Dissolved quartz in supercritical water: Insights from *ab initio* molecular dynamics simulations

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We have carried out ab initio molecular dynamics (AIMD) simulations of SiO_2 in supercritical water at temperatures of 900 K and 1200 K and a pressure of 1.5 GPa at concentrations of 5 and 16 wt% [1]. The different polymeric forms monomer (SiO_4H_4), dimer ($Si_2O_7H_6$), and trimer ($Si_3O_{10}H_8$) are found to be stable during the 10 ps time span of the simulations. A Raman spectrum recorded of the SiO_2/H_2O fluid in a diamond-anvil cell, comparable to spectra presented in the literature [2-4], has been compared to the vibrational spectra obtained from the AIMD simulations by Fourier transform of the velocity autocorrelation function. Determination of relative monomer and dimer concentrations from the relative intensities of the Raman bands is found to be problematic as both species contribute to the most intense band [1]. The mechanism of dimerisation and the associated free energy profile along the reaction coordinate have been obtained using coordination-constrained AIMD together with thermodynamic integration [5-7]. The calculated relative free energies of monomer and dimer suggest that both species should coexist at high P, T conditions.

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Characterization of carbon materials in metasediment hosted gold deposits (NW Portugal) by micro-Raman spectroscopy

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Introduction

Micro-Raman spectroscopy (MRS) is a powerful technique used for the characterization of dispersed carbon materials (DCM) in metasediments, giving information about their evolution during metamorphic process (graphitization).

The aim of this study is to characterise the DCM by MRS in order to estimate the maximum P-T conditions reached during regional metamorphism.

Results

Using a Labram Dilor-Jobin Yvon spectrometer attached to an Olympus microscope and an excitation of 633 nm lines of a He-Ne laser, MRS analyses were performed on samples from metasedimentary rocks of borehole cores obtained during an exploration survey at Três-Minas roman open-pits. The criterion of sample selection was the presence of non-outcroping black-carbonate lithologies. Four samples were studied and ten Raman spectra were recorded for each sample.

The first-order Raman spectrum of DCM exhibit a graphite G band at around 1580 cm^{-1} and defect bands D2 around 1616 cm^{-1} and D1 around 1332 cm^{-1}. For the second-order spectrum a symmetric S1 band and a broad S2 band appear near 1700 cm^{-1} and 1900 cm^{-1}, respectively (Fig.1).

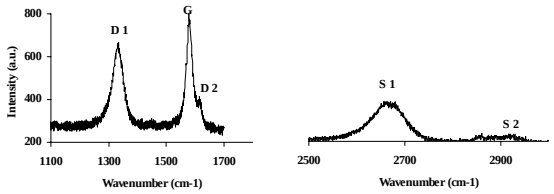

Figure 1: Representative Raman spectra obtained for DCM at Três-Minas.

After the calculation of the Raman parameters for the different first-order Raman spectrum and using Beyssac *et al*. (2002) graphite geothermometer in order to estimate the peak temperature of metamorphism the obtained temperatures are in the range of 360 to 490 ºC.

This data will be further compared and constraint with others geothermometers, fluid inclusion and mineral assemblages.

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