

Water contents in the Cenozoic subcontinental lithospheric mantle beneath the Cathaysia block, SE China

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Refractory subcontinental lithospheric mantle (SCLM) is produced by the removal of partial melts from mantle rocks; this process includes the removal of H₂O. The nature and stability of the SCLM are also strongly influenced by hydrous melts and fluids, which affect the physical and chemical properties of mantle minerals and rocks.

Our recent work has focussed on determining the H₂O contents of peridotite xenoliths from the Cathaysia block, SE China using Fourier transform infrared spectrometry (FTIR). The xenoliths consist mainly of nominally anhydrous minerals (NAMs, e.g., olivine, pyroxene) and are direct samples that may reflect the actual H₂O budget of SCLM.

The homogeneity in H₂O distribution within single pyroxene grains, equilibrium partitioning of H₂O between cpx and opx ($D_{\text{cpx/opx}} \approx 2.3$) and correlations between H₂O contents and major elements suggest that the xenoliths preserve the H₂O contents of their mantle source. The average whole-rock water contents calculated from mineral modes is 60±20 ppm. This is much higher than the H₂O contents of peridotites from the North China Craton (average 26±17 ppm). However, it is still low compared to other SCLM inferred from typical cratonic (122±54 ppm) and off-cratonic (81±40 ppm) peridotites.

This medium-dry SCLM can be explained by the refertilization of old lithospheric mantle which has undergone multiple geological events through time, e.g., hydration due to paleo-Pacific plate subduction and massive H₂O extraction during large-scale Late Mesozoic magmatism in SE China. The redox state is another factor in controlling the H₂O contents in the SCLM. This is supported by the negative correlations between pyroxene H₂O contents and spinel Fe³⁺/ΣFe in xenoliths from Niutoushan (Mg#<90). This locality lies astride the Changle–Nan'ao fault, which facilitated the infiltration of peridotites by oxidized fluids or melts rising from the subducting Pacific plate.

Automated fitting of XRD profiles of interstratified phyllosilicates

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Phyllosilicate minerals are common constituents of soils and many rocks, but quantitative analysis of such materials using X-ray diffraction (XRD) is difficult due to the presence of interstratification within many phyllosilicates. Interstratification refers to the occurrence of two or more types of layers in a single crystallite (also termed “coherent scattering domain”). Diffraction from interstratified phyllosilicate minerals has been successfully modeled, and several software codes (e.g., NEWMOD [1], Diffax [2] and Sybilla [3]) have been developed. However, these programs rely on trial-and-error methods, making the results sensitive to user input. FITMOD, an automated parametric fitting program based on Reynolds' [6] methodology and incorporating recent progress in the structures of phyllosilicate minerals, has been developed [4]. The downhill simplex method [5] was applied in FITMOD to minimize the discrepancies between experimental and simulated XRD profiles by simultaneously varying all adjustable model parameters including the chemical composition (e.g., cation content) and structure (e.g., proportion of the two components, crystal-size distribution, stacking order). Both previously simulated and experimental XRD profiles were used to evaluate the performance of FITMOD in terms of the goodness of fit (R_{wp} , R_p), accuracy, as well as efficiency. Fits to simulated profiles yielded values of R_{wp} as low as <0.3%. Very good fits to experimental profiles were also obtained, with results in excellent agreement with previously published data. Importantly, final results were quite insensitive to starting model parameters, and the method allows fitting with minimal operator intervention.

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