Effect of experimental, optical, and geometrical variables on the laser heating of inclusions during Raman spectroscopic analysis

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Raman spectroscopy for fluid, melt, and mineral inclusions provide direct insights into the physicochemical conditions of the environment surrounding the host mineral at the time of trapping. However, the obtained Raman spectral characteristics such as peak position are modified due to the local temperature enhancement of the inclusions by the excitation laser, which may lead to systematic errors and incorrect conclusions if the effect is not corrected. Despite the potentially non-negligible effect of laser heating, laser heating coefficient (B) ($^{\circ}C/mW$) of inclusions have remained unsolved. Here, we determined B by two independent experiments and heat transport simulation to evaluate how various parameters such as experimental conditions, mineral properties, and inclusion geometry affect B of inclusions. To determine the influential experimental parameters on laser heating, we measured B of a total of 21 CO₂-rich fluid inclusions hosted in olivine, orthopyroxene, clinopyroxene, Cr-spinel, and quartz. Our results revealed that the measured B of fluid inclusions in spinel show highest (approx. 6° C/mW) and those in quartz is lowest (approx. 1×10^{-2} °C/mW), consistent with previous inferences and our simulation results that absorption coefficient of the host mineral ($a_{spinel} = 20$ and $a_{quartz} = 0.02$ cm⁻¹) is linearly correlated with B and is the most influential parameter when absorption coefficient of the host mineral (a_h) is larger than those of a inclusion (a_{inc}) . Furthermore, our results show that both inclusion size and depth have little impact, whereas thickness and radius of host mineral have significant influence on B . This suggests that the differences in inclusion size and depth to be analyzed in a given sample do not cause any systematic errors in the Raman data due to laser heating, but the host radius and thickness, which can be adjusted to some extent at the time of sample preparation, can be the cause of systematic errors between samples.

Our results show that even with a laser power of 10 mW, which is typical for inclusion analysis, the inclusion temperature rises to tens to one-hundred of degrees during the analysis depending especially on the host mineral geometry and optical properties. Therefore, correction of the effect of heating will be necessary to obtain reliable data from the Raman spectroscopic analysis of inclusions. In this study, we propose some correction methods for the non-negligible effect of laser heating.

Keywords: Raman spectroscopy, Laser heating, Fluid inclusion, Mineral inclusion, Melt inclusion, Finite element method