The Effects of Surface Roughness on the NEAR XRS Elemental Results: Monte-Carlo Modeling

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The NEAR XRS Spectra: 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. The X-ray Spectrometer (XRS) system measured 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.

Various investigators, using both laboratory experiments and computer simulations (e.g. [3, 4, 5, 6]) have established that X-ray fluorescent line ratios can be influenced by small-scale surface roughness at high incidence or emission angles. The effect on the line ratio is specific to the geometry, excitation spectrum, and composition involved. In general, however, the effect is only substantial for ratios of lines with a significant energy difference between them: Fe/Si and Cu/Si are much more likely to be affected than Al/Si or Mg/Si.

All of the NEAR XRS data were taken at relatively high phase angle, since the XRS was boresighted at 90° to the direction of the sun (as constrained by the pointing needs of the solar panels). During the major solar flares (Table 4 of [7]) which accounted for all of the XRS results for S, Ca, and Fe, either the incidence angle of the Sun or the emission angle toward the NEAR detectors was generally above 45°. Thus, the NEAR XRS fluorescent line ratios could certainly have been affected by surface roughness.

Although the results of the XRS experiment [8, 9, 7] strongly support the MSI/NIS (Multi-Spectral Imager, Near-Infrared Spectrometer) conclusion that 433 Eros has an ordinary chondritic composition, the bulk Fe/Si content of the asteroid remains uncertain. Thus, it is unclear whether Eros represents an H, L, or LL composition. The MSI/NIS data are relatively insensitive to metallic iron. The NEAR GRS experiment measured a substantially lower Fe/Si than the XRS, but sampled a localized area (the NEAR landing site) to a greater depth than was available to the XRS owing to the greater penetrating power of cosmic-ray induced neutrons and gamma rays. Thus, the GRS sample may have been subject either to less space weathering (because of the sampling depth) or more (because of ponding of weathered material at the landing site) than the near-surface regions measured by the various XRS solar flare measurements.

In order to address these problems, we apply a Monte-Carlo code to the specific geometry and spectrum of a major NEAR XRS solar flare observation, using an H chondrite composition [10] as the substrate. The seventeen most abundant elements were included in the composition model, from oxygen to titanium.

Monte-Carlo Simulations: Monte-Carlo simulations were carried out using the PENELOPE code [11, 12]. The solar spectrum of the 10 July 2001 solar flare was used as the input spectrum. This spectrum was calculated using CHIANTI [13, 14] from two-temperature models applied to the NEAR solar monitor data from the flare [7]. In order to make efficient use of processing time, the incident spectrum was limited to energies above 1.83 keV. As the K edges of Si, S, Ca, and Fe are all above this value, lower-energy X-rays have no effect on the K emission from these elements (1.74–7.06 keV).

Two substrate geometries have been constructed so far, representing "smooth" and "rough" cases. The smooth geometry is a simple homogeneous slab of material with chondritic composition. In the rough case, the surface is a cylindrically symmetric square wave shape in which the width and height dimensions of each ring are 100 microns.

The source (solar) spectrum has been applied at three different angles: normal to the surface, 45° from normal, and 60° from normal. (The actual solar incidence angle for the NEAR observation of the July 10 flare (Table 1) ranged from 55°–59° over the course of the flare.) The emission (fluorescence + scatter) spectrum was tallied at three angles: normal, +45° (opposite from the incident spectrum, at 90° phase for a 45° incidence angle), and -45° (zero phase). NEAR observed this flare at emission angles of 40–49°.

Preliminary Results: The effect of surface roughness was only evident in the Fe/Si ratios. The rough surface has no observable effect on the Fe/Si line ratio when observed from straight above, but at high emission angles (45 or 60 degrees) the Fe/Si line ratio is consistently higher by 10–20% than in the smooth-surface cases. There is no comparable effect on S/Si or Ca/Si, however, within the uncertainties of these simulations. Thus, based on these preliminary simulations, the NEAR Fe/Si compositional estimate from this solar flare may be 10–20% high. However, the S/Si and Ca/Si results are unlikely to have been affected by surface roughness.

Comparison with NEAR data: The photon ra-
tios were in reasonable agreement with the NEAR results. Both the smooth-surface Monte-Carlo prediction of Fe/Si (photon) = 0.035 ± 0.001 and the rough-surface results are higher than the 0.028 ± 0.005 measured by NEAR during this flare. However, although the XRS results were consistent with H chondritic Fe/Si overall, the July 10 flare alone resulted in a lower Fe/Si ratio.

The measured S/Si from the July 10 flare is half the value predicted from an ordinary chondritic composition, consistent with the significant sulfur depletion previously reported [8]. This is unaffected by the roughness model.

Future work: Future applications of the Monte-Carlo code will include testing a variety of roughness models, lower-iron (L and LL) compositions, modeling compositional inhomogeneity (e.g. "Brazil-nut" sorting), and modeling the solar spectra and geometries from the seven other major NEAR solar flares.

Table 1: Monte-Carlo Simulations of the 10-Jul-2001 NEAR Solar Flare

<table>
<thead>
<tr>
<th>INC. ANGLE</th>
<th>EMISS.</th>
<th>PHASE</th>
<th>FE/SI</th>
<th>S/SI</th>
<th>CA/SI</th>
</tr>
</thead>
<tbody>
<tr>
<td>55–59°</td>
<td>40–49°</td>
<td>81–89°</td>
<td>0.028 ± 0.005</td>
<td>0.031 ± 0.012</td>
<td>0.036 ± 0.007</td>
</tr>
<tr>
<td>Smooth Surface</td>
<td>0°</td>
<td>0°</td>
<td>0°</td>
<td>0.034 ± 0.002</td>
<td>0.062 ± 0.003</td>
</tr>
<tr>
<td>Smooth Surface</td>
<td>45°</td>
<td>+45°</td>
<td>90°</td>
<td>0.025 ± 0.001</td>
<td>0.060 ± 0.002</td>
</tr>
<tr>
<td>Smooth Surface</td>
<td>60°</td>
<td>+45°</td>
<td>105°</td>
<td>0.033 ± 0.004</td>
<td>0.064 ± 0.005</td>
</tr>
<tr>
<td>Rough Surface</td>
<td>45°</td>
<td>0°</td>
<td>45°</td>
<td>0.035 ± 0.002</td>
<td>0.062 ± 0.003</td>
</tr>
<tr>
<td>Rough Surface</td>
<td>45°</td>
<td>+45°</td>
<td>90°</td>
<td>0.039 ± 0.002</td>
<td>0.062 ± 0.003</td>
</tr>
<tr>
<td>Rough Surface</td>
<td>45°</td>
<td>-45°</td>
<td>0°</td>
<td>0.040 ± 0.003</td>
<td>0.062 ± 0.003</td>
</tr>
<tr>
<td>Rough Surface</td>
<td>60°</td>
<td>+45°</td>
<td>105°</td>
<td>0.038 ± 0.002</td>
<td>0.063 ± 0.002</td>
</tr>
</tbody>
</table>

Figure 1: Monte-Carlo (PENELOPE) generated spectra of an H chondrite composition as illuminated by the solar flare of 10-July-2010, with $\theta_1=45^\circ$, $\theta_2=45^\circ$, $\alpha=90^\circ$. Black (+): smooth surface; blue (diamonds) = rough-surface model.

References