ANALYSIS OF MÖSSBAUER DATA FROM MARS: A DATABASE AND ARTIFICIAL NEURAL NETWORK FOR IDENTIFICATION OF IRON-BEARING PHASES. P. A. de Souza Jr.<sup>1</sup>, R. V. Morris<sup>2</sup>, G. Klingelhöfer<sup>3</sup>, and the Athena Science Team, <sup>1</sup>Departamento de Pelotização, Companhia Vale do Rio Doce, 29090-900 Vitória, ES, Brazil, eMail: paulo.antonio.souza@cvrd.com.br, <sup>2</sup>Aeromaterials Research Center, NASA Johnson Space Center, 77058 Houston, TX, USA, eMail: r.v.morris@nasa.gov, <sup>3</sup> Institut für Anorganische und Analytische Chemie, Staudinger Weg 9, Johannes Gutenberg Universität, 55099 Mainz, Germany; eMail: klingel@mail.uni-mainz.de

Introduction: The exploration of the planet Mars is one of the major goals within the Solar system exploration programs of the US-American space agency NASA and the European Space Agency ESA. In particular the search for water and life and understanding of the history of the surface and atmosphere will be the major tasks of the upcoming space missions to Mars. The miniaturized Mössbauer spectrometer MIMOS II [1] has been selected for the NASA Mars-Exploration-Rover twin-mission to Mars in 2003 and the ESA 2003 Mars-Express Beagle 2 mission (Figure 1). Reduced in size and weight, in comparison to ordinary laboratory setup, the sensor head just weights approximately 400 g, with a volume of (50x50x90) mm<sup>3</sup>, and holds two gamma-ray sources: the stronger for experiments and the weaker for calibrations. The collimator (in sample direction) also shields the primary radiation off the detectors. Around the drive four detectors are mounted. The detectors are made of Si-PIN-photodiodes in chip form (100 mm<sup>2</sup>, thickness of 0.5 mm). The control unit is located in a separate electronics board. This board is responsible for the power supply, generation of the drive's velocity reference signal, read of the detector pulses to record the spectrum, data storage and communication with the host computer.

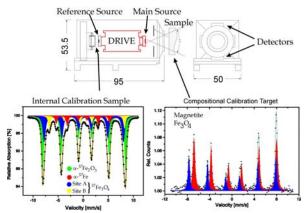


Figure 1. Drawing of the MIMOS II and a spectrum from the Compositional Calibration Target (CCT, magnetite) for the Mössbauer spectrometer on board of the Mars Exploration Rovers (MER) and a spectrum obtained in transmission geometry from an internal calibration sample placed inside the instrument.

After more than four decades from the discovery of the Mössbauer effect, more than 400 minerals were studied at different temperatures. Their Mössbauer parameters were reported in the literature, and have been recently collected in a data bank [2, 3]. Previous Mars-missions, namely Viking and Mars Pathfinder, revealed Si, Al, Fe, Mg, Ca, K, Ti, S and Cl to be the major constituents in soil and rock elemental composition of the red planet. More than 200 minerals already studied by Mössbauer spectroscopy contain significant amounts of these elements. A considerable number of Mössbauer studies were also carried out on meteorites and on Moon samples. Looking backward in the studies of the whole Mössbauer community, we have built a specific library containing Mössbauer parameters of those possible Mars minerals. The selected minerals, their Mössbauer parameter values (min. max. s.d and number of available data), main site substitution, behaviour as a function of temperature and a ranking as expected to be found on Mars were organized. Mars-analogue Fe-bearing minerals not studied by Mössbauer spectroscopy are being collected and investigated. In addition, it an identification system based on Artificial Neural Networks (ANN) was implemented which enables fast and precise mineral identification from the experimental Mössbauer parameters at a given temperature [4].

Processing the Information: Minor differences on Mössbauer parameters can seen be a result of all the properties described above and, also, imprecision, misinterpretation of the Mössbauer spectra [3] or even mistyping on papers. Despite of these small disadvantages, all information is still useful. An implemented software based on artificial neural networks is robust to minor differences and can, without any additional information, identify Mössbauer phases from its parameters. From a proper learning process, the ANN extract all relevant information from a given set of data (published Mössbauer parameters) forgetting most of the deviations coming from misinterpretations, imprecision and mistyping on reports.

Data Base. A Mössbauer data base was compiled from published Mössbauer parameters on minerals at different temperatures. All minerals containing the elements found on previous Mars missions were selected. Since temperature on Mars varies from -100°C to 10°C, only room and liquid nitrogen temperatures were selected. Literature on the selected Mars-analogue minerals were investigated considering the following aspects:

Chemical Formula and Mineral Identification. The chemical formula is given for each selected mineral. Those minerals were classified according to the standard mineralogical pattern, as: (a) oxides and (oxy)hydroxides; (b) Fe-S-bearing minerals; (c) phosphates; (d) carbonates; (e) Mn-rich minerals; (f) silicates (nesosilicates, sorosilicates, cyclosilicates, inosilicates, phyllosilicates, tektosilicates); and (g) minerals not studied by Mössbauer spectroscopy.

Statistical analysis on the recorded Mössbauer data. The average value, the standard deviation, the minimum and maximum values of a given site were calculated.

Behavior as function of temperature and grain size. The studied mineral may suffer magnetic transitions as a function of temperature and grain sizes. Also, the Mössbauer parameters of isomer shift, quadrupole splitting and internal magnetic field may change as function of temperature or, including the line width, its crystallinity.

Changes as a function of site substitution (e.g.  $\alpha$ -Fe<sub>2-x</sub>Al<sub>x</sub>O<sub>3</sub>) and vacancies. There are rich literature describing the effects of isomorphic substitution of cations in iron sites. This substitutions lead to changes in the Mössbauer parameters well defined at the literature.

Genisis. The Mössbauer spectrum of a given mineral may change according to the formation process. This situation, when pertinent, is reported and described on the basis of previous studies [e.g. 5, 6].

Other Fe-bearing phases usually reported join the considered mineral. Smectites (e.g. montmorillonite and notronite) are usually found together with hematite and/or goethite). The weathering process of palagonites leads to Ferich smectite phases and oxyhydroxide and ferric oxide. This may be a supporting information during the analysis process of a Mössbauer spectrum.

Final Remarks. Some minerals were reported at the literature with a single site up to, for example, four. This difference may be a result of differences among the analyzed samples, analysis method, spectrum statistics, etc. When such situation is detected, a specific note is registered at this mineral records. Finally, color, common impurities, other iron-free mineral phase reported, as so on. This information may be useful, specially considering the cameras and other scientific instruments carried out by the Mars landers.

Tentative Ranking. Previous lander and orbiter missions to Mars obtained relevant information on the mineralogy of the neighbor planet. Each mineral is being assign to a rank according to the available information on the its possibility to be found on Mars (e.g., based on SCN meteorites, previous Mars landers and orbiters data, and Martian analogue sample studies). Additional minerals, not found as studied by Mössbauer spectroscopy, are being collected and studied from room temperature down to – 100°C. Up to now, over 2,600 references are stored and classified according to the criteria described above. Is the intention of the authors to make available the whole data set and programs by the end of the Mars missions.

Fast Mineral Identification: A hybrid artificial neural network [2, 3], associated with the data base, was implemented. The program, written in C++ language, consists in a *learning vector quantization* (LVQ) network. Specific trainings were performed using Mössbauer parameters at room and at liquid nitrogen temperature. The neural identification is robust to minor changes at the reported parameters. This capability comes from its ability to see through noise. After the adequate training, the ANN could successfully and quickly identify the studied Febearing mineral from its Mössbauer parameters.

Conclusions: A very specific Mössbauer data base was built taking into consideration the needs of the Mars Missions. The information published in the literature was carefully analyzed. The most relevant variables that may lead to changes of the Mössbauer parameters of each mineral were recorded in the data base records. The stored Mössbauer parameters were used to train an artificial neural network making possible a fast and accurate mineral identification from measured Mössbauer parameters. Before the first Mössbauer spectrum is obtained on Mars surface, early in 2004, several and exhaustive tests are planed to be carried out. Very detailed calibration and data validation is an important upcoming issue in the present investigation.

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