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A software tool to evaluate crystal types and morphological developments of accessory zircon

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ABSTRACT

Computer programs for an appropriate visualization of crystal types and morphological developments of accessory zircon are not available hitherto. Usually, typological computations are conducted by using simple calculation tools or spread-sheet programs. In practice, however, high numbers of data sets including information of numerous zircon populations have to be processed and stored. The paper describes the software ZIRCTYP, which is a macro-driven program within the Microsoft Access database management system. It allows the computation of zircon morphologies occurring in specific rock samples and their presentation in typology diagrams. In addition, morphological developments within a given zircon population are presented (1) statistically and (2) graphically as crystal sequences showing initial, intermediate, and final growth stages.

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1. Introduction

Databases are programs allowing the storage and management of various kinds of information. Whilst in economy and communication sciences databases have become an irreplaceable part of electronic administration and public recording, in earth sciences these programs have not gained acceptance in the same way hitherto. Only in geoscientific fields, where large amounts of data are produced (e.g. petrography, thermodynamics, geophysics), respective programs for data management have been published during the past decades. For an appropriate computation of igneous petrologic data, the database IGBA was developed in the early 1980s (Chayes, 1983, 1985). According to the programmers, this database should represent a type of electronic library containing igneous petrology data intended for general use and published in different countries and languages. A more recent update of the program was documented by Brändle and Nagy (1995). Concerning the administration of mineral assemblage data and related thermodynamic results, the relational database ParaDIS provided by Schmatz et al. (1995) represented a significant innovation due to its interfacing with external thermobarometric programs (e.g. TWEEQ; Berman, 1991) and Geographic Information Systems (GISs), allowing the suitable display of local P-T data. Geological and geophysical information is e.g. available from the database PANGAEA published by Diepenbroek et al. (2002), whilst SPECCHIO (Bojinski et al., 2003) offers comprehensible data of the spectral properties of natural and artificial materials on the earth's surface. For a more effective search of geological data in the world-wide web, specific internet applications were recently introduced by Laxton and Becken (1996) and Guillen et al. (2001). In most recent times, database programming was focused on specific geoscientific fields. Thereby most publications concerning the storage and administration of data were provided for GIS (e.g. Xie et al., 2005; Mixon et al., 2008), geological mapping (e.g. Zanchi et al., 2009a), and three-dimensional geological modeling (e.g. Kaufmann and Martin, 2008; Zanchi et al., 2009b). Due to the rapid increase of internet connections and continuous acceleration of data transfer, use of the world-wide web as a powerful source for geological information will be also an important topic for future publications in geoinformatics.

This paper presents a database program, which could awake interest among mineralogists and petrologists. The program termed ZIRCTYP enables the morphological description of zircon crystals separated from igneous rocks. Furthermore, zircon morphologies may be subjected to a statistical evaluation using previously published methods (Pupin and Turco, 1975; Pupin, 1980; Fig. 1). In the past, studies on the rock-specific growth behavior of accessory zircon provided a chance to solve e.g. the question of earth crust formation in a given terrain (Pupin, 1980) or a possible petrogenetic relationship between two rocks (e.g. Steyrer and Sturm, 2002; Sturm, 2010). Early morphological investigations yielded evidence that zircon crystals are characterized by a strong dependence of their growth process on the chemistry of their crystallization medium (Poldervaart, 1956; Hoppe, 1963). Due to chemical changes of the magmatic source during rock crystallization zircon crystal growth may be subject to significant morphological changes from

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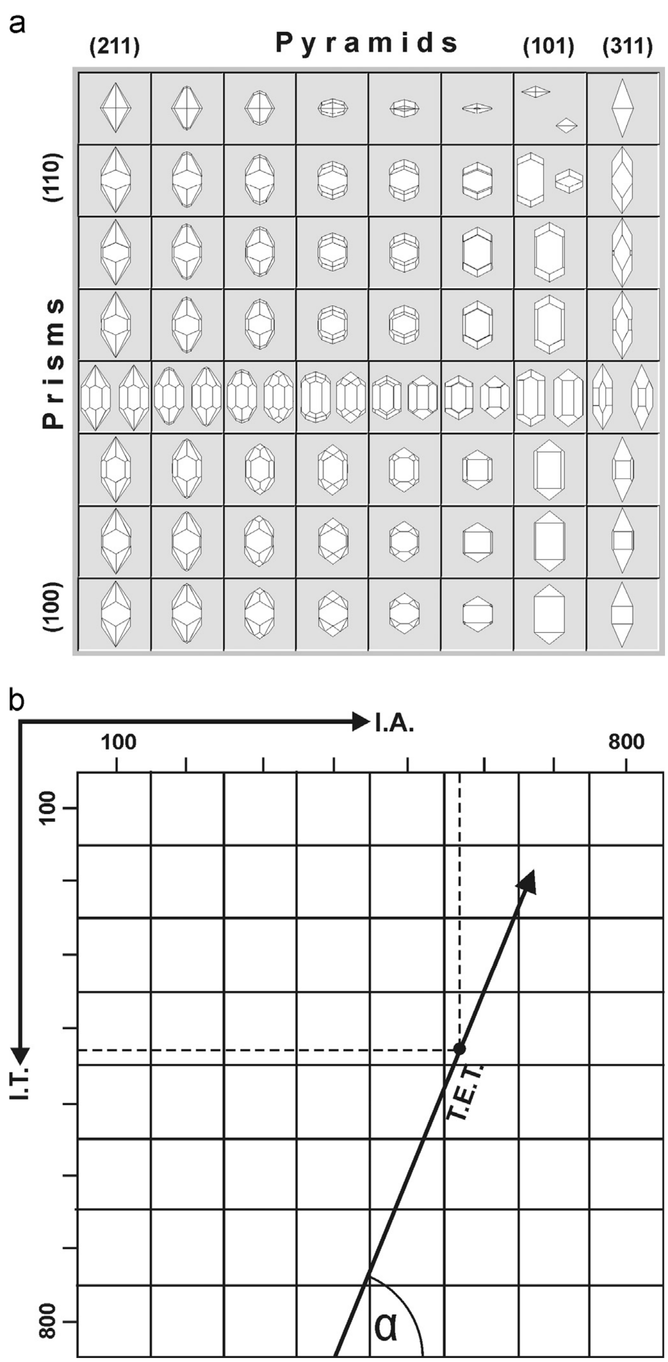

Fig. 1. (a) Typology diagram outlined by Pupin and Turco (1975). (b) Determination of the morphological evolutional trend (see text); $\alpha=\tan(S_T/S_A)$.

initial to final growth stages (Sturm, 1999, 2004, 2010). During the past 15 years, the relationship between zircon morphology and rock petrogenesis was appreciated by numerous scientific studies dealing with examplary cases (e.g., Wang et al., 1998, 2002; Wang and Kienast, 1999; Belousova et al., 2006). The results of previous petrological and mineralogical investigations were summarized in part by Corfu et al. (2003), who describe zircon textures occurring in various granitic rocks and their possible implications for petrogenesis. Concerning the theoretical modeling of external zircon morphologies, only few studies and related computer codes have been outlined hitherto, among which MARVIN (Gay and Rohl, 1995) crystallized out as most applicable. ZIRCTYP, however, also offers a possibility to illustrate morphological developments of accessory zircon in different lithologies.

2. Materials and methods

2.1. Methodologies used in the database program

Distinction of zircon crystal types is based on the theory of Pupin and Turco (1975), according to which a total of 64 zircon crystal types may be detected in igneous rocks. Specific rock chemistries result in the predominance of specific crystal types. The crystal types have been summarized in a diagram containing 64 fields (Fig. 1a). Statistical evaluation of crystal types separated from a given rock is usually carried out under the microscope, whereby each investigated crystal is attributed to a specific field of the diagram.

Estimation of morphological growth trends is based on the typological statistics, which were formerly introduced by Pupin (1980). The coordinates of the so-called typological mean point of a certain zircon population, $\overline{I.A.}$ and $\overline{I.T.}$, are calculated according to the following formulas:

$$\overline{I.A.} = \sum_{I.A.=100}^{800} I.A. \cdot n_{I.A.} \tag{1}$$

$$\overline{I.T.} = \sum_{I.T.=100}^{800} I.T. \cdot n_{I.T.}. \tag{2}$$

In Eqs. (1) and (2) $n_{I.A.}$ and $n_{I.T.}$ denote the relative frequencies of each value of *I.A.* and *I.T.* (note: *I.A.* and *I.T.* represent the fields of the respective rows and columns of the typological diagram; Fig. 1b). The following convention has to be fulfilled:

$$\sum n_{I.A.} = \sum n_{I.T.} = 1 \tag{3}$$

The morphological trend line runs through the typological mean point and has the slope *a*, which is computed according to the following mathematical expression:

$$a = S_T/S_A. \tag{4}$$

in Eq. (4) S_T and S_A represent the standard deviations of the *T* index and the *A* index, respectively, which may be computed according to the simple formulas:

$$S_T = \sqrt{\sum_{i=1}^{N} (T_i - \overline{T})^2/N} \tag{5}$$

$$S_A = \sqrt{\sum_{i=1}^{N} (A_i - \overline{A})^2/N}. \tag{6}$$

in the two equations noted above, *N* is the overall number of zircon crystals that have been included into the statistical analysis.

2.2. Basic description of the program

ZIRCTYP was programmed in Microsoft Access (Version 2002) using the macro-editor and Visual Basic code editor for the generation of specific command buttons. The program consists of an entrance mask, from which the user can navigate to the input forms for (1) the statistical analysis of zircon morphologies and (2) the evaluation of morphological growth trends (Figs. 1 and 2). Within both parts of the database program, processing of data includes three main steps:

1. Input of information describing the studied rock (sample name, petrology, trace-element data, U-Pb age data, Lu-Hf and O-isotope data) and typological data. At the current developmental stage of the database, however, trace-element data, isotope data or information concerning zircon age cannot be submitted to further calculation processes, since the main focus

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