

First-principle partitioning and disequilibrium of chromium in garnet - clinopyroxene assemblage

AIM: partitioning of Cr to test equilibrium between garnet and clinopyroxene

CONTEXT OF THE STUDY

Using partition coefficients is extremely useful to model melting processes and fluid-rock interactions. However, partition coefficients values remain scarce in regard of their sensitivity to mineral composition and to the variability of mineral composition.

In addition, the inferred equilibrium between phases is not necessarily reached, even in high-grade metamorphic conditions associated to melting. *Disequilibrium may dramatically hamper the effective mobility of species and lead to element distribution far from the predicted values.*

This contribution aims at estimating partition coefficients for chromium (Cr) between garnet and clinopyroxene, and testing them in natural rocks of various metamorphic grades. As a poorly mobile trivalent element, *Cr is chosen as a proxy to rare earth elements.*

A COMBINED APPROACH

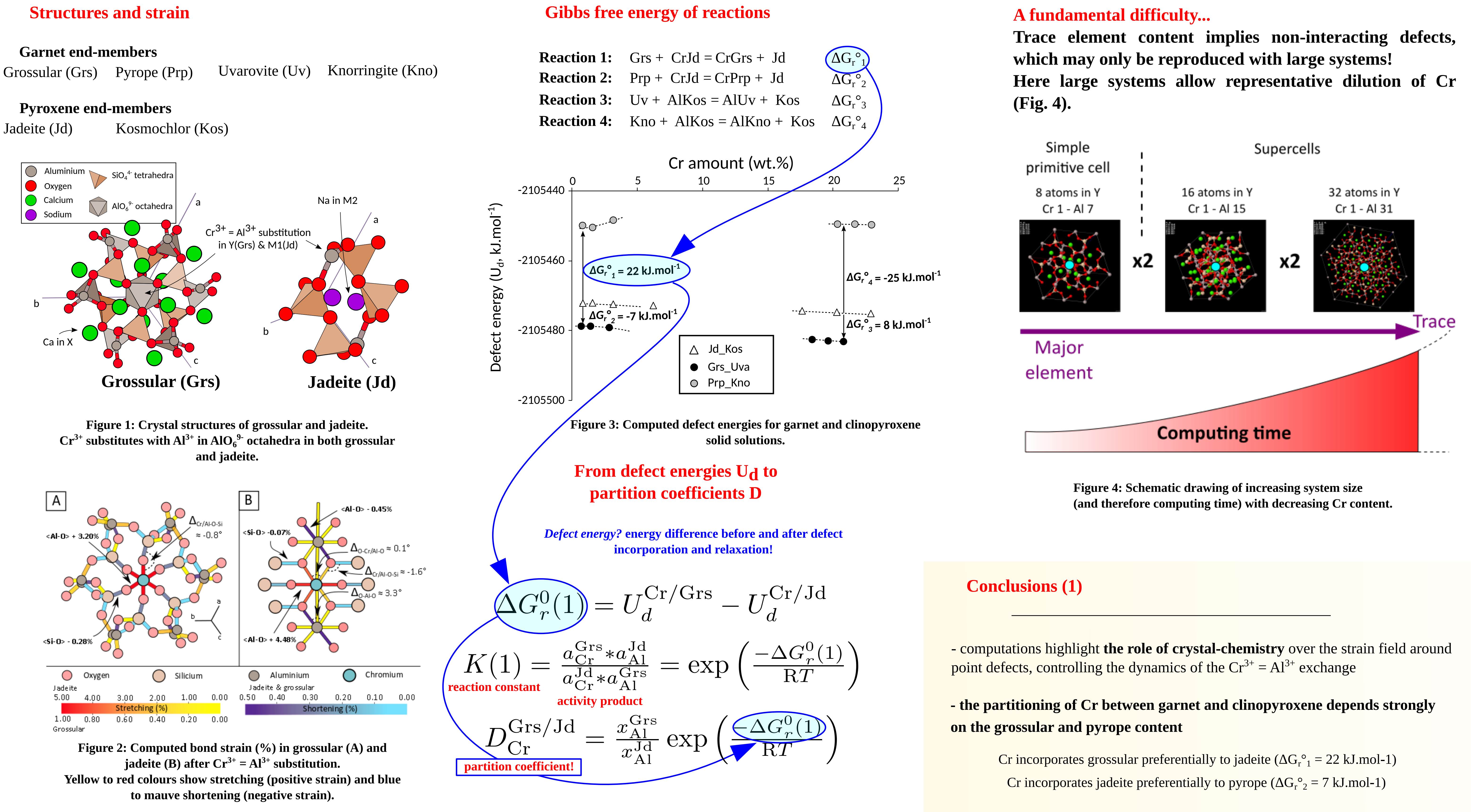
Theoretical partition coefficients for Cr between garnet and clinopyroxene are calculated *ab initio* from structures where Cr³⁺ is modelled as a defect in Al³⁺ sites using CRYSTAL17 (Dovesi et al., 2009, 2018) and the thermodynamic description of Dubacq and Plunder (2018).

The distribution of Cr in natural samples is measured with *electron microprobe* (EPMA) in garnet-clinopyroxene assemblages containing 10s to 10 000s of ppm of Cr. Element mapping is crucial for correct interpretation of zoning.

Comparison between predicted and measured partition coefficients allows estimating the deviation from equilibrium.

For more, check out: *Figowy et al., Partitioning of chromium between garnet and clinopyroxene: first principles modelling versus metamorphic assemblages*, accepted with minor revisions in *European Journal of Mineralogy*

Ab initio modelling of Cr in garnet and clinopyroxene



APPLICATION: Mapping trace and minor Cr content shows disequilibrium

