

QUANTIFICATION OF THE MINERALOGY OF ORDINARY CHONDRITES USING POSITION SENSITIVE X-RAY DIFFRACTION T.L. Dunn¹, H.Y. McSween, Jr.¹, G. Cressey², P.A. Bland^{2,3} and T.J. McCoy⁴ ¹Department of Earth and Planetary Sciences, University of Tennessee, Knoxville, TN, 37996 USA (tdunn@utk.edu); ² Department of Mineralogy, Natural History Museum, London, SW7 5BD, UK; ³Impacts & Astromaterials Research Centre (IARC), Department of Earth Science and Engineering, Imperial College, London, SW7 2AZ, UK; ⁴Department of Mineral Sciences, Smithsonian Institution, Washington, DC, 20560, USA.

Introduction: Few credible determinations of phase abundances in ordinary chondrites exist because of the difficulty associated with measuring accurate modes using traditional techniques, such as optical point counting. Microprobe phase mapping, which has been used to determine modal abundances in previous studies, is too time-consuming for many determinations, is inaccurate for small grain sizes because the beam tends to overlap grain boundaries, and may be compromised by analyzing unrepresentative thin-section areas. In an attempt to more accurately quantify modal abundances of chondrites, [1,2] first applied a technique for quantification of multi-phase samples using position-sensitive X-ray diffraction to several chondrites. This technique differs from traditional XRD in that it uses a position-sensitive detector (PSD), which enables diffraction patterns to be collected simultaneously at all angles over a 120° arc.

Position Sensitive Detector X-ray Diffraction Methodology: The PSD X-ray diffraction (PSD-XRD) technique was first applied to phase quantification of clay samples by [3]. PSD-XRD was further developed by [4], who incorporated procedures to correct for differences in attenuated radiation of multi-phase mixtures and single-phase standards. PSD-XRD was first applied to phase quantification chondrites by [1,2], who determined the modal abundances of a few carbonaceous and ordinary chondrites, respectively. These studies demonstrated that accurate phase quantification of multi-phase samples is possible using this technique.

The PSD-XRD quantification method utilizes a curved position-sensitive detector (PSD) with an output of 4096 channels representing an arc of 120° 2θ. The position-sensitive detector simultaneously measures diffracted intensity at all angles, resulting in rapid collection of diffraction patterns. The use of an anode blade rather than a traditional anode wire allows for rapid recording of high precision diffraction patterns. In addition to Bragg scattering from crystalline phases, the interaction of CuKα radiation with Fe results in the emission of Fe fluorescence radiation. This characteristic fluorescence signal is useful in the fitting process [4]. Accurate phase quantification can be accomplished using diffraction patterns acquired in as little as 5 minutes [4]. However, multiphase meteorite samples (such as those in this study) require additional counting time (60

minutes) to ensure proper fitting of the diffraction pattern.

Fitting Procedure. The PSD-XRD method for phase quantification uses a whole-pattern fitting procedure, which can be summarized by the expression:

$$X_i = \left(\frac{t'}{t} \right) \left(\frac{I'_0}{I_0} \right) \left[\frac{(\mu/\rho)_i}{(\mu/\rho)'} \right] w_i$$

where X_i is the pattern intensity fraction relative to pure i , t and t' are the counting times for the standard and mixture, respectively, I_0 and I'_0 are the incident beam flux for the standard and mixture, $(\mu/\rho)_i$ is the mass absorption coefficient of phase i , $(\mu/\rho)'$ is the mass absorption coefficient of the mixture, and w_i is the actual weight of phase i present in the mixture.

This whole-pattern fitting procedure requires considerable data processing [4]. The amounts of individual phases are estimated using a computer least squares fitting program, which compares peak intensities of the standard to those in the mixture [3]. Each standard pattern is then decreased by the appropriate factor and is subtracted from the original sample until the sum of identified phases totals 100%. The mass absorption coefficient (μ/ρ) of each standard is used to calculate weight proportions of each phase present in the mixture. Provided well-matched standards are available, mineral abundances can be determined with an relative accuracy of ~1% for each phase [1].

Standards. To ensure an accurate fitting, standards representative of the minerals present in a multi-phase mixture must be available. Mineral standards appropriate for unequilibrated ordinary chondrites, including the entire range of olivine solid solution, clino-enstatite, Na-plagioclase, and troilite, were procured and utilized by [2]. Because mineral chemistries differ between unequilibrated and equilibrated chondrites, these standards do not represent the full range of mineral compositions present in equilibrated ordinary chondrites. Minerals such as high-Ca pyroxene, chromite, Ca-plagioclase, and chlorapatite are currently being obtained from the Smithsonian Institution.

Application to Ordinary Chondrite Mineralogy: Quantified mineral modes can directly address two long standing questions that have hindered our understanding of thermal metamorphism in the asteroidal parent bodies of ordinary chondrites:

1. Does oxidation or reduction occur during progressive metamorphism in equilibrated ordinary chondrites?
2. What is the best geothermometer to constrain peak metamorphic temperatures in type 6 H, L, and LL ordinary chondrites?

Obtaining accurate modal abundances of olivine, pyroxene, and plagioclase in ordinary chondrites should enable us to resolve these questions. In this study, we will determine the modal abundances of ordinary chondrites using the PSD X-ray diffraction method. First, we will address the question of hypothesized redox changes during thermal metamorphism by examining modal olivine/low-Ca pyroxene ratios, which should increase from petrologic types 4-6 if oxidation is occurring. We will then examine the accuracy of using the plagioclase geothermometer [5] to determine peak temperatures in ordinary chondrites (as an alternative to pyroxene geothermometers [e.g. 6]) by determining the metamorphic grade at which plagioclase is completely crystallized. Peak temperatures estimated using the plagioclase geothermometer are only valid if plagioclase continued to crystallize from chondrule glass through type 6 conditions.

Sample Selection. To date, thirty-five equilibrated ordinary chondrites representing each of the ordinary chondrites groups (H, L, and LL) and corresponding petrologic categories 4-6 [7] have been analyzed using PSD-XRD (Table 1). Most petrologic groups are well represented by the samples already analyzed; however, this is not the case for the LL4 and LL5 groups. To ensure that the entire range of ordinary chondrites is represented in our data set, we are in the process of obtaining several LL4 and LL5 samples for analysis.

Table 1: Chondrites Analyzed Using PSD-XRD

Name	Class	Name	Class
Bandong	LL6	Farmville	H4
Cherokee Spring	LL6	Forest Vale	H4
Karatu	LL6	Kabo	H4
Saint-Severin	LL6	Marilia	H4
Attara	L4	Sao Jose	H4
Bald Mountain	L4	Schenectady	H4
Rio Negro	L4	Allegan	H5
Rupota	L4	Ehole	H5
Guibja	L5	Itapicuru-Mirim	H5
Mabwe-Khoywa	L5	Lost City	H5
Malakal	L5	Pribram	H5
Messina	L5	Uberaba	H5
Apt	L6	Andura	H6
Aumale	L6	Butsura	H6
Karkh	L6	Canon City	H6
Kunashak	L6	Guarena	H6
Kyushu	L6	Ipiranga	H6
New Concord	L6		

All samples selected for analysis are unbrecciated falls with minimal weathering. Because metal fractions

were removed from these powders prior to spectral analysis, characteristic metal peaks will be absent from these X-ray diffraction patterns. Metal abundances will be added back into XRD silicate modes using the proportion of metal to silicate minerals reported by [8]. Removing the metal portion of powders also prevents XRD analytical problems previously encountered with metal in ordinary chondrites [2].

Results: To test the accuracy of the PSD-XRD method in mixtures with compositions similar to ordinary chondrites, diffraction patterns of several powder mixtures consisting of varying but known proportions of plagioclase, pyroxene, and olivine have been collected and deconvolved using the fitting procedure described by [3]. Our results confirm that modal abundances can be determined with an accuracy of <1 vol %.

Calculated and measured abundances of a mixture of olivine and low-Ca pyroxene (mixture A) are presented in Table 2. Figure 1 shows the whole pattern matching and stripping of this mixture. Note, the irradiated volume of the mixture was less than that of the standards, leading to <100% total fit. However, when normalized the validity of the experiment is confirmed.

Table 2: X-ray Diffraction Data for Mixture A

Mineral	XRD		wt%	
	% fit	μ/ρ	XRD	actual
Olivine	28.0	48.6	69.4	70.0
Low-Ca Px	12.5	47.9	30.6	30.0

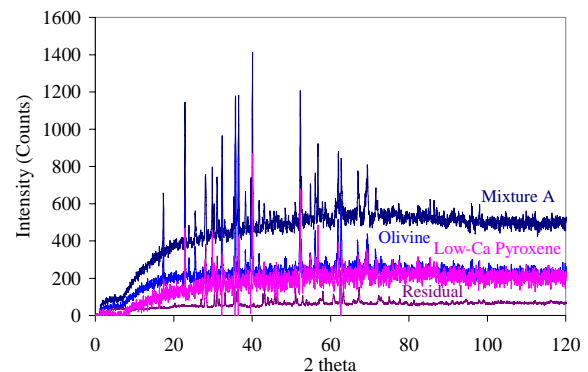


Figure 1: Whole pattern matching and stripping of mixture A.

References: [1] Bland P.A. et al. (2004) *MAPS*, 39, 3-16. [2] Menzies O.N. et al. (2005) *MAPS*, 40, 1023-1042. [3] Cressey G. and Schofield P.F. (1996) *Powder Diffraction*, 11, 35-39. [4] Batchelder M. and Cressey G. (1998) *Clays and Clay Minerals*, 46, 183-194. [5] Nakamutu Y. and Motomura Y. (1999) *MAPS*, 34, 763-772. [6] McSween H.Y. Jr and Patchen A.D. (1989) *Meteoritics*, 24, 219-226. [7] Van Schmus W.R and Wood J.A. (1967) *GCA*, 31, 747-765. [8] Jarosewich E. (1990) *Meteoritics*, 25, 323-337.