

**ACCURACY OF DERIVED PLAGIOCLASE COMPOSITIONS FROM THERMAL EMISSIVITY SPECTRA OF MULTI-COMPONENT MIXTURES OF PURE PLAGIOCLASE.** K. A. Milam<sup>1</sup>, H. Y. McSween, Jr.<sup>1</sup>, J. E. Moersch<sup>1</sup>, and P. R. Christensen<sup>2</sup>, <sup>1</sup>Planetary Geosciences Institute, Dept. of Earth & Planetary Sciences, Univ. of Tennessee, 306 EPSB, Knoxville, TN 37996-1410 (kmilam@utk.edu), <sup>2</sup>Dept. of Geological Sciences, Arizona State Univ., Tempe, AZ.

**Introduction:** Remote sensing studies indicate that plagioclase feldspar is the dominant mineral phase in the martian crust [1-2], present in both surface types 1 and 2 identified by the Mars Global Surveyor Thermal Emission Spectrometer (TES) [1]. Martian meteorites, commonly thought to have sampled isolated areas on Mars, contain plagioclase in abundances secondary only to pyroxene.

Terrestrial basalts and andesites are comprised of primary plagioclase feldspar that is calcic-intermediate (An<sub>50-75</sub>) in composition. Primary plagioclase with sodic (>An<sub>30</sub>) compositions is found in felsic and alkali-rich volcanic rocks and as an alteration phase in metamorphic and hydrothermally altered rocks. Primary plagioclase compositions vary with the extent and type of crystallization processes and with a variety of emplacement mechanisms. In low-temperature (<200°C) aqueous environments, plagioclase is commonly converted to clay minerals through hydrolysis. At hydrothermal temperatures, calcic plagioclase converts to more sodic compositions (<An<sub>30</sub>) through a process known as albitization [3-5].

Our ability to accurately derive plagioclase compositions from thermal infrared (TIR) emission spectra of martian surface materials affects our ability to identify and distinguish evidence for primary igneous and alteration (low vs. high T) processes that may have been at work on Mars. A previous study [6] demonstrated that average plagioclase compositions of two-component, coarse plagioclase sand mixtures can be derived to within 4 An (1σ) at laboratory, TES, and Miniature-Thermal Emission Spectrometer (Mini-TES) spectral resolutions and 6 An (1σ) at Thermal Emission Imaging System (THEMIS) resolution. The accuracy is less for volcanic rocks [6-8], with compositions modeled to within 10-15 An of measured values. This discrepancy may be due to the fact that volcanic rocks rarely contain bimodal plagioclase compositions (as in controlled sand mixtures), but are commonly zoned and can span intermediate sub-ranges of the plagioclase solid-solution series. Thus, two-component mixtures only reflect this variability to first order.

We have taken the next step towards approximating the complexity of natural samples by constructing increasingly complex mixtures of pure plagioclase components. We examine the accuracy with which

we can derive plagioclase compositions from TIR spectra of such mixtures. As in [6], we also examine whether or not component proportions, compositional ranges, and/or the endmember sets used affect modeled results.

**Methods:** Fifteen physical mixtures of multiple pure coarse plagioclase sand samples were prepared using the same components (ranging from An<sub>2</sub> to An<sub>73</sub>) that were used in [6]. In that study, mixtures varied in their average composition (from An<sub>19</sub> to An<sub>72</sub>) and proportions (25-75%) of each component were used. Here we have taken a comparable approach, mixing pure components in variable proportions (from 1-80%), with average plagioclase compositions of mixtures ranging from An<sub>35</sub> to An<sub>51</sub> (Table 1). We refer to these as multi-component mixtures, with the term *component* meaning a particular solid solution

Mixture	Percentages	Average An
<i>Three Component<sup>(1)</sup></i>		
III-A	80-15-5%	51
III-B	60-25-15%	45
III-C	40-35-25%	40
III-D	33-33-33%	36
III-E	20-45-35%	35
<i>Four Component<sup>(2)</sup></i>		
IV-A	80-10-5-5%	51
IV-B	60-20-15-5%	46
IV-C	40-30-20-10%	44
IV-D	25-25-25-25%	44
IV-E	20-30-30-20%	40
<i>Five Component<sup>(3)</sup></i>		
V-A	80-10-5-4-15%	51
V-B	60-20-10-6-4%	50
V-C	40-30-15-10-5%	48
V-D	20-20-20-20-20%	50
V-E	10-15-25-30-20%	49

Samples used: <sup>(1)</sup>=0022b, 4512A-L, 5851, <sup>(2)</sup>=<sup>(1)</sup>+SS, <sup>(3)</sup>=<sup>(2)</sup>+1382a – see [6] for details.

**Table 1.** Multi-component mixtures used in this study. Subscripts refer to specific plagioclase used as in [6].

composition (An value) of plagioclase.

TIR spectra were collected using a Nicolet Nexus 670 spectrometer at Arizona State University. Each mixture spectrum is the average of 270 scans collected over 2000–200 cm<sup>-1</sup> (2.5–50 μm) with 4 cm<sup>-1</sup> spectral sampling. Sample radiance was then converted to emissivity and calibrated using techniques described

by [9-10]. As in [6], lab spectra ( $4 \text{ cm}^{-1}$  sampling), were degraded to TES/Mini-TES ( $10 \text{ cm}^{-1}$ ) and THEMIS (10 bands from  $1480\text{-}796 \text{ cm}^{-1}$ ) resolutions to simulate the effects of lower spectral resolution collected by these instruments.

Mixture spectra were deconvolved using a linear deconvolution technique [9] over  $1300\text{-}400 \text{ cm}^{-1}$ , a range that includes most silicate absorption features and is directly comparable to the results from previous studies [6-8]. Five plagioclase endmember sets [6] were used including: (1) a set containing spectra only from endmembers used in physical mixtures, (2) a restricted set using spectral endmembers spaced 15 An apart across the plagioclase solid-solution series, (3) another restricted set (from [8]), (4) a set containing all currently available plagioclase endmembers, and (5) all available plagioclase excluding those used in mixtures. Set 1 was used as a "check" on the deconvolution technique and to determine whether or not each mixture was adequately mixed. Sets 2 and 3 were used to determine the suitability of using more restricted endmember sets in deriving compositions. Set 4 represents a "best case" scenario, where some endmembers are the same as those present in each mixture. Set 5 is more representative of a remote sensing scenario, because it is unlikely that spectral libraries contain endmembers that are exact matches for plagioclase on Mars.

**Results.** Deconvolution results were used to calculate average plagioclase compositions (average An) for each mixture to compare with measured compositions. Variations between measured and modeled plagioclase values are reported to within  $1\sigma$  standard deviation and are hereafter referred to as *An variation* ( $\Delta\text{An}$ ).

*$\Delta\text{An}$  Per Number of Components:* Results indicate that, with an increasing number of components used in plagioclase mixtures,  $\Delta\text{An}$  does not vary significantly. Likewise,  $\Delta\text{An}$  values from this study are comparable to those reported from deconvolutions of 2-component mixtures [6]. Modeled plagioclase compositions for 3, 4, and 5-component mixtures are within  $\Delta\text{An}=3$ ,  $\Delta\text{An}=5$ , and  $\Delta\text{An}=5$ , respectively, of measured compositions.  $\Delta\text{An}$  values reported above include deconvolutions at all spectral resolutions using all endmember sets. RMS errors were low (mostly within 0.002-0.003) and any variabilities do not correlate with the number of components used in each mixture.

*$\Delta\text{An}$  At Different Spectral Resolutions:* At lab resolution, compositions were modeled to within  $\pm 4$  An of measured values, whereas at TES and Mini-TES resolutions,  $\Delta\text{An}=5$  An. At THEMIS resolution, modeling accuracy is further degraded, with a  $\Delta\text{An}=6$  An. Values reported here include deconvolutions of all mixtures and incorporate those using all endmember

sets. Again, RMS errors varied little (0.002-0.003) and did not correlate with spectral resolution.

*$\Delta\text{An}$  Per Endmember Set.* Deconvolutions of all mixtures at variable resolutions produced  $\Delta\text{An}$  values of 4 An for endmember sets 1, 3, 4, and 5, while set 2 modeled compositions to within 5 An. This indicates that all endmember sets modeled average plagioclase compositions sufficiently well. RMS errors remained between 0.002-0.003, with only deconvolutions with set 3 producing values near 0.004.

**Discussion.** Results suggest that, with an increasing number of compositional components of a plagioclase in multi-component, coarse-grained sand mixtures, modeled compositions do not vary significantly and are comparable to results reported for 2-component sand mixtures in [6]. Thus, the increasing number of components does not account the discrepancy between higher  $\Delta\text{An}$  values (10-15 An) for rocks [6-8] and lower values (4-6 An) for plagioclase sand mixtures [6 & this study]. The presence of other phases or grain size effects may account for this.

This study further constrains the ability to which plagioclase compositions can be modeled at varying resolutions as sample mixtures increase in complexity, approaching that of volcanic rocks. Combined results from this study and [4] suggest that plagioclase compositions can be modeled to within 4 An at laboratory spectral resolution, 5 An at TES and Mini-TES resolutions, and within 6 An at THEMIS resolution for coarse sand mixtures. Presently, we are addressing potential effects of lower and variable (by instrument and temperature) signal-to-noise ratios on our ability to derive plagioclase compositions. Results reported above do not take this into account.

All spectral libraries used in deconvolutions adequately modeled average plagioclase compositions., contrary to the conclusion drawn in [6] suggesting larger endmember sets better modeled measured compositions. While set 2, with a limited number of endmembers, modeled average plagioclase to within  $\pm 5$  An, another restricted set (3), produced  $\Delta\text{An}$  values identical to those (sets 4 & 5) with more endmembers.

**References:** [1] Bandfield et al (2000) *Science*, 287, 1626-1630. [2] Hamilton et al. (2001) *J. Geophys. Res.*, 106, 14733-14746. [3] Hardie (1983), *Contrib. Mineral. Petrol.*, 82, 205-213. [4] Alt & Emmermann (1985), *Initial Rep. DSDP*, 83, 249-262. [5] Stakes & Schiffman (1999), *GSA Bull.*, 3, 1294-1314. [6] Milam et al. (2004) *J. Geophys. Res.*, 109. [7] Hamilton & Christensen (2000) *J. Geophys. Res.*, 105, 9717-9733. [8] Wyatt et al. (2001) *J. Geophys. Res.*, 106, 14711-14732. [9] Ramsey & Christensen (1998) *J. Geophys. Res.*, 103, 579-596. [10] Ruff et al. (1997) *J. Geophys. Res.*, 102, 14899-14913.