DERIVATION OF VELOCITY SCALES FOR MARS MÖSSBAUER DATA. David. G. Agresti[1], M. Darby Dyar[2], and Martha W. Schaefer[3], [1]Dept. of Physics, U. of Alabama at Birmingham, Birmingham, AL 35294-1170 (agresti@uab.edu), [2]Dept. of Astronomy, Mount Holyoke College, 50 College St., South Hadley, MA 01075 (mdyar@mtholyoke.edu), [3]Dept. of Geology and Geophysics, E235 Howe-Russell, Louisiana State University, Baton Rouge, LA 70803 (schaefer@geol.lsu.edu).

Introduction: In terrestrial studies of rocks and soils, Mössbauer spectroscopy has not found routine application for mineral identification because other methods such as x-ray diffraction are usually more definitive. On the Mars Exploration Rovers (MERs), however, Mössbauer spectrometers [1] have been called upon to assist in defining the mineralalogy, despite the overlapping Mössbauer parameters of most rock-forming silicates, sulfates, and oxides. Published interpretations of MER Mössbauer data have revealed some very interesting results, including the presence of olivine and magnetite or hematite at Gusev [2] and olivine, hematite, and jarosite at Meridiani [3].

The strength (and uniqueness) of the interpretation of such data lies in the degree to which peak positions can be determined with accuracy and precision, and the data must be understood in the context of the conditions under which they were collected. Recognizing that interpretation of any data set is enriched by scrutiny of multiple research teams, with their different perspectives and approaches, it has been our purpose since release of the first MER data set in August 2004 [4] to enable non-MER team members easy access to MER Mössbauer data in a form that is readily usable by commonly available data analysis routines.

The *MERView* Program: MER data for each sol are contained in an Experimental Data Record (EDR), a single file in binary format containing, among other data, Mössbauer spectra of surface material and an internal reference target, acquired in up to 13 temperature windows, as well as a drive error signal. As reported last year [5], the Windows-based computer program, *MERView*, was developed in response to the MER data release. With help of menus and interactive dialog boxes, it provides decimal listings and graphical displays of all the EDR spectra and exports spectral data to individual files for use by other programs.

Subsequently, *MERView* was enhanced to compensate for the fairly large velocity non-linearity of the MER Mössbauer drives by automatically adjusting the amount of the drive error signal, *ErrAmp*, added to a linear (V-shaped) velocity waveform of amplitude, ±*Vmax*, and phase shifting by an amount, *PShift*, the modified waveform in channel space [6]. To accomplish this, *MERView* employs a least-squares criterion based on the requirement that the two mirror halves of a Mössbauer spectrum must overlap perfectly when plotted versus a properly calibrated velocity. The result is a proportional scale, in effect, *Vmax* = 100%.

Velocity Calibration: In this report, we present the most recent enhancement to *MERView*, the capability to determine *Vmax* in mm/s, which completes the derivation of the velocity scale. To do this, we refer to the nature of the reference targets, which consist of an α-Fe foil overlaid with undetermined amounts of α-Fe_2O_3 and Fe_3O_4, all enriched in ^{57}Fe. *MERView* graphs of reference spectra for MER-A (Spirit) and MER-B (Opportunity) are shown in Figures 1 and 2.

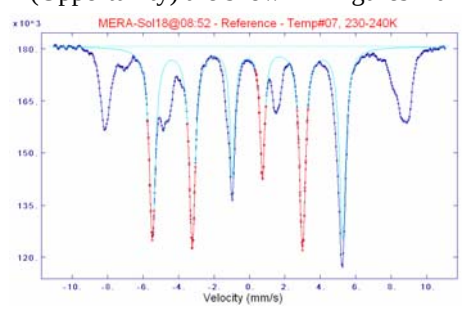

Figure 1. MER-A reference spectrum (blue) and same-temperature α-Fe spectrum (green) with a computed baseline (dotted). The velocity scale (*Vmax*) was adjusted to maximize overlap of selected parts of four α-Fe peaks (red) with the reference spectrum.

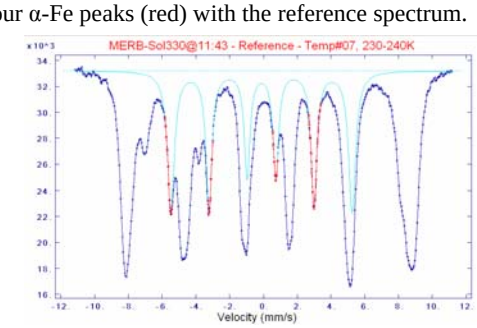

Figure 2. MER-B reference spectrum and same-temperature α-Fe spectrum. Remarks as in Figure 1.

The characteristic feature of the reference spectrum that allows its use to calibrate the velocity, i.e. to determine *Vmax*, is the presence of the α-Fe subspectrum, four of whose peaks (red in Figures 1 and 2) are relatively free of overlap by the hematite and magnetite subspectra. Unlike hematite and magnetite, whose spectra depend strongly on preparation conditions, the structure of α-Fe is essentially invariable. For this reason, the room-temperature spectrum of α-Fe is a velocity standard for the Mössbauer community.

For this study, low-temperature data for α-Fe, which are not readily available, were measured in our laboratory. Thus given the magnetic hyperfine field, B_{hf}, for each MER temperature window, *MERView* models the α-Fe spectrum at each temperature (solid lines in Figures 1 and 2), and compares it with the reference spectrum under control of a dialog box such as that of Figure 3, with manual or automatic adjustment of the parameters, *Vmax*, α-Fe spectrum center, α-Fe spectrum intensity, and the widths and relative intensities of four α-Fe peaks. The portion of each peak selected for comparison (left, right widths) is held fixed during *AutoAdjust*, but may be changed manually.

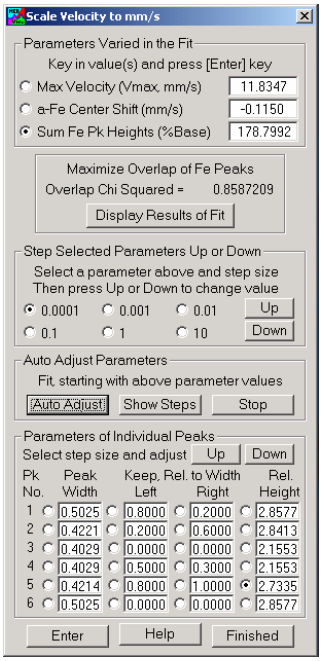

Figure 3. Velocity scaling dialog box, as it appears after auto adjustment for Figure 2.

In this way, *MERView* now routinely and quickly calibrates velocity for the entire MER data set. The user opens an EDR for a particular MER-A or MER-B sol, presses a designated key, and *MERView* automatically compensates for velocity non-linearity and determines the mm/s scale for each temperature window for which a measurement was made. Press another key and the velocity data for the entire sol are exported to a file. Press a different key and individual spectra are exported with accompanying velocity information.

***MERView* Results:** The new *MERView* capability allows trends in fitting parameters and velocity scales to be investigated, too numerous to be presented here. Figure 4 shows a typical variation in *Vmax* as function of temperature, which leads to a temperature dependence of the velocity scale. For this reason, the MER team has provided a universal set of velocity scales [7], for temperature windows 03 to 11, advising the user to independently calibrate each case of interest for greater precision. Note that a few sols have data extending into windows 02, 12, and 13, requiring user calibration in any case. The sol-to-sol variation in *Vmax* (Figure 5) further emphasizes this point, illustrating the dependence of velocity scales on environmental conditions and details of the sensor head placement.

The team-provided velocity scales are fairly accurate for most sols, with deviations from *MERView*-derived true velocity typically ~0.02-0.04 mm/s, or <0.1 line width. For some sols, however, the error is unacceptably large, as shown in Figure 6, which exhibits a large phase shift not properly taken into account. For other sols, the spectrometer was set to a reduced velocity to increase resolution of the central doublets, and the team-provided calibration does not apply.

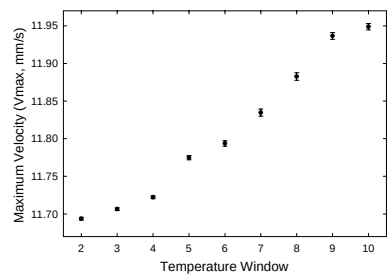

Figure 4. Typical variation of *Vmax* with temperature (example for MER-B, Sol 330).

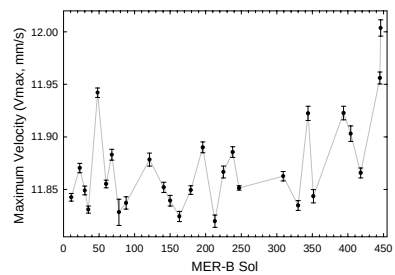

Figure 5. Variation of *Vmax* from sol to sol for MER-B, temperature window 07 (selected sols only).

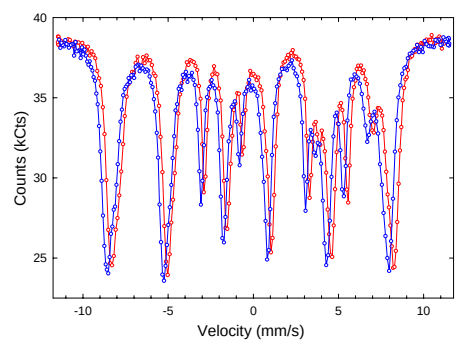

Figure 6. Raw data for MER-B, Sol 48, window 11, plotted versus corresponding team-provided velocity .

References: [1] Klingelhöfer et al. (2003) *JGR*, *108*, ROV 8-1–8-18. [2] Morris et al. (2004) *Science*, *305*, 833-836. [3] Klingelhöfer et al. (2004) *Science*, *306*, 1740-1745. [4] MER Analyst's Notebook, http://anserver1.eprsl.wustl.edu/. [5] Agresti, Dyar & Schaefer (2005) *LPS XXXVI*, Abstract #1941. [6] Agresti, Dyar & Schaefer (2006), Proceedings ICAME 2005, *Hyperfine Interactions*, to be published. [7] Folder *calib* at http://pds-geosciences.wustl.edu/missions/mer/geo_mer_datasets.htm.