APPLICATION OF MONTE-CARLO SIMULATION TO OUTSTANDING PROBLEMS IN X-RAY FLUORESCENCE SPECTROSCOPY. L.F. Lim[1], L.R. Nittler[2], [1]*NASA/Goddard Space Flight Center (lucy.f.lim@nasa.gov),*[2]*Carnegie Institution of Washington (DTM)..*

Introduction

The objective of the NEAR-Shoemaker X-ray Gamma-Ray Spectroscopy ("XGRS") investigation [1, 2] was to determine the elemental composition of the near-Earth asteroid 433 Eros. Two techniques were used. The X-ray Spectrometer (XRS) system detected the characteristic fluorescence of six major elements (Mg, Al, Si, S, Ca, Fe) in the 1–10 keV energy range excited by the interaction of solar X-rays with the upper 100 microns of the surface of 433 Eros. The Gamma-Ray Spectrometer (GRS) detected gamma rays in the 1–10 MeV energy range produced by natural radioactivity in K and by the interaction of cosmic rays with the nuclei of O, Mg, Si, and Fe in the upper meter of Eros' surface.

Iron, silicon, and magnesium abundances were measured with both XRS and GRS techniques. Unlike the Mg/Si ratio, which was consistent in the XRS and GRS data, the two Fe/Si measurements differed substantially from one another The NEAR-Shoemaker Gamma-Ray Spectrometer (GRS) determined that Fe/Si = 0.8 [3] whereas the XRS-derived Fe/Si is 1.68 +/- 0.34 [4, 5].

The evidence from other XGRS-derived elemental ratios and from the IR spectra as measured by MSI/NIS (Multi-Spectral Imager, Near-Infrared Spectrometer) strongly suggests that, apart from its space-weathering induced sulfur depletion, 433 Eros has an ordinary chondritic composition [6]. Recently, a chondritic Cr/Fe ratio has also been derived from the XRS data [7, 8]. However, because of the conflicting Fe/Si results there is no consensus on which subclass (H, L, or LL), if any, is its closest analogue; the GRS-derived value would imply an LL composition, but the XRS value would be consistent only with H chondrites.

Although the solar X-ray spectra have since been reassessed using a new model of the efficiency of the NEAR gas solar monitor [9, 5], reanalysis of the flare data with the new solar spectra did not reduce the XRS-derived Fe/Si.

It has been proposed [10, 11, 12] that if the surface of Eros has significant surface roughness, the combination of roughness with the relatively high phase angles of the NEAR observations might have distorted the Fe/Si results without affecting the Mg/Si or Al/Si results, since surface roughness was not taken into account in the original XRS analysis. This hypothesis can be tested using Monte Carlo methods. These methods can also be used to address several other problems relevant to XRS analysis, such as the effects of mineral mixing and of compositional segregation within the asteroid regolith.

The PENELOPE Code

PENELOPE [13, 14] is a Monte Carlo code for coupled transport of electrons, photons, and positrons and has especially accurate cross sections and transport of low-energy photons and electrons. Photon transport is simulated with a "detailed" method, in which each photon is followed throughout its history and each of its interactions is simulated chronologically.

Setting up a model in PENELOPE is done by generating the appropriate input files and a "MAIN" program. The input files specify the geometry, material composition and density of each material body in the simulation as well as the energy spectrum and geometry of the excitation source The MAIN program is the steering program that applies the PENELOPE transport routines to the simulation setup as specified in the input files. It also tallies the outcomes (energies and directions of emitted photons, dosages received within materials) of the simulation as it progresses, and writes the results out to files.

X-ray interaction with rough surfaces at high angles

With a Monte-Carlo code such as PENELOPE, it is possible to construct geometry files representing surfaces of varying degrees of roughness, then model the interaction of solar X-ray spectra with them at various incidence and emission angles. By reproducing the sun-asteroid-spacecraft geometries of various solar flares that occurred during the NEAR mission, it will be possible to determine whether surface roughness can account for the discrepancy between NEAR XRS and GRS Fe/Si results.

"Mosaic" or mineral-mixing effects

The effects of compositional inhomogeneity were addressed analytically in [4], in which "correction factors" were introduced to account for the differences between the X-ray spectra of homogeneous compositions and those of real rocks, in which atomic species are found in different proportions in different mineral grains. The correction factors were derived by calculating the fluorescent spectra of the various mineral species found in chondritic meteorites, then combining them in the proportion in which they are found in the meteorites. This approach of course does not account for intimate mixing of mineral grains. By contrast, in PENELOPE it would be relatively simple to put together a geometry file based on a thin section of an actual meteorite. Individual photon histories would then be able to include traverses through several mineral grains of appropriate sizes and distinct compositions, as in X-ray transport through rocks in nature.

Compositional Segregation by Regolith Processes

Another explanation that has been advanced for the discrepancy between the XRS and GRS Fe measurements is that iron-rich phases have been segregated from silicate phases in the regolith, since their physical properties are likely to be different. This could occur via the "Brazil-nut" process described in [15], in which shaking an inhomogeneous mixture causes hard spheres with larger-than-average diameters to rise to the top; or by the reverse process [16] in which if the bed is sufficiently deep and the amplitude of vibration sufficiently large, the large particles can segregate to the bottom.

With a Monte-Carlo code, it would be straightforward to set up a simulation in which the grains sitting on top are different in composition from the substrate, and thus discover how much segregation is necessary to produce the observed spectra from various bulk compositions.

This modeling approach can the question of whether the discrepancy between the NEAR XRS- and GRS- derived iron abundances can be reconciled by accounting for the effect of surface roughness on the XRS spectra. If it turns out that the XRS measurements are consistent with the lower GRS measurement (Fe/Si = 0.8) when roughness is taken into account, the case for Eros being related to the lower-iron subgroups of ordinary chondrites will be strengthened. If the discrepancy between XRS and GRS Fe/Si remains, however, that would be evidence that the surface layer of Eros' regolith is inhomogeneous in iron abundance, implying that regolith processes have operated differently at the major locations sampled (the GRS landing site and the locations of the XRS footprint during the largest solar flares).

Monte-Carlo modeling of solar X-ray interactions with rough surfaces will also be applicable to the XRS on MESSENGER [17]. Because of MESSENGER's extremely elliptical orbit, most of its XRS observations will be made at high incidence, emission, or phase angles. Understanding the behavior of X-ray spectra of rough surfaces at these geometries under solar illumination will be crucial for the interpretation of these data.

XRF spectra were also measured by the Japanese Hayabusa mission as it orbited 25143 Itokawa [18] and a similar XRS is included on the lunar orbiting mission SELENE, now known as Kaguya [19]. This type of modeling will be useful for understanding these spectra as well.

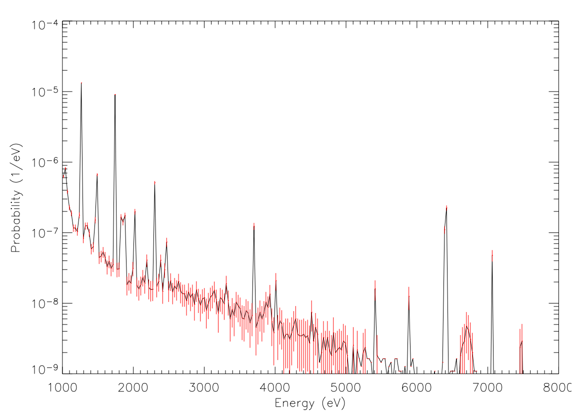

Figure: PENELOPE simulation of the spectrum of an H chondrite as illuminated by the solar flare of 10 July 2000. Both fluorescent and scattered photons are simulated. The computation time represented is 7400 seconds.

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