

EXAFS ANALYSES OF COMET 81P/WILD2. J. C. Bridges¹, H. G. Changela¹ and S. J. Gurman², ¹Space Research Centre, Dept. of Physics & Astronomy, University of Leicester LE1 7RH, UK j.bridges@le.ac.uk, ²Dept. of Physics & Astronomy, University of Leicester LE1 7RH, UK.

Introduction: Extended X-ray Absorption Fine Structure (EXAFS) allows the determination of bond lengths and atomic co-ordination in minerals [1]. As it can be performed *in-situ* on aerogel tracks, with non destructive analyses of micron-size grains, it is an ideal technique to start applying to the *Stardust* cometary minerals. It can also readily be combined with complementary XANES and microRaman analyses [2] with the tracks preserved for other techniques. In addition to mineral identification one of our aims is to establish whether capture has had an influence on the oxidation state of the grains.

Samples and Methods: XRF and EXAFS analyses were made using the I18 Microfocus Spectroscopy Beamline of the UK *Diamond* Synchrotron. This can provide a $2 \times 2.5 \mu\text{m}$ spot size. XRF mapping for elements with $Z > 20$ were made to locate grains in the tracks and provide some elemental compositions. EXAFS were studied using an energy spectra range from 6900 to 7500 eV, with 0.2 - 0.4 eV energy steps. The results of Fe K XANES studies from the energy range 7000 - 7200 eV have previously been reported for some grains in track #41, identifying ferric and ferrous iron-bearing minerals [2]. Here we provide new Fe-K XANES analyses from track #162.

The EXAFS spectra were fitted using *DL_EXCURV* which produces reciprocal, k-space parameters, and followed by a Fourier Transform to produce bond lengths, within different shells [1]. Results were compared to expected values for different phases from the Chemical Database Service [3] and also to powdered mineral standards of similar composition.

Track samples. C2044,0,41,0,0 (Type B, track #41), C2012,10,134,0,0 (Type A, track #134), C2062,2,162,0,0 (Type A, track #162). A range of mineral standards were also analysed: magnetite, hematite, goethite, Mg-rich olivine from the Admire pallasite meteorite ($\text{Mg}\# = 0.88$ and Fe-sulphide – pyrrhotite Fe_{1-x}S).

XRF analyses of Wild2 tracks: Synchrotron XRF mapping of Wild2 tracks (#41, #134, #162) shows up the Fe- and Ni-bearing minerals very clearly. Some of the $\sim 1\text{-}10 \mu\text{m}$ size ‘hotspots’ were then studied by EXAFS and Fe K XANES.

An important feature revealed by synchrotron XRF mapping and Fe K XANES is the ubiquitous presence of Fe oxide grains along the tracks and the oxidation of FeNi metal [2,4].

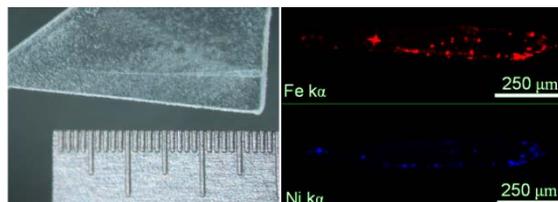


Fig. 1. Track #162 XRF maps. Total track length 2.9 mm.

EXAFS analyses of Comet Wild2 tracks: Examples of EXAFS mineral identifications are given in Table 1 and Fig. 2. Forsterite in track #162 with an Fe-O bond distance of 2.07 \AA is identified. The terminal grain of track #134 has an EXAFS showing 4 nearest neighbouring S atoms at a distance of $2.29 \pm 0.05 \text{ \AA}$.

The #134 midtrack grain has a 95% fit to magnetite [4,5] and our EXAFS are consistent with this. Our identifications of Fe oxides are also informed by microRaman analyses which show magnetite and hematite in track #41 rather than the ferric oxide goethite [2].

Fe K XANES on Track #162. Fe-K XANES were taken approximately $100 \mu\text{m}$ in from the track entrance of track #162 (Fig. 1). The Fe-XANES in (Fig 2) shows hotspot 4 to closely match our olivine standard whilst the others are iron oxides with their distinctive edge positions, which indicate the presence of ferric iron. This signature has been found on all of the hotspots we have studied, with the exception of hotspot 4. Table. 1 summarises their edge positions.

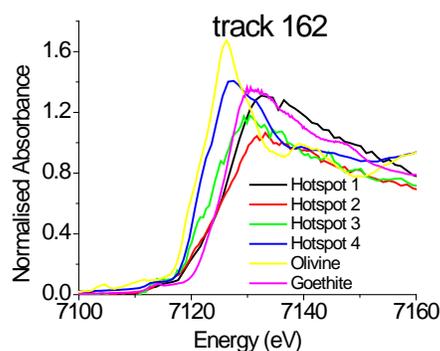


FIG 2. Fe-XANES region of four hotspots from track #162 showing the abundance of ferric iron hotspots.

Table 1. EXAFS Mineral Identification in Wild2

Track	1 st Shell (Fe-O) Å	½ Edge position (eV)	Closest fit XANES	Closest fit EXAFS
#162, 1	2.01	7124.6	Hematite	Hem/Mag
#162, 2	2.01	7124.2	Hematite	Hem/Mag
#162, 3	1.99	7122.1	Hematite	Hem/Mag
#162, 4	2.07	7120.6	Olivine	Forsterite
#41, 1	2.01	7122.4	Hematite	Hem/Mag
#41, 2	2.00	7122.6	Hematite	Hem/Mag
#134, midtrack	1.96	7121.4	Magnetite	Hem/Mag
#134 terminal	2.31 (Fe-S)	7117.9	Pyrrhotite	Pyrrhotite

Error in bond lengths ~ 0.03 Å.

Discussion: Bond length information of the first co-ordination shells from Fe-bearing ‘hotspots’ have been determined in all of our track samples. A key assumption made when interpreting these results is that the calculated bond distances have been derived from a dominant phase that has contributed most to the EXAFS signal. The relatively weak EXAFS signal and potentially heavily modified phases at the track entrances have allowed calculation of only Fe-O bond lengths. The EXAFS spectra have, however, been shown to complement the XANES analyses [2] well in identifying oxides, sulphides and silicates.

Each track we have studied by EXAFS and XRF and XANES is found to contain abundant evidence of oxidised grains. Oligioren et al. [6] studied a terminal particle from track #41 that was found to be a large grain of Fe-Ni metal – a mixture of kamacite and taenite. This is consistent with our observations of the ferric oxides in the tracks we have studied here and previously [2] and oxidation of Fe-Ni metal in our track #41 slice, in an uncertain process but perhaps during capture.

Following EXAFS and XANES these tracks are now available for other analyses. For instance, the #134 sample has now had its terminal grain identified – pyrrhotite – in a non destructive EXAFS analysis leaving the track and terminal grain for ongoing analyses by other techniques.

References: [1] Gurman S. J. (1984) *Journal of Physics C: Solid State Physics* 17, 143-151. [2] Bridges J. C. et al. (2010) *Meteoritics & Planet. Sci.* 45, 55-72. [3] Fletcher D. A. et al. (1996) *J. Chem. Inf. Comput. Sci.*, 36, 746-749. [4] Changela H. G. unpub. PhD, *Univ. of Leicester*, in prep. [5] Changela H. G. et al. (2010) *Meteoritics & Planet. Sci.* 45, A32. [6] Oglione R. C. et al. (2008), 39th LPSC, #2363. [7] Lee P. A. and Pendry J. B. (1975) *Physics Review B* 11, 2795-2811.

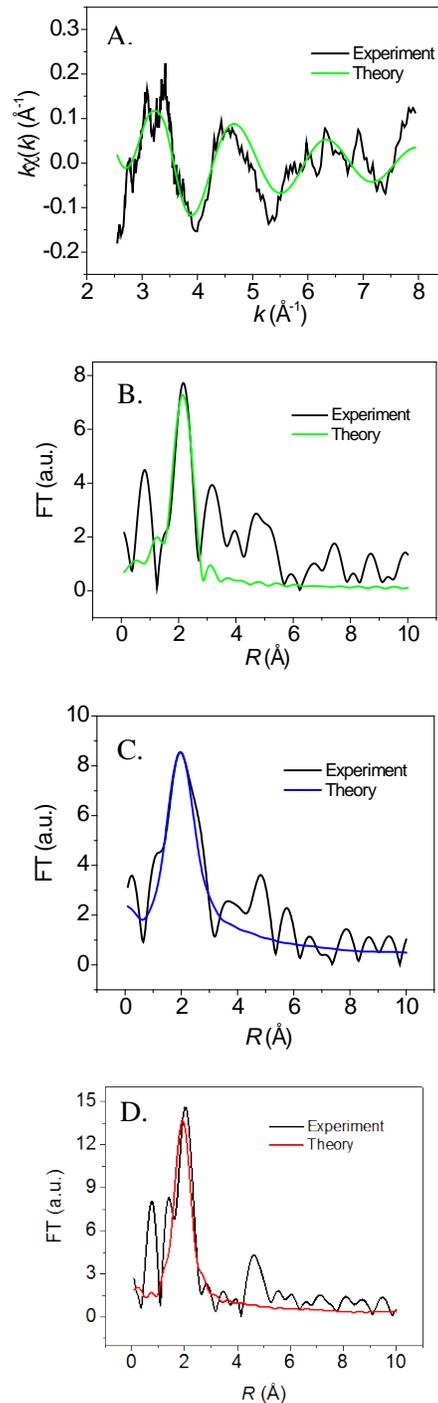


Fig. 2. (A) Pyrrhotite Fe_{1-x}S , k -weighted EXAFS, terminal grain, track #134. (B) Pyrrhotite Fourier Transform (arbitrary units) consistent with 4 nearest neighbouring S atoms at a distance of 2.31 ± 0.05 Å. (C) Fourier Transform of forsterite EXAFS, track #162, hotspot 4. Fe-O distance 2.07 Å ± 0.03 Å. (D) Fourier Transform of hematite from track 41, hotspot 2, Fe-O distance of 2.00 ± 0.03 Å. Theory data from [7].