Attenuated total reflection infrared (ATR–IR) spectroscopy of antigorite, chrysotile, and lizardite

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Attenuated total reflection infrared (ATR–IR) spectroscopy allows measurements to be made directly from the surface of one-sided, diamond polished thin sections of geological samples. This method greatly reduces the sample preparation time when compared to other IR spectroscopy methods and opens the possibility of using infrared spectroscopy to study thin-section scale microstructures. ATR–IR spectroscopy of antigorite, chrysotile, and lizardite in samples from the Mt. Shiraga serpentinite body, central Shikoku, SW Japan, reveals clear spectral differences in the 650–1250 cm\(^{-1}\) region associated with the vibration of the Si–O bonds in SiO\(_4\) tetrahedra and in the 3300–3750 cm\(^{-1}\) region associated with the vibration of the O–H bond in MgO\(_2\)(OH)\(_4\) octahedra. A data-processing algorithm developed in this study allows the absorbance intensity and wavenumber of a particular absorbance peak to be used to create serpentine mineral phase maps based on the highest intensity Si–O absorbance bands for antigorite, chrysotile, and lizardite. Our methodology can be used to map serpentinite microstructures in thin sections illustrating the potential of ATR–IR as a relatively un-explored analytical tool in petrological studies. A combination of ATR–IR and electron microprobe data shows that for antigorite the wavenumber of the O–H absorbance band is correlated with the Fe content. Metamorphic reactions of serpentine minerals play a key role in the hydrodynamics of the earth’s lithosphere, and the new information on serpentine mineral hydroxyl group behavior obtained by applying the technique outlined in this study are of great potential interest to researchers in a wide range of different fields.

Keywords: Attenuated total reflection infrared (ATR–IR) spectroscopy, ATR–IR mapping, Serpentine minerals, Antigorite, Chrysotile, Lizardite

INTRODUCTION

Serpentine minerals, antigorite, chrysotile, and lizardite are hydrous sheet silicates that contain approximately 13 wt% of water. They are the main constituents of serpentinite rocks, which are formed when ultramafic rocks are hydrated. Metamorphic reactions of serpentine minerals play an important role in many subduction zone processes. For instance, it is thought that the dehydration of serpentine minerals can trigger partial melting in the subduction zone (Ulmer and Trommsdorff, 1995; Hattori and Guillot, 2003; Rüpeke et al., 2004). There is also evidence that fluids released from serpentine minerals could be the cause for seismicity occurring in subduction zones at intermediate depths (~ 50–300 km) (Peacock, 2001; Dobson et al., 2002; Hacker et al., 2003; Jung et al., 2004).

Different serpentine minerals are stable in different metamorphic conditions, and their formation is controlled by \(P–T\) conditions, kinetic factors, and the composition of the metasomatic fluid (Evans, 2004). Furthermore, the differing coefficients of friction of serpentine minerals, especially the low coefficient of friction for chrysotile, have a significant impact on the faulting behavior of serpentinite rocks (Scholz, 2019). Therefore, reliable identification of antigorite, chrysotile, and lizardite and microstructural analysis of natural serpentinite samples are an important part of developing a better understanding of the metamorphic processes and fault zone dynamics of serpentinite rocks. However, this kind of research is hampered by a limited range of easy to use techniques that can distinguish different types of serpentinite minerals in standard petrographic thin sections.

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Identifying antigorite, chrysotile, and lizardite in thin section using a polarizing microscope or an electron microprobe can be challenging due to the similarity of their optical properties and chemical composition. A simplified general chemical formula for serpentine minerals is \( X_2Y_3O_5(OH)_4 \), where \( X \) is usually occupied by Mg and \( Y \) by Si. However, natural samples exhibit considerable compositional variation. For instance, Mg can be substituted by various cations such as Fe\(^{2+}\), Fe\(^{3+}\), Al, Cr, Ni or Mn and Si by cations such as Al and Fe\(^{3+}\) (Moody, 1976; O’Hanley and Dyar, 1993).

Different types of serpentine show somewhat different ranges of chemical composition, but there is a large overlap and the main distinguishing feature is the crystal structure. The basic structure of all serpentine minerals is comprised of sheets of SiO\(_4\) tetrahedra that are covalently linked to a layers of MgO\(_2\)(OH)\(_4\) octahedra (Evans et al., 2013). In each of the main types of serpentine mineral, sheets of these basic units are stacked and bound together in a specific way forming a distinct crystal structure. Antigorite has a wavy, layered structure in which the orientation of the tetrahedral SiO\(_4\) layers is periodically reversed, chrysotile forms layered tubular structures that give chrysotile its typically fibrous appearance, and lizardite has a simple, layered structure.

Vibrational spectroscopic methods—Raman and infrared spectroscopy—can be used to identify minerals through observing the characteristic molecular vibration of the different functional groups. Raman spectroscopy and infrared spectroscopy are complementary methods as vibrational modes that are infrared active cannot be Raman active and vice versa. Several Raman studies have documented the characteristic Raman spectra of antigorite, chrysotile, and lizardite (e.g., Rinaudo et al., 2003; Enami, 2006). However, Raman spectroscopy of serpentine minerals tends to suffer from fluorescence effects (Groppo et al., 2006), which can make mineral identification more difficult.

Several previous studies (e.g., Farmer, 1974; Post and Borer, 2000; Šontevska et al., 2007) also describe the infrared spectra of serpentine minerals. Nearly all of these previous studies use transmission IR spectroscopy. Transmission IR spectroscopy requires that samples are either ground into a fine powder and pressed into discs thus losing microstructural information, or made into double polished thin sections of a specific thickness. In the case of serpentine minerals, the sample needs to be thinner than about 20 micrometers for a successful measurement. Preparation of such samples is time consuming and technically challenging.

Attenuated total reflection infrared (ATR-IR) spectroscopy is an alternative IR method, which utilizes an internal reflection element (IRE), also known as an ATR crystal, that allows measurements to be made directly from the surface of a normal polished thin section, which significantly reduces the time needed for sample preparation. In this paper, we studied the suitability of the ATR-IR method to distinguish antigorite, chrysotile, and lizardite. In addition, we applied the ATR-IR method to map areas with multiple mineral phases in order to demonstrate the possibilities of this technique in analyzing thin section scale microstructures.

**METHODS**

**Attenuated total reflection infrared (ATR-IR) spectroscopy**

The ATR-IR spectra was measured with a Fourier transform infrared (FTIR) spectrometer (Nicolet iS10 by Thermo Fisher Scientific) equipped with a mercury cadmium telluride (MCT) detector at the Petrology Laboratory at Nagoya University. The FTIR spectrometer was attached to an infrared microscope (Nicolet Continuum by Thermo Fisher Scientific) and the instrument was purged with dry air and cooled by liquid nitrogen. The measurements were made using a germanium ATR crystal with an angle of incidence of 28° and refractive index of 4. The individual spot measurements were made from thin sections polished by diamond paste (grainsize 1 \( \mu \)m). The thin sections used for mapping were further polished using colloidal silica. 100 \( \times \) 100 \( \mu \)m aperture, which corresponds to a 25 \( \times \) 25 \( \mu \)m spot size, was used for the ATR-IR measurements. The step size for ATR-IR mapping varied between 25–50 \( \mu \)m. 32 scans were recorded for each individual measurement. In order to limit the mapping time, only 16 scans were recorded for each measurement during the ATR-IR mapping. A spectral range of 650–4000 cm\(^{-1}\) was recorded with a 4 cm\(^{-1}\) resolution for all ATR-IR measurements.

**Electron microprobe (EMPA)**

The compositions of the serpentine minerals were analyzed quantitatively by wavelength-dispersive spectrometer (WDS) by an electron probe microanalyzer (JXA–8900R; JEOL) at the Petrology Laboratory of Nagoya University. The accelerating voltage of individual quantitative measurements was set to 15 kV with a 12 nA beam current and a 5 \( \mu \)m beam spot diameter. For mapping, the accelerating voltage and the beam current were set to 20 kV and 100 nA, respectively. The step size used for mapping was 5 \( \mu \)m. The correction factors calculated by Kato (2005) were employed for matrix correction.
SAMPLE DESCRIPTION

Samples analyzed for this study are from the Mt. Shiraga serpentinite body, which is located in the Sanbagawa metamorphic belt in central Shikoku, SW Japan. The originally dunitic rocks of mantle wedge origin have been completely serpentinized and are surrounded by mafic, pelitic, and siliceous schists (Kawahara et al., 2016).

The most common serpentinite mineral found in the Mt. Shiraga serpentinite body is antigorite. Antigorite is typically platy (Fig. 1a) but can also have a fibrous appearance. Chrysotile and lizardite were formed after the main antigorite-dominated serpentinization, and they are present in a limited number of samples, mostly found between the contact zone of the serpentinite body and the surrounding metasedimentary rocks. The chrysotile found in the Mt. Shiraga serpentinite body is characteristically fibrous (Fig. 1b). Lizardite is fine-grained and occurs in anastomosing veins, which appear reddish (Fig. 1c) due to the existence of iron oxides. Remarkably, several samples contain all three serpentine minerals (Fig. 1d). These samples are of particular interest as they contain various reaction textures between serpentine minerals, which can be studied in detail using infrared spectroscopy. Raman spectroscopy was used to make the preliminary mineral identifications of the serpentinite minerals using the characteristic peaks proposed by Enami (2006). The Raman spectra of antigorite, chrysotile, and lizardite presented in this paper (Fig. 2) were measured from the same samples as the representative ATR-IR spectra for each respective serpentinite mineral. In addition to the three serpentinite minerals, the samples also contained olivine (of metamorphic origin), magnetite, brucite, and Cr-spinel as well as some other minor accessory minerals, such as talc.

RESULTS

ATR-IR spectra of serpentine minerals

In order to choose representative spectra of antigorite, chrysotile, and lizardite, we selected 30 ATR-IR measurements (10 measurements of each mineral) and determined the wavenumber value of each absorbance band using the spectral peak fitting software PeakFit 4.12. From these 30 measurements, we chose the most representative spectra of antigorite, chrysotile, and lizardite to present in this study (Fig. 3). The measurement locations of these ATR-IR spectra of antigorite, chrysotile, and lizardite are shown in Figure 1. All three serpentine minerals have two dominant vibrationally active domains in their crystal structure, which absorb radiation in two distinct parts of the mid-infrared region that was measured for this study (650–4000 cm⁻¹). Detailed wavenumber values of all absorbance bands that were detected are listed in Table 1 along with results from previous IR studies of serpentine minerals made using the transmission IR method.

The lower wavenumber region (650–1250 cm⁻¹) is associated with the vibration of the Si-O bonds in the SiO₄ tetrahedra of serpentine minerals (Deer et al., 2009). In this region, the biggest difference between the three serpentine minerals is the position of the highest intensity absorbance band. The highest intensity absorbance bands of antigorite, chrysotile, and lizardite are at ~ 959, ~ 941, and ~ 930 cm⁻¹, respectively. Antigorite also has several low-intensity peaks in the low wavenumber region (650–1250 cm⁻¹) that are not present in the spectra of chrysotile and lizardite. These absorbance bands are related to various lower energy Si-O vibrational modes (Šontevska et al., 2007) caused by the complex undulating crystal structure of antigorite.

The high wavenumber region (3300–3750 cm⁻¹) is associated with the vibration of the O-H bond in the MgO₅(OH)₄ octahedra. In this region, the largest difference between the serpentine minerals is in the absorbance intensity and the overall number of absorbance peaks. In addition to the main absorbance peak at 3671 cm⁻¹, antigorite has 4 subsidiary low-intensity peaks in the 3300–3750 cm⁻¹ region. Mellini et al. (2002) suggest the main antigorite peak is related to the inner O-H stretching, and that the lower wavenumber peaks are related to variations in the O-H bond strength, which can be caused by octahedral substitutions of Mg by other cations. The chrysotile spectrum in this region is characterized by two peaks at ~ 3680 and ~ 3643 cm⁻¹, which are related to the inner and outer stretching vibration of the O-H bond (Viti and Mellini, 1997). The 3300–3750 cm⁻¹ region of lizardite is characterized by a sharp main absorbance peak at 3683 cm⁻¹, which is also related to in-phase vibrations of O-H groups (Balan et al., 2002a).

Chemical compositions of serpentine minerals

The chemical compositions of the representative antigorite, chrysotile, and lizardite are shown in Table 2. Antigorite is enriched in silicon in comparison to chrysotile and lizardite. This is because the crystal structure of antigorite can accommodate slightly more silicon due to the periodic reversals of the SiO₄ tetrahedra in antigorite (Evans et al., 2013). Other minor compositional differences that we observed are: the higher aluminum content of chrysotile and the higher iron content of lizardite, which might be partly caused by the iron oxides in the lizardite veins. These compositional variations are within

ATR-IR spectroscopy of serpentine minerals
the limits of regular serpentine mineral compositions published previously (e.g., Brindley and Wan, 1975; Peacock, 1987).

**ATR–IR mapping**

In order to examine the variation of serpentine mineral absorbance band wavenumber values in more detail, we developed an algorithm to process the ATR–IR mapping data. The algorithm uses the ‘findpeaks’ function, available in several software packages for numerical–analysis, to determine the wavenumber value and intensity of the highest intensity absorbance band in a set region of the ATR–IR spectra (Figs. 4a and 4b).

*Figure 1.* Thin section images of serpentine minerals from Mt. Shiraga serpentinite body taken in cross polarized light (XPL) and plane polarized light (PPL). (a) Antigorite from sample NSY7–15, XPL. (b) Chrysotile vein that also contains antigorite in a matrix of antigorite and olivine. Sample NSY5–7, XPL. (c) Iron–oxide stained anastomosing lizardite veins running through a matrix of antigorite, olivine and magnetite. Sample KSY64, PPL. (d) A reaction zone of co–existing antigorite, lizardite and chrysotile with fine–grained olivine and magnetite. Sample KSY71, PPL. Atg, antigorite; Ctl, chrysotile; Lz, lizardite; Ol, olivine; Mgt, magnetite. The measurement locations of the ATR–IR spectra of antigorite, chrysotile and lizardite presented in this study are indicated.
Since each serpentine mineral has a characteristic highest intensity Si-O absorbance band, it is possible to use this algorithm to create serpentine mineral phase maps (Fig. 5). In addition to antigorite, chrysotile, and lizardite, the sample used in this study also contains a significant amount of olivine and some magnetite. The highest ATR-
IR absorbance peak of olivine is at \( \approx 866 \text{ cm}^{-1} \), and it is included in the calculations (Fig. 4a). Magnetite does not have a distinct absorbance band in the 650–4000 cm\(^{-1}\) range (Chamritski and Burns, 2005), and thus the locations with magnetite are left blank in Figures 5 and 6.

In addition to mineral phase mapping, it is possible to use ATR–IR mapping to examine spectral variation of a single mineral. In order to illustrate this, we mapped a sample from Mt. Shiraga with antigorite veins running through an antigorite matrix (Fig. 6a). In this sample, the wavenumber values of the highest intensity O–H absorbance peak vary between the veins and the matrix (Fig. 6b). The wavenumber values of O–H absorbance bands of antigorite grains in the matrix are between 3660 and 3666 cm\(^{-1}\), while the antigorite grains in the veins tend to show higher values between 3666 and 3670 cm\(^{-1}\). To find out if the differences in the wavenumber values of O–H absorbance bands might be caused by chemical composition, we mapped the chemical compositions of the sample using an electron microprobe. We measured the distribution of Si, Al, Mg, Fe, Mn, Cr, Ni, and Ti in the sample and found that variations in the Fe concentration (Fig. 6c) were correlated with the O–H absorbance values of antigorite (Fig. 6b). Quantitative mi-

| Antigorite                  | This study | Post and Borer, 2000 | Šontevska et al., 2007 | Mellini et al., 2002 | Farmer, 1974 |
|-----------------------------|-----------|----------------------|------------------------|----------------------|--------------|
| 959                         | 990       | 987                  | 983                    | 994                  |              |
| 1035                        | 1076      | 1083                 | 1082                   | 1077                 |              |
| 1072                        | -         | -                    | -                      | -                    |              |
| 1204                        | 1202      | 1205                 | -                      | -                    | 1205         |
| 3572                        | 3568      | -                    | 3561                   | -                    |              |
| 3618                        | 3620      | -                    | 3622                   | -                    |              |
| 3637                        | 3652      | -                    | 3637                   | -                    |              |
| 3671                        | 3673      | 3678                 | 3678                   | 3675                 |              |
| 3700                        | 3697      | 3699                 | 3700                   | 3700                 |              |

| Chrysotile                  | This study | Post and Borer, 2000 | Šontevska et al., 2007 | Anbalagan et al., 2010 | Viti and Mellini, 1997 |
|-----------------------------|-----------|----------------------|------------------------|------------------------|------------------------|
| 941                         | 958       | 961                  | 965                    | 956                    | 956                    |
| 1024                        | 1068      | 1078                 | 1079                   | 1072                   | 1072                   |
| 1073                        | -         | -                    | -                      | -                      | -                      |
| 3557                        | -         | -                    | -                      | -                      | -                      |
| 3643                        | 3647      | 3646                 | 3648                   | 3640                   | 3640                   |
| 3680                        | 3685      | 3688                 | 3689                   | 3688                   | 3688                   |

| Lizardite                   | This study | Post and Borer, 2000 | Balan et al., 2002a | Mellini et al., 2002 | Viti and Mellini, 1997 |
|-----------------------------|-----------|----------------------|---------------------|----------------------|------------------------|
| 930                         | 959       | 948                  | 951                 | 952                   | 952                    |
| 1043                        | 1075      | 1080                 | 1084                 | 1088                   | 1088                   |
| 1073                        | -         | -                    | -                    | -                      | -                      |
| 3545                        | 3558      | 3584                 | 3585                 | 3586                   | 3586                   |
| 3651                        | 3653      | 3645                 | 3651                 | -                      | -                      |
| 3683                        | 3685      | 3684                 | 3684                 | 3685                   | 3685                   |
| 3703                        | -         | 3703                 | 3703                 | -                      | -                      |

| Mineral Sample              | Antigorite | Chrysotile | Lizardite | | |
|-----------------------------|------------|------------|-----------| | |
| SiO₂ w%                     | 44.27      | 41.60      | 39.29     | | |
| TiO₂                        | 0.00       | 0.03       | 0.03      | | |
| Al₂O₃                       | 0.51       | 1.63       | 0.01      | | |
| Cr₂O₃                       | 0.33       | 0.38       | 0.00      | | |
| FeO                         | 1.04       | 2.03       | 3.89      | | |
| MnO                         | 0.03       | 0.02       | 0.08      | | |
| MgO                         | 40.42      | 40.18      | 40.21     | | |
| NiO                         | 0.14       | 0.08       | 0.25      | | |
| Total                       | 86.75      | 85.95      | 83.75     | | |

| Numbers of ions on the basis of O = 7 | | | | | |
| Si  | 2.05 | 1.96 | 1.94 | | |
| Ti  | 0.00 | 0.00 | 0.00 | | |
| Al  | 0.03 | 0.09 | 0.00 | | |
| Cr  | 0.01 | 0.01 | 0.00 | | |
| Fe  | 0.04 | 0.08 | 0.16 | | |
| Mn  | 0.00 | 0.00 | 0.00 | | |
| Mg  | 2.79 | 2.83 | 2.95 | | |
| Ni  | 0.01 | 0.00 | 0.01 | | |
| Sum cation                   | 4.93       | 4.98       | 5.06      | | |
| Mg#                          | 0.986      | 0.972      | 0.949     | | |

Table 1. Representative ATR–IR absorbance band values (in cm\(^{-1}\)) of serpentine minerals and the corresponding transmission IR absorbance band values from previous studies.

Table 2. Chemical composition of the representative ATR–IR spectra of antigorite, chrysotile, and lizardite.
croprobe analyses show that Fe contents of antigorite range from 0.05 to 0.09 pfu with lower concentrations in the veins than in the matrix (Fig. 6d).

**DISCUSSION**

The ATR–IR method has proven to be a reliable and simple method to measure the infrared spectrum of serpentine minerals. There are clear differences between the three serpentine minerals in the wavenumber values and overall shape of the spectra (Fig. 3). For instance, the highest intensity absorbance bands of antigorite, chrysotile, and lizardite have characteristic values of ~ 959, ~ 941, and ~ 930 cm⁻¹, respectively. The differences observed between the highest intensity absorbance bands of the three serpentine minerals are due to different Si–O bond energies, which are the result of varying bond lengths related to the contrasting crystal structures of different serpentine minerals (Mellini et al., 2002).

The majority of the ATR–IR spectroscopy absorbance bands of serpentine minerals recognized in this study are in good agreement with previously published studies (Table 1). A larger number of low-intensity bands in the ATR–IR spectra were observed in this study than in some of the previous transmission IR studies. This could be due to the difficulty of distinguishing the lower absorbance peaks from background noise or simply due to the difference in how previous workers catalogued their observations. The high-intensity absorbance bands in the transmission IR spectra tend to have higher wavenumber values than the high-intensity ATR–IR absorbance bands. For example, in the transmission IR studies...
the highest intensity absorbance band of antigorite has a wavenumber value nearly 30 cm\(^{-1}\) higher than the corresponding band observed in the ATR–IR spectra. The differences in the serpentine mineral absorbance band positions observed between the ATR–IR measurements and the previously published transmission IR studies are caused by the different ways in which light interacts with the sample in the different infrared spectroscopy methods. Spectral distortions are common in transmission IR measurements made using KBr pellet samples because electrostatic interactions between different particles in a powdered sample influence the whole macroscopic electric field of the sample (Balan et al., 2011). The ATR–IR method is also susceptible to spectral distortions, because the difference in refractive indices of the sample and the ATR crystal causes anomalous dispersion of infrared radiation at the interface resulting in shifts of the spectral peaks (Woods and Bain, 2014). This means that the ATR–IR spectra of serpentine minerals will be slightly different when measurements are made with ATR crystals with different refractive indices.

This study clearly highlights some of the difficulties faced when trying to distinguish different serpentine minerals from each other using polarizing microscope techniques and how ATR–IR mapping can resolve some of these issues. For example, in the thin section image of sample KSY71 (Fig. 5a) both the lizardite and antigorite domains show similar discoloration by iron–oxides, and there is no clear contrast in the associated crystal habits meaning that the boundary between these two mineral domains is unclear. However, an overlay of the ATR–IR map on the thin section image (Fig. 5c) clearly reveals the location of the boundary. The inverse situation can also be observed. The boundary between chrysotile and lizardite domains appears sharp in the thin section image of sample KSY71 (Fig. 5a). However, the ATR–IR map reveals the presence of a boundary zone between the two domains with a symplectitic intergrowth of lizardite and chrysotile (Fig. 5b). On closer inspection, symplectitic intergrowths can also be observed in some other sections.
of the boundary between chrysotile and lizardite (Fig. 5a). Such intergrowths in serpentine minerals have been previously reported (Bailey and Banerjee, 1995; Dódony and Buseck, 2004), and the ATR–IR technique offers a simple way to recognize and image them. We also note that although coloration and other features may allow different types of serpentine to be distinguished under the polarizing microscope, these features are not consistent between different samples and some other method, such as that proposed here, is required to identify the particular mineral species.

Other factors that can also have an effect on the observed infrared spectra are variations in crystallographic orientation and compositional changes. Balan et al. (2002b) studied the effect of crystallographic orientation on the ATR–IR spectra of chrysotile. According to their observations the wavenumber value of the highest intensity absorbance peak of chrysotile varied between 938–957 cm$^{-1}$ depending on the crystallographic orientation. Such large variation was not observed in this study, perhaps suggesting that chrysotile in our sample has a strong crystallographic preferred orientation.

Studying variations in serpentine mineral O–H absorbance bands is of particular interest to many researchers as it can further our knowledge of the hydration and dehydration reactions of serpentinites. Figure 6 illustrates how changes in chemical composition can affect the O–H absorbance bands of serpentine minerals. A comparison between the ATR–IR map of wavenumber values of the O–H absorbance band of antigorite and the EMPA map of Fe distribution shows a close correspondence (Figs. 6b and 6c). Areas with high iron contents (~ 0.09 pfu) have up to 10 cm$^{-1}$ lower O–H absorbance values than areas with lower iron contents (~ 0.05 pfu) (Figs. 6b and 6d). This observation is in line with the suggestion made by Mellini et al. (2002) that the octahedral substitution of Mg by Fe$^{2+}$ would shift the main O–H absorbance band of antigorite to lower wavenumbers. Other elemental substitutions for example Si by Al, have also been observed to have a large impact on the IR spectra of serpentine minerals (e.g., Serna et al., 1979; Velde, 1980). However, any other clear correlations between the ATR–IR and EMPA maps were not observed in this study.

While ATR–IR maps of individual absorbance bands are useful in illustrating spectral variations and studying their connection to serpentine microstructures, it is better to examine the whole serpentine mineral spectrum when making a mineral identification. As mentioned above, the intensities and wavenumber values of individual absorbance bands can be affected by several factors, such as variations in mineral microstructure, crystallographic orientation, and chemical composition, and more work is necessary to study how such factors affect the ATR–IR spectra of serpentine minerals.

**CONCLUSIONS**

Our study shows that the ATR–IR method is well suited to the in situ identification of serpentine minerals. The ease of making measurements directly from the surface of a thin section means the ATR–IR method has a considerable as yet largely un-explored potential in the field of mineral spectroscopy. This study also demonstrates that using a data-processing algorithm can be useful in teasing out small-scale fluctuations in absorbance intensities and wavenumber values of individual absorbance peaks in large ATR–IR mapping datasets. Such an approach shows that Fe concentration can have a noticeable effect on the wavenumber values of antigorite O–H absorbance bands. More detailed ATR–IR mapping of serpentine microstructures, such as veining, in combination with other petrological methods, such as EPMA mapping, can further improve our knowledge of the serpentinization processes.

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