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Inverse Stefan problem - application to geology

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SUMMARY

The growth of zircon crystals in cooling magmas is modelled by the one-phase Stefan problem, with a growth rate that depends on the magma cooling rate. The one-phase Stefan problem is an advection-diffusion equation in a free-boundary domain, where a non-linear boundary condition takes into account different thermodynamic equilibria at the crystal/melt interface. The velocity of the interface is also an unknown of the non-linear problem, which in our case depends on the temperature through the saturation constant and diffusion coefficient of zirconium.

Some rare elements (like e.g. U, Th, Hf) are also incorporated in the crystal at trace concentration. These elements have different temperature-dependent diffusion and partition coefficients. As a consequence their final spatial repartition in the crystal depends on the temperature evolution of the magma during the cooling. The direct problem consists of knowing the magma cooling evolution, and determining the trace elements concentration in the crystal.

The present work proposes to reconstruct the temperature evolution from the measurements of trace elements concentration in natural zircon. For simplicity (and due to available measurements), we assume spherical symmetry, and the one-phase Stefan problem is expressed as a one-dimensional PDE.

The inverse problem is solved by minimizing the L2 misfit between calculated and measured trace element concentrations. The tangent model to the one-phase Stefan problem provides the sensitivity matrix, and the quadratic cost-function is minimized using Gauss-Newton method. The algorithm is tested on two synthetic datasets, and on real data obtained in a zircon crystal from Early Fish canyon tuff eruption. Reconstructed temperature ranges and cooling duration are in good agreement with available petrological interpretation.

Keywords: One phase Stefan problem, inverse problem, accessory minerals, crystal growth

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