

MINERALOGY OF SNC METEORITE EET79001 BY SIMULTANEOUS FITTING OF MÖSSBAUER BACKSCATTER SPECTRA. D. G. Agresti¹ and R. V. Morris², ¹Department of Physics, University of Alabama at Birmingham, Birmingham, AL 35294-1170 (agresti@uab.edu), ²NASA Johnson Space Center, Houston, Texas (richard.v.morris@nasa.gov)..

Introduction: We have acquired Mössbauer spectra for SNC meteorite EET79001 with a MIMOS II backscatter Mössbauer spectrometer [1] similar to those now operating on Mars as part of the Mars Exploration Rover (MER) missions. We are working to compare the Fe mineralogical composition of martian meteorites with in-situ measurements on Mars.

Our samples were hand picked from the >1 mm size fraction of saw fines on the basis of lithology, color, and grain size (Table 1). The chips were individually analyzed at ~300K by placing them on a piece of plastic that was in turn supported by the contact ring of the instrument (oriented vertically). Tungsten foil was used to mask certain areas from analysis. As shown in Figure 1, a variety of spectra was obtained, each resulting from different relative contributions of the Fe-bearing minerals present in the sample.

Because the nine samples are reasonably mixtures of the same Fe-bearing phases in variable proportions, the nine spectra were fit simultaneously (simfit) with a common model, adjusting parameters to a single minimum chi-squared convergence criterion [2]. The starting point for the fitting model and values of hyperfine parameters was the work of Solberg and Burns [3], who identified olivine, pyroxene, and ferrous glass as major, and ilmenite and a ferric phase as minor (<5%), Fe-bearing phases in EET79001.

Data Processing: A 512-channel backscatter Mössbauer spectrum was acquired for each sample. The velocity range was set to around ± 10 mm/s to keep to the usual practice for MIMOS on Mars. An iron foil spectrum was acquired and the differential velocity signal was recorded. The velocity calibration was performed by *MERView* [4] after adapting the program to read and process data supplied by the laboratory instrument. Before exporting from *MERView* for analysis by *MERFit* [2], the data were interpolated to a uniformly spaced velocity scale, the spectral halves summed, and the 256-channel fold-summed spectrum referenced to the center of the α -Fe spectrum.

Simfitting: To simfit a set of spectra, a model, typically a sum of Lorentzian doublets and sextets, is chosen that applies to all spectra. Single-spectrum constraints are established, relating parameters within a given spectrum in the same way for all spectra. Then, multi-spectrum constraints, relating the same parameter among several spectra, are chosen.

Table 1. Samples (>1 mm chips) of EET79001,N studied in this work.

^a ID	^b N	Appearance; Processing
A	65	Selected light green clasts
B	65	Selected light green clasts
C	65	Lithology C
D	12	Grey chip
E	65	Lithology C
F	12	Black chips (fusion crust)
G	12	Black side of grey chip (fusion crust)
H	65	Grey chip with large clast
I	65	Coarse-grained grey chip

^aSample sequence identifier

^bSaw fine identifier

Because there is no sextet in any spectrum and we are equating doublet peak widths and areas pairwise, each doublet subspectrum is defined by four parameters: Center Shift (δ), Quadrupole Splitting (ΔE_Q), Line Width (Γ), and Doublet Area, which we report here as percent of total spectrum area. As a measure of mineral content, Area is adjusted for differences in recoil-free fraction f , using $f(\text{Fe}^{3+})/f(\text{Fe}^{2+}) = 1.21$ [5,6].

Following [3], our initial model consisted of 6 Lorentzian doublets: Olivine (Ol), Pyroxene (Px), Glass or glass-like phase (G11, G12), a Fe^{3+} phase, and Ilmenite (Ilm). Later, we tried a second doublet for pyroxene, but found unacceptable values for δ and ΔE_Q , and for Γ (~ 0.22 mm/s). We started Ilm at typical values for δ and ΔE_Q , but they consistently drifted away to values for another ferrous phase (Fe^{2+}) (listed in Table 2).

On the other hand, we were successful in stably fitting two “glass” doublets with δ and ΔE_Q close to those of [3]. To refine the “glass” distribution, we added a third doublet between G11 and G12 and found it to stabilize, constraining only Γ by holding it equal for the 3 doublets (Table 2). In Figure 1, the “glass” subspectrum is the sum of these 3 doublets. To keep the same subspectral shape for all spectra, Area ratios of the “glass” doublets were constrained equal for all spectra.

We found that modeling Ol as a sum of Lorentzian plus Gaussian lineshapes improved the fit somewhat, but had little effect on parameter values of any phase.

Our final simfit is displayed on Figure 1, with f -corrected Areas on Figure 2. The final parameter set is listed in Table 2.

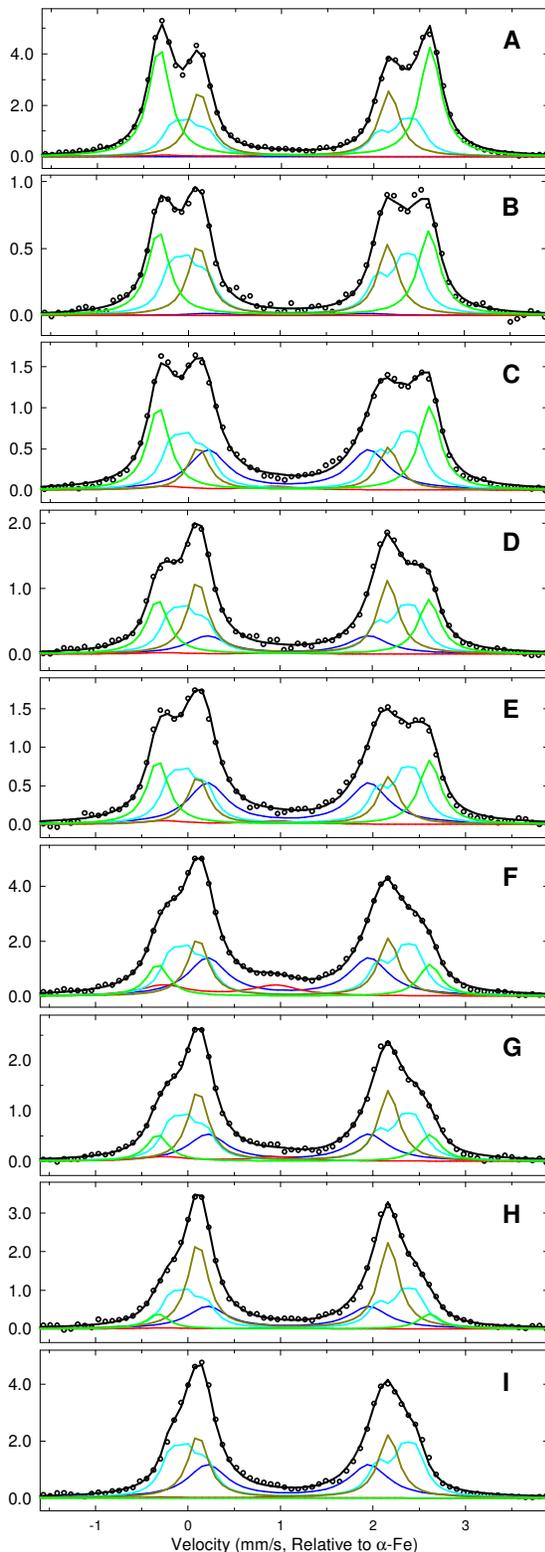


Figure 1. Spectra with fitted curves for 9 EET79001 samples. Only the central part of the spectra are shown. Sample codes A-I are given in Table 1. Sub-spectral curves are color coded as on Figure 2. The vertical scale is backscattering as % above baseline.

Table 2. ^aValues of parameters obtained in the simfit.

	OI	Px	G11	G12	G13	Fe ³⁺	Fe ²⁺
δ	1.14	1.14	1.14	1.15	1.12	0.34	1.08
ΔE_Q	2.94	2.06	2.66	2.33	1.86	1.21	1.74
Γ	0.28	0.27	0.24	^b 0.24	^b 0.24	0.63	0.51

^aUnits are mm/s. Errors are estimated as ± 0.01 mm/s for OI and Px, and ± 0.02 - 0.03 mm/s for the others.

^bHeld equal to Γ (G11).

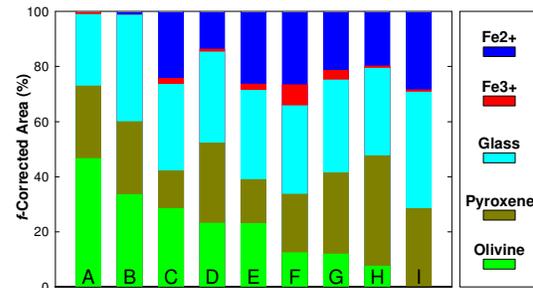


Figure 2. Relative Fe content in Fe-bearing phases detected in the simfit of the nine EET79001 samples, ordered and labeled A-I according to f -corrected olivine spectral areas.

Conclusion: We have shown in this experiment simulating a Mars measurement on SNC meteorite EET79001 with a MIMOS II spectrometer and high counting statistics that resolution and data are sufficient to perform a successful Mössbauer analysis of the Fe mineralogy of this martian material, providing that: 1) a number of targets are selected with different proportions of Fe-bearing minerals and 2) the data are fit simultaneously. Simfitting takes advantage of the different ways in which identically shaped subspectra influence the overall spectrum, in effect breaking the strong correlation among fitting parameters present in a single-spectrum fit.

As for the mineralogy of EET79001, we found narrow lines (i.e. good crystallinity) for olivine and pyroxene (M2 site), but no evidence for pyroxene (M1). We confirm the presence of a minor ferric phase, and we modeled an abundant phase with three doublet components we assigned to Fe²⁺ “glass.” We note that the values of ΔE_Q are outside the normal range for Mars-like basaltic glass [7], so these doublets reasonably result from an Fe²⁺-bearing phase other than glass. We did not detect the presence of ilmenite, but we did find evidence for a different Fe²⁺ phase, with parameters $(\delta, \Delta E_Q) = (1.08, 1.74)$.

References: [1] Klingelhöfer G. et al. (2003) *JGR*, 108, 8067. [2] Agresti D. G. and Gerakines P. A. (2009) *Hyp. Interact.*, 188, 113. [3] Solberg T. C. and Burns R. G. (1989) *LPSC*, 19, 313. [4] Agresti D. G. et al. (2006) *Hyp. Interact.*, 170, 67. [5] DeGrave E. and Van Alboom A. (1991) *Phys. Chem. Miner.*, 18, 337. [6] Morris R. V. et al. (1995) *JGR*, 100, 5319. [7] Morris R. V. et al. (2008) *JGR*, 113, E12S42, doi:10.1029/2008JE003201.