Computers & Geosciences 59 (2013) 90–97

Contents lists available at SciVerse ScienceDirect

Computers & Geosciences

journal homepage: www.elsevier.com/locate/cageo

MinSORTING: An Excel® worksheet for modelling mineral grain-size distribution in sediments, with application to detrital geochronology and provenance studies

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ARTICLE INFO

Article history:
Received 20 March 2013
Received in revised form
28 May 2013
Accepted 29 May 2013
Available online 5 June 2013

Keywords:
Heavy minerals
Size–density sorting
Settling equivalence
Detrital geochronology
Mineral separation
Provenance analysis

ABSTRACT

MinSORTING is an Excel® spreadsheet devised to model mineral distributions in different size-classes within sediment samples and maximize mineral recovery during separation procedures for single-grain analysis. It is based on the physical laws of settling by tractive currents, both in water and air, applied to the different minerals in silt to sand-sized terrigenous sediments. Input values are: (i) grain size and sorting, (ii) depositional medium (seawater, freshwater or air), (iii) sediment composition (selected from a range of tectonic settings).

The software's output includes the distribution of 27 different detrital components contained in sediments in size intervals of 0.25, 0.5, or 1 phi. Researchers can thus select the most appropriate size window for their own analyses and obtain valuable information on the amount of minerals lost in finer and coarser grain-size classes, allowing to accurately constrain the significance of their results.

1. Introduction

Detrital minerals are receiving increasing attention in the Earth Sciences, due to development of single-grain analytical techniques that are currently applied to constrain sediment fluxes and exhumation/erosion of sediment sources (von Eynatten and Dunkl, 2012).

Single grain U/Pb analyses are routinely performed on detrital zircon (e.g. Amidon et al., 2005; Gehrels et al., 2008), apatite (e.g. Chew et al., 2011; Thomson et al., 2012; Zattin et al., 2012), rutile (e.g. Zack et al., 2011; Meinhold, 2010; Small et al., 2013), monazite (Hietpas et al., 2010; Rubatto et al., 2013), and titanite (McAteer et al., 2010; Gao et al., 2012). Fission-track and (U-Th)/He analyses are currently applied to detrital zircon and apatite (Garver et al., 1999; Carter and Bristow, 2003; Bernet and Garver, 2005; Heberer et al., 2011; Tranel et al., 2011; Malusà and Balestrieri, 2012; Resentini and Malusà, 2012). Hf and Nd isotopes are measured in detrital zircons (Dhuime et al., 2011). K/Ar and Ar/Ar dating is applied to muscovite (Kundic et al., 2012), *k*-feldspar (Chetel et al., 2005), biotite, and hornblende (Pierce et al., 2011). OSL dating is performed on feldspars and quartz grains (Stokes, 1999; Tsukamoto et al., 2011; Fuchs et al., 2009), and quartz is also routinely used for the analysis of cosmogenic nuclides (Norton et al., 2008; Wittmann et al., 2007; Schaefer and Lifton, 2007).

Sampling and concentration procedures of all these minerals are crucial steps in order to retrieve as much information as possible from sediments. When inaccurate, they can influence the reliability of results, possibly leading to incorrect interpretation. Moreover, mineral species must be extracted from bulk sediment in a convenient amount, to ensure that datasets are statistically robust (e.g. Vermeesch, 2004). Heavy minerals relevant for single-grain studies are commonly diluted in sediment sample (e.g. zircon typically represents ~0.02% of the bulk sediment, Garzanti et al., 2012), and they concentrate in specific grain-size classes as an effect of hydraulic sorting during settling (Fig. 1; Rubey, 1933; Rittenhouse, 1943; Garzanti et al., 2008). Heavy minerals usually represent no more than 5% in weight in modern first-cycle sediments, and their abundance drastically decreases in ancient sedimentary successions and recycled sediments (Garzanti and Andò, 2007). As a consequence, one of the major problems faced not only by detrital geochronologists, but also by ore prospectors, is extracting minerals from bulk sediments/sedimentary rocks in a convenient amount for analysis. A common strategy is to collect very large samples, but this implies logistic issues, greater costs and longer time for mineral separation. Moreover, this approach does not ensure that the required amount of material is finally obtained. In most detrital studies, only specific

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http://dx.doi.org/10.1016/j.cageo.2013.05.015

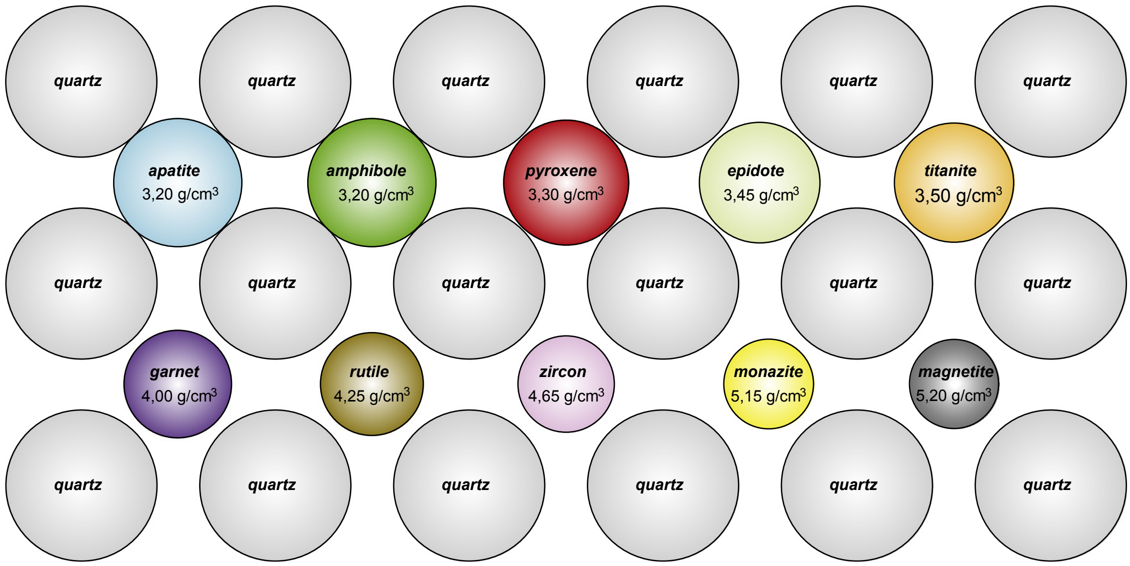

Fig. 1. Pictorial representation of size relationships between quartz (2.65 g/cm^3) and settling-equivalent minerals of different densities. All depicted spheres are hydraulically equivalent and settle at 2.67 cm/s in freshwater. Differences in density correspond to variations in grain-size: quartz diameter 250 μm; magnetite diameter 148 μm (size shifts calculated with Cheng's, 1997 formula).

grain-size classes are sieved from the bulk deposit and further processed for analysis, for (i) the need to standardize procedures and collect grains big enough for analysis (but still small enough to be easily processed in large amounts) and (ii) the false belief that precision can be increased by narrowing the analysed size-window (Garzanti et al., 2009). For these reasons, the mineral-separation process quite commonly ends with an insufficient amount of retrieved material, because the processed grain-size class was too fine or too coarse. Last and most important, missing the information contained in other grain size fractions may lead to biased results (Yang et al., 2012).

To solve all of these problems, we present here a MS Excel® spreadsheet that calculates the size–frequency distribution of any detrital component in sediments according to the physical rules that govern particle settling in fluids.

Applications of this program are manifold:

(i) in detrital geochronology, it enables us to choose the correct size of sediment samples and maximize mineral recovery during standard laboratory-separation procedures;
(ii) in bedrock studies performed on sedimentary rocks, it enables us to calibrate separation procedures after sample disaggregation, provided that the original grain size distribution is preserved;
(iii) in sediment budgets based on narrow-window single-grain analyses, it allows us to estimate the amount of mineral lost in finer and coarser grain-size classes;
(iv) in classic sedimentary petrography, it helps us to improve provenance information, as it gives insights on the representativeness of results from single-window analyses and can give clues on anomalous mineral assemblages and intrasample variability.

2. Theoretical background

Detrital grains in sediments are efficiently sorted during erosion, transport and deposition according to their size, density and shape (Komar, 2007).

Size–density distributions in sand laid in water, where fluid viscosity plays an important role, can be predicted by empirical formulas, such as that of Cheng (1997):

$$v=((25+1.2((g\times\Delta_x\times D_x^3/\eta^2)^{2/3}))^{1/2}-5)^{3/2}\times\eta/D_x \quad (1)$$

$$SS_x=\log_2(\Delta_x/\Delta_{\text{ref}})-3/2\log_2(\Xi_x/\Xi_{\text{ref}}) \quad (2)$$

where v is settling velocity, g is gravity, Δ_x is the submerged density (mineral density δ_x—fluid density δ_f), D_x is the diameter of mineral grain x, η is the fluid viscosity. SS_x is the size-shift, i.e. the expected difference in size between a mineral x and the sediment mean size, where $\Xi=v/\eta+((v/\eta)^2+48\ (g\times\Delta_x/\eta^2)^{2/3})^{1/2}$ (Garzanti et al., 2008). Theoretical size-shifts of different minerals relative to quartz are reported as a function of grain size in Fig. 2.

The grain-size distribution in sand laid in air is influenced by fluid turbulence rather than fluid viscosity, and empirical results show that it can be described by the Impact law:

$$v=(2/3g\times\Delta_x\times D_x/\delta_f)^{1/2} \quad (3)$$

$$SS_x=\log_2(\Delta_x/\Delta_{\text{ref}}) \quad (4)$$

Instead, for sediments laid in water and finer than 3.5 phi (i.e. very fine sand to silt), the turbulence effect is negligible and settling velocity and size shift can be calculated with the Stokes law:

$$v=g\times\Delta_x\times D_x^2/18\eta \quad (5)$$

$$SS_x=\log_2(\Delta_x/\Delta_{\text{ref}})/2 \quad (6)$$

Note that size shifts calculated with Stokes law are half of those calculated with the Impact law.

MinSORTING applies these equations to model sediment settling both in subaerial and subaqueous environments, and calculates for different types of fluids (air, freshwater, seawater) the expected size-shift for each particle and its distribution in different size classes. Analyses of different grain size-classes in sediments deposited in fluvial, shallow-marine and eolian environments indicate that the discrepancies between observed and calculated size shifts associated with differences in shape are negligible for most minerals, with the only major exception of flaky micas and fibrous sillimanite (Garzanti et al., 2008, 2009). For simplicity, most detrital components were thus considered of the same spherical shape. To account for slower settling of micas and fibrous