Total Scattering Techniques: A powerful tool to investigate size, shape and growth mechanisms of minerals at the nanoscale

A. GUAGLIARDI[1*], A. CERVELLINO[2], R. FRISON[1], J. M. DELGADO LÓPEZ[3], J. GÓMEZ-MORALES[3] AND N. MASCIOCCHI[4]

[1]Istituto di Cristallografia, CNR, I-22100 Como, Italy (*correspondence: antonella.guagliardi@ic.cnr.it).
[2]SLS Laboratory for Synchrotron Radiation - Condensed Matter, PSI, CH-5232 Villigen, Switzerland.
[3]Laboratorio de Estudios Cristalográficos, IACT (CSIC-UGR, E-18100 Armilla, Granada, Spain.
[4]DiSAT, Università dell'Insubria, I-22100 Como, Italy.

Nanoscaled crystals (NCs) and the processes governing their nucleation and growth play a fundamental role in relevant, and diverse, fields, such as (to mention a few) geochemical cycling, mining and biomineralization. The limited coherence length of NCs, the presence of compositional and structural defects and the interaction with organic components make these systems highly complex, with a *short-range order only*. In the diffraction space, these features turn into diffuse scattering, falling between and below the Bragg peaks. The Debye equation [1] is a *Total Scattering* approach treating Bragg and diffuse scattering on an equal basis and, therefore, is able to use the *entire* information present in the experimental diffraction pattern. Conversely, conventional single-crystal and powder X-ray and neutron diffraction methods deal with Bragg intensies only. Recently, we have proposed a new, original and computationally efficient implementation of the Debye Function Analysis [2], which enabled us to *quantitatively* characterize, in terms of structure, size and shape distributions, different kinds of nanocrystalline materials [3]. Among these, citrate-controlled biomimetic apatites [4], very similar in size, shape and composition to bone apatites, have been for the first time characterized by DFA. Combining DFA and AFM, we were able to unravel the mechanism forming platy-shaped NCs from an amorphous calcium phosphate precursor. A major role of citrate in controlling the growth mechanism of the apatitic mineral clearly emerges.

[1] Debye (1915) *Ann. Phys.* **351**, 809-823. [2] Cervellino *et al.* (2010) *J. Appl. Cryst.* **43**, 1543-1547. [3] Cernuto *et al.* (2011) *Angew. Chem. Int. Ed.* **50**, 10828-10833, and references therein. [4] Delgado-López *et al.* (2012) *Acta Biomater.* **8**, 3491-3499.

High-silica rhyolites and granites: Products of the shallow crust

GUILHERME A. R. GUALDA[1] AND MARK S. GHIORSO[2]

[1]Earth & Environmental Sciences, Vanderbilt University, Nashville, TN 37235, USA; (g.gualda@vanderbilt.edu)
[2]OFM Research - West, Seattle, WA 98115, USA; (ghiorso@ofm-research.org)

High-silica rhyolites and granites (>75 wt. % SiO_2, anhydrous) are common features of the crust, as part of both the volcanic and plutonic records. While low crystallization pressure (<250 MPa) is typically inferred, it has been suggested that they form via polybaric evolution, with initial crystallization at relatively high pressures (> 500 MPa).

We use glass compositions derived from the EarthChem portal, selected natural examples from the literature, and rhyolite-MELTS calculations to probe the depth at which different magma compositions can form within the crust.

We demonstrate that the phase relations in the Qz-Ab-Or ternary dictate the silica content of silicic melts and cause silica content to increase with decreasing pressure. Our analysis has profound implications for the origin of silicic melts and magmas within the continental crust, specifically:

(a) *Silicic magmas are expected to show stratification in silica contents within the crust*. Melts within the crust will show a gradient in maximum silica content; while dacites can occur over much of the crust, high-silica rhyolites are confined to the shallow levels of the crust.

(b) *High-silica rhyolite glass can only form at low P, requiring crystallization in the shallow crust*. Polybaric evolution of magmas is confined to their possible range of occurrences. While dacites can evolve via decompression-driven crystallization over a large range of pressures (as recorded in glass inclusions), high-silica rhyolites are confined to the shallow crust (consistent with narrow range of silica contents in glass inclusions).

(c) *The existence of high-silica pumice requires fractionation or melting at low pressure*. Whole-pumice with high-silica rhyolite composition requires melting or fractionation in the shallow crust, which precludes direct derivation of high-silica magmas from high pressures without substantial fractionation at low pressure, and shows that high-silica rhyolites and granites are intrinsic to the shallow crust.

(d) *Low-pressure cumulates or melting residues must exist in the shallow crust*. If shallow-level fractionation is required, then crystal cumulates or partial melting residues must be present within the upper crust. The crystal cumulates necessary to form high-silica rhyolites are to be found within upper crustal granitoid plutons.

DOI:10.1180/minmag.2013.077.5.7