative extreme quartz grains were measured along a 250 μm long line of 50 points in each. Afterwards, ten microstructurally transitional grains were studied in a similar way.

The statistical analysis displays, that the microscopically defined extreme grains have significantly different spectral attributes, so the microstructurally different quartz grains can accordingly be divided based of certain spectral variables of their Raman spectra as well.[4] The extreme grains appear as rather tight clouds of points, and so their centers define a triangle...
in the F1-F2 spectral space (Fig. 2). The most important spectral attributes that describe best the difference between the T0 and T1 grains are the integrated areas of the 128 and 206 cm\(^{-1}\) bands. The difference between T1 and T2 grains is mainly characterized by the positions of 128, 206 and 464 cm\(^{-1}\) bands.\(^{[4]}\) By the application of the F1 and F2 discriminant functions the spectral positions of the ten transitional grains were calculated, too. The results exhibit that, each transitional grain is situated inside the triangle defined by T0, T1 and T2 extreme grains (Fig. 2).\(^{[5]}\)

**Figure 2.** Position of T0-T1-T2 extreme quartz grain types in the spectral space (T0-T1-T2 spectral triangle) with transitional grains.\(^{[4]}\)

**Discussion:** The microstructure of available detrital quartz grains may provide valuable information about the evolution of a subsurface shear zone. Using Raman microspectroscopy single quartz grains and monomineralic domains, which are characterized by different deformation conditions can be identified and so separated. In this study three microstructurally extreme quartz grain types were discriminated from a subsurface shear zone; T0 grains with undulose extinction, T1 grains with subgrains and T2 grains consisting of small, undeformed recrystallized grains. The above extremes have significantly different spectral attributes, so the microstructurally different quartz grains can accordingly be divided on the basis of the certain spectral variables of their Raman spectra. Spectra of all extreme grains (T0, T1, T2) define closed groups of points in the spectral space, while each transitional grain is situated inside their triangle. The three extreme quartz grain types were formed by different deformation mechanisms, so they represent different deformation conditions, which are associated with increasing temperatures from T0 state up to T2 (\(\Delta T \approx 250-500^\circ\text{C}\)).\(^{[4]}\) Thus the T0-T1-T2 spectral space is actually considered as a virtual deformational space. Each complex quartz grain measured in the sample appears a little bit elsewhere in the deformation process defined by T0-T1-T2 extreme conditions, but they together determine a deformation development pathway. It can be supposed that this combined pathway is characteristic for the whole rock volume in study.

The obtained virtual deformational space allows the reconstruction of the deformation history of the examined shear zone on the basis of available detrital quartz grains.

**Applications:** Characterization of single quartz grain microstructures using the above technique along the whole well enables localization of the ductile shear zones inside the crystalline complex. These zones coincide very well with the brittle horizons defined by well-log evaluation. This behavior may suggest two different evolution schemes. (1) If the firstly evolved ductile shear zones caused softened regions inside the crystalline mass, it could reactivate later in a brittle way due to strain localization during a subsequent tectonic event independent of the early one. (2) Provided, these structures formed due to the same tectonic event, these zones may represent a detachment fault maintaining subsequent deformation regimes of different ages. These structures develop as the result of continental extension, when the middle and lower continental crust deformed in a ductile way is uplifted to the brittle upper crust. As a consequence, ductile and brittle deformation overlaps along the same shear zones.\(^{[5]}\) These large scale faults usually divide crystalline blocks of significantly different metamorphic evolutions in the footwall and the hanging wall (metamorphic core complexes), what is a well-known phenomenon in the metamorphic basement of SW Transdanubia, close to the studied well.