Correlations between Hf, O and trace element concentrations in zircon from rhyolitic rocks
(NE German Basin)

E. DEJA[1]*, A. PIETRANIK[1], J. KIERCZAK[1], R. MILKE[2] AND C. BREITKREUZ [3]

[1]University of Wrocław, Institute of Geological Sciences, Poland; (elka_deja@yahoo.com)
[2]Freie Universität Berlin; (milke@zedat.fu-berlin.de)
[3]TU Bergakademie Freiberg, Germany; (cbreit@geo.tu-freiberg.de)

Hundreds of deep hydrocarbon exploration wells exposed the Late Paleozoic volcanic province in NE Germany, which covers the area 500 by 800 km^2 and comprises rhyolites (ca. 70%), andesites and basalts (ca. 30%) [1]. SHRIMP zircon emplacement ages of volcanic rocks in NE Germany range from 303 to 290 Ma with the major peak of the volcanic activity being 299 - 295 Ma [2,3].

The range of εHf and δ^{18}O values in these magmatic zircons in the three sites investigated have been modelled by simple assimilation - fractional crystallization processes of mantle derived magma contaminated by sediments with model ages of ca. 2.1 Ga.

Trace element composition of zircons do not correlate with the isotopic composition, but zircons from the least contaminated sample have different chemical characteristic to that of zircons from more contaminated samples. For example distribution of Hf is bimodal in the least contaminated sample, whereas Hf has intermediate values in the more contaminated ones. The implication is that the least contaminated sample contains zircons from various sources recording different stages of fractional crystallization, whereas more contaminated samples contain one population of zircons, probably crystallized from the surrounding magma.

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Melts in the deep mantle: Insights from first principles molecular dynamics

NICO DE KOKER[1], LARS STIXRUDE[2] AND BIJAYA KARKI[3]

[1]Bayerisches Geoinstitut, Bayreuth, Germany, (nico.dekoker@uni-bayreuth.de)
[2]University College London, UK
[3]Louisiana State University, Baton Rouge, USA

As the primary medium through which planetary differentiation occurs, silicate melts are a key entity in the study of the thermal and chemical evolution of Earth. Over the past few years we have used first-principles molecular dynamics simulations to investigate the liquid state physics of the magnesio-, calsio- and aluminosilicate melts at pressure and temperature conditions relevant to the entire mantle. First-principles methods characterize bonding directly in terms of the electronic charge density computed via density functional theory, and is equally robust at ambient and extreme pressure and temperature conditions. This allows accurate predictions of the physics of melts at extreme conditions to be made.

Liquid state diffusion and thermodynamics have been investigated in detail, with special attention to dependence on pressure, temperature and composition. Comparison to corresponding changes in liquid structure enables us to understand thermodynamic and diffusive behavior in a detailed atomistic context. Our results provide a rigorous test for a new fundamental thermodynamic relation for melts, which we derived to accurately describe liquid state thermodynamics. The relation is unique in that it accounts for electronic free energy contributions and displays the correct limiting behavior at extreme volume and temperature, capturing the thermodynamics of liquid-vapor coexistence.

Our work has allowed for deeper insight into the evolution of terrestrial planets, including the thermal state and mode of crystallization of magma oceans, the possible presence of melt in the deep earth, and their relative buoyancy. This insight in turn acts as a guide for questions to be addressed in the future, as first-principles simulations of systems of larger numbers of atoms and complex chemical compositions representative of natural systems become feasible.