Portable energy dispersive x-ray diffraction analyser for lunar applications

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As rocket technology makes further advancements, space mining, space exploration and human occupation of extra-terrestrial bodies becomes a more realistic endeavour. However, to sustain human life and to create rocket fuel for exploratory missions deeper into the solar system, a supply of oxygen is needed [1]. On the moon specifically, the mineral ilmenite (FeTiO$_3$) has been targeted for mining since upon reduction by hydrogen gas, oxygen gas and metallic iron are produced [2]. In order to increase the efficiency of such a reaction, it is desirable to know the concentration of ilmenite as well as impurity minerals in a reactor feedstock. To resolve this issue, a prototype portable Energy Dispersive X-ray Diffraction (EDXRD) analyser in a reflection geometry has been constructed that could be attached to a lunar rover to detect regions on the lunar surface with high ilmenite concentrations. Monte Carlo simulations using modified EGS code [3] were used to optimise geometrical parameters of the device, particularly to choose angles of diffraction that separate diffraction and fluorescence parts of the measured spectrum to obtain both types of information. The prototype analyser was used to analyse samples of Lunar Highlands (LHS-1) [4] which is simulant doped with ilmenite in the range of 0 wt% - 24 wt%. A curve fitting algorithm was developed in Python, the integrated intensity of diffraction and fluorescence peaks were used for linear regression analysis and results are presented in Fig. 1.

![Figure 1](https://example.com/figure1.png)

**Figure 1.** The linear regression results of the calculation of ilmenite diffraction and fluorescence peak integrated intensity.

Samples were also measured on a PANalytical Empyrean II benchtop XRD, equipped with a cobalt anode and analysed using Rietveld refinement software. The analysis performed by the prototype EDXRD analyser was found to be more accurate than the Rietveld refinement analysis, largely due to low availability of appropriate patterns. The results obtained by the EDXRD analyser demonstrate promise for measuring real lunar samples.

Further, samples of calcite (CaCO$_3$) and dolomite (MgCO$_3$) mixtures were also measured and analysed with custom curve fitting software resulting in linear regression analysis predictions with an RMS error of ~0.95 wt%. Similarly, samples of ilmenite acquired from a pottery supply store containing ilmenite, hercynite (FeAl$_2$O$_4$) and rutile (TiO$_2$) were mixed with quartz (SiO$_2$) then measured and analysed. Linear regression analysis predictions of ilmenite wt% had a RMS error of ~2.55 wt%.