

Upper mantle and metasomatic processes on Eastern Moroccan Anti-Atlas

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The Jbel Saghro alkaline complex was emplaced close to the eastern edge of the Moroccan Anti-Atlas. Two types of nephelinite were recognized in the northern part [1]: a) olivine-rich nephelinite (between 9.6 and 7.5 ± 0.1 Ma), b) pyroxene nephelinites (2.9 ± 0.1 Ma) bearing metasomatised peridotite xenoliths [2].

In the nephelinites of Jbel Saghro there are mantle spinel lherzolites and spinel harzburgites enriched in LREE relative to HREE and have U-shaped REE patterns, with strongly depleted middle REE. Since [3], U-shaped REE patterns are generally attributed to chromatographic effects resulting from interstitial percolation of small melt fractions through LREE-depleted peridotites. However, the Foum El Kouss (North of the South-atlasic-fault) xenoliths display more complex distributions of trace elements, are enriched in LILE (Rb, Ba, Th, LREE and Sr) and shows negative anomalies of HFSE (Nb, Ta, Zr and Hf). Such trace-element distribution is generally attributed to carbonate melt metasomatism [4].

In pyroxene nephelinite there are megacrysts of green diopside rich in fluid inclusions of CO₂, olivine, chromite (Cr/(Cr+Al) = 0.72 to 0.79), interstitial anorthoclase (Ab₅₂ - Ab₅₆, Or₄₁ - Or₄₅, An₀₁ - An₀₂) and apatite phases.

The Mössbauer spectroscopy gives more precise evaluation of Fe³⁺ in spinels [5] and the oxygen fugacity in peridotitic xenoliths which were higher ($\log(fO_2) - \log(fO_2)$) FMQ averaging 0.18 to 0.25).

[1] Ibhi, Nachit, Abia & Hernandez (2002) *Bull. Soc. Géol. France* **173**, 37–43. [2] Ibhi & Nachit (1999) *Géol. Méditerranéenne* **XXXVI**, 1/2, 19–28. [3] Navon & Stopler (1987) *J. Geol.* **95**, 285–307. [4] Rudnick, McDonough & Chappel (1993) *Earth Planet. Sci. Letters* **114**, 463–475. [5] Ibhi, Khatib & Hernandez (1999) *Ann. Chim. Sci. Mat.* **24**, 487–492.

Interfacial morphology of iron oxide α -Fe₂O₃ in aqueous equilibrium studied with *ab initio* thermodynamics

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Ab initio thermodynamics, used to study interfacial energetics for metal oxides in equilibrium with gas phase constituents, has been previously employed to understand surface morphologies over a wide range of gas pressures and temperatures. These methods are applied to the 1 $\bar{1}$ 02 (r-cut) surface of hematite, and have shown good agreement with experimental results.

We have extended these methods to application over a varying range of aqueous conditions. This allows the modelling of surface equilibrium with dissolved surface constituents at varying temperatures, pH conditions and redox potentials.

The applicability of these studies can be wide ranging. Typically DFT methods are used in cooperation with solvation models to understand free energies of the system constituents. Further analysis of the results is necessary to ascertain the range of applicability for this aqueous *ab initio* thermodynamic model, and these studies motivate further extension to include other dissolved cations and anions.