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ATOMIC ENVIRONMENTS IN IRON METEORITES USING EXAFS

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1. Introduction

Extended X-ray Absorption Fine Structure (EXAFS) is observed as a modulation on the high energy side of an X-ray absorption edge. It occurs when the photo-ejected electron wave is scattered by neighbouring atoms in a solid, and interference occurs between the outgoing and scattered waves. The result is that the absorption spectrum carries a signature that is characteristic of the identity and disposition of scattering atoms around the absorbing atom (see e.g. Stern 1978). It may be shown that the Fourier transform of the normalized EXAFS gives directly the distance, co-ordination number and identity of scattering atoms around the absorbing atom. An analysis of EXAFS can therefore provide detailed information about the immediate environment of specific atoms in a solid and is ideally suited to the study of cosmic dusts.

We have initiated a study of cosmic dusts, using EXAFS and other techniques, at the SERC Synchrotron Radiation Source (SRS) at Daresbury, U.K. We have started this work by investigating what seems to be the simplest type of cosmic material, namely the iron meteorites, the morphology of which has been well-studied using conventional techniques.

2. Iron Meteorites

Iron meteorites have nickel content typically in the range ~ 4 - 40%. The metal normally occurs as two co-existing phases, namely kamacite (which has b.c.c. structure) and taenite (f.c.c.). A portion of the Fe-Ni phase diagram is shown in Fig. 1. Meteorites having high Ni content consist mainly of taenite, whereas those having low Ni content are mainly kamacite.

The iron meteorites investigated in the present study are Uwet (5.6% Ni), Steinbach (9.1%), Mount Edith (9.4%), Butler (15.2%) and Santa Catharina (33.6%) (see Graham et al. 1985). In some cases meteorites having intermediate nickel content were first treated to separate the kamacite and taenite phases.

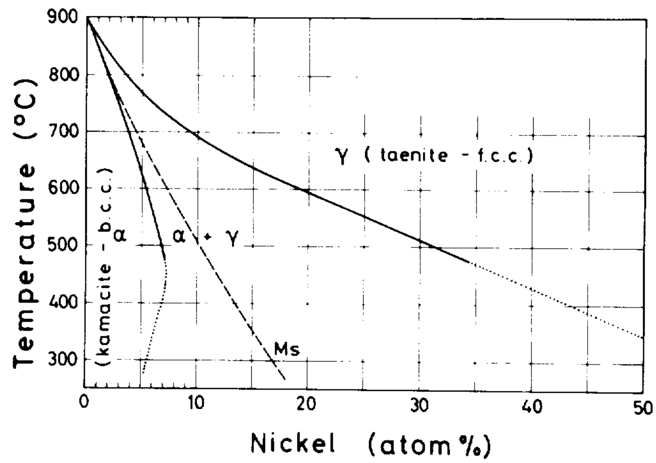


Fig. 1: Fe-Ni phase diagram (after Wasson 1974).

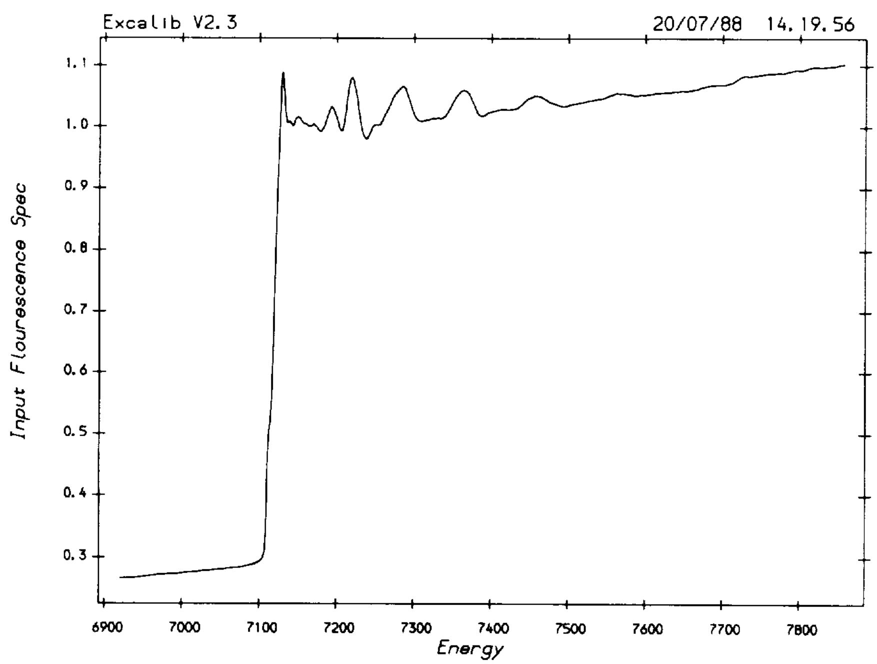


Fig. 2: Relative absorption at the Fe K-edge vs. photon energy (eV) for Butler meteorite.

3. EXAFS

We have measured the Ni and Fe K-edge EXAFS using (i) transmission mode, (ii) fluorescence mode and (iii) a photo-yield ion chamber filled with helium. Iron (b.c.c.) and nickel (f.c.c) foils were used as 'spectroscopic standards'. A typical meteoritic (Butler) EXAFS spectrum - at the Fe K-edge - is shown in Fig. 2.

Fig. 3a shows the spectrum of Ni foil, background subtracted and normalized to the post-edge region where the EXAFS is no longer visible. The Fourier transform is shown in Fig. 3b, the broken curve being a theoretical fit - including multiple scattering effects - for an f.c.c. lattice with 12 nearest neighbour Ni atoms at distance (r) 2.49 Å, 6 Ni atoms at 3.52 Å etc. Figs. 4a,b show the corresponding plots for Fe foil.

The Fourier transform of the EXAFS spectrum of the Uwet meteorite at the Fe K-edge is shown in Fig. 5a (full line); the broken curve is the Fourier transform of the Fe foil spectrum and clearly the Fe b.c.c. structure gives an extremely good fit to the meteoritic data. This result is consistent with the low Ni content of the Uwet meteorite.

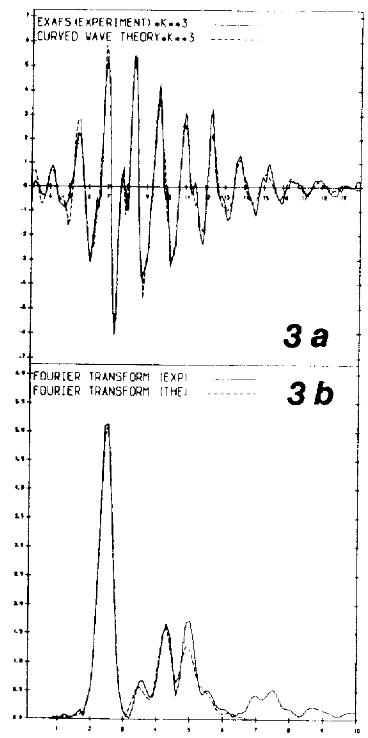
The Santa Catharina meteorite consists of a mixture of kamacite and taenite phases. The Fe K-edge EXAFS for this meteorite is shown in Fig. 5b. In this case neither the Fe nor the Ni alone can adequately fit the data. Instead we find that a combination consisting of 10-20% b.c.c. and 80-90% f.c.c. fit the data well; Fig. 5b shows the fit for a 15:85 combination (broken curve). [Note that, while the general features of the Fourier transform are well described the amplitudes differ because the meteorite and foil EXAFS were obtained using photo-yield and transmission techniques respectively.]

The Butler meteorite also consists of a kamacite-taenite mixture. In this case the data at the Fe K-edge are consistent with a 60-80% b.c.c. and 20-40% f.c.c. mix (see Fig. 6a, which shows the fit for a 70:30 combination). To demonstrate that neither pure b.c.c. nor pure f.c.c. can fit the data, Fig. 6b compares the Butler Fourier transform with the Fe standard only, while Fig. 6c compares Butler with Ni only.

Again the Steinbach meteorite is a kamacite-taenite mix and the data are best fitted by a 80-100% b.c.c. + 0-20% f.c.c. combination. Fig. 7 again compares the Fourier transform for the meteorite data (Fe K-edge) with that for a 90:10 combination.

4. XANES

In addition to the EXAFS, which extends over $\geq$ 100 eV past the absorption edge, information can also be derived from the X-ray Absorption Near Edge Structure (XANES); this is the structure in the absorption close ($\leq$ 40 eV) to, and in, the edge step itself. Fig. 8a shows the XANES around the Fe K-edge for the Mount Edith meteorite (thin line). The thick line is the corresponding XANES for Fe foil, indicating that the bulk of the Mount Edith meteorite is b.c.c., consistent with its known composition. Fig. 8b shows the corresponding



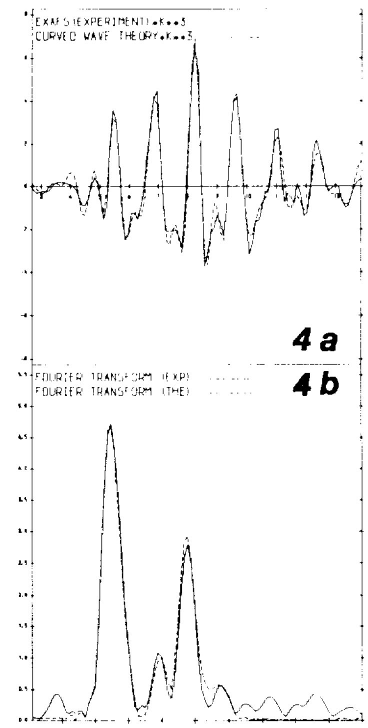
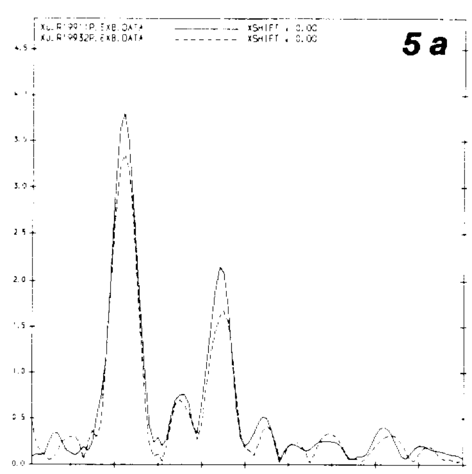


Fig. 3: (a) Normalized EXAFS of Ni foil at K-edge;
(b) Fourier transform of (a).

Fig. 4: (a),(b) As 3(a),(b) but for Fe foil.



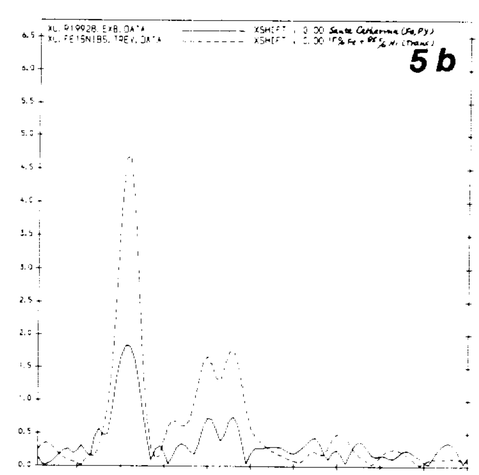
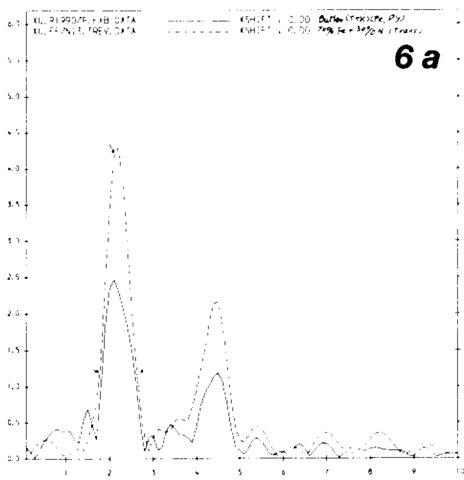


Fig. 5: (a) Fourier transform of normalized Fe K-edge EXAFS for Uwet; see text for details.

Fig. 5: (b) As 5(a) but for Santa Catharina.



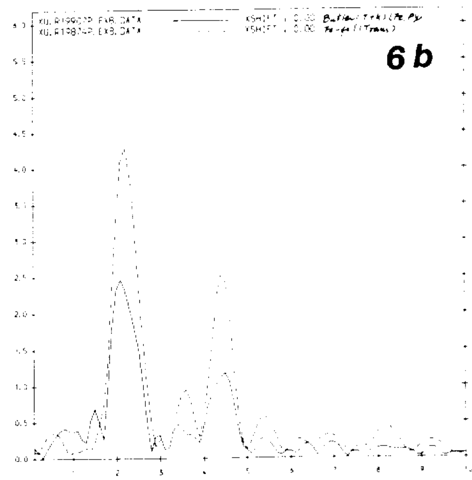
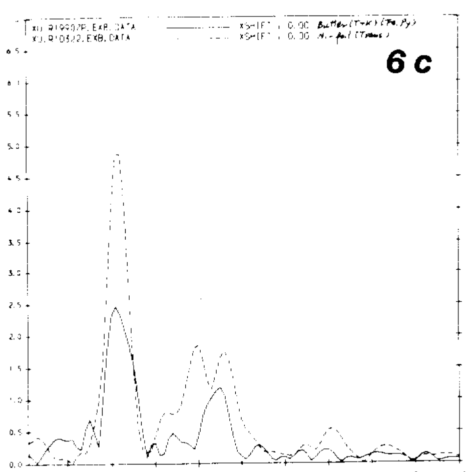


Fig. 6: (a) As 5(a) but for Butler.
Fig. 6: (b) Fourier transform of Butler Fe K-edge EXAFS + Fe foil.



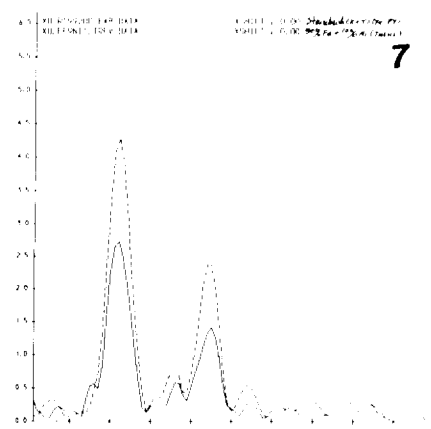


Fig. 6: (c) Fourier transform of Butler Fe K-edge EXAFS + Ni foil.
Fig. 7: As 5(a) but for Steinbach.

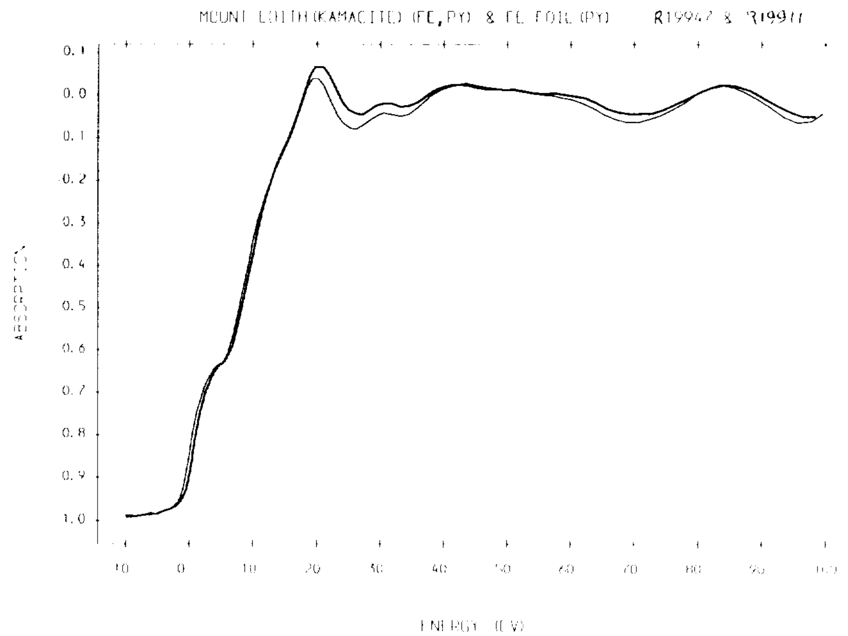


Fig. 8: (a) XANES in Fe K-edge spectrum of Mount Edith.

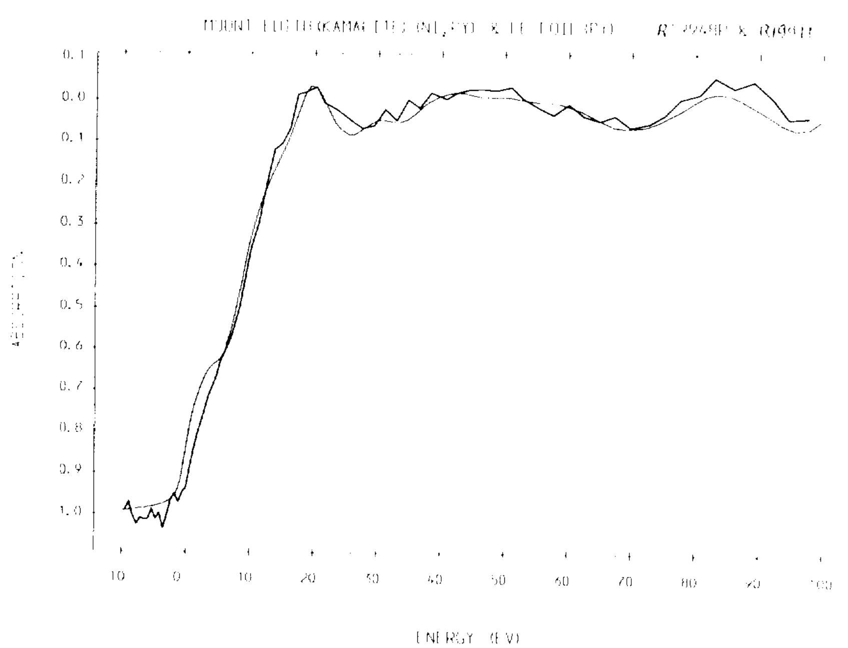


Fig. 8: (b) XANES in Ni K-edge spectrum of Mount Edith.

XANES at the Ni K-edge.

5. Conclusions and further work

Our results to date demonstrate that the relative proportions of kamacite and taenite in bulk samples can be determined with accuracy using EXAFS. Previous determinations have had to rely on optical micrograph and SEM techniques, which provide kamacite-taenite ratios in terms of the relative surface area occupation of the section under consideration; as such previous determinations have tended to be somewhat less representative of the actual bulk value. Since the kamacite-taenite ratio has direct bearing on the thermal history of iron meteorites EXAFS is capable of providing information on the cooling history of these materials (Saikumar & Goldstein 1988).

Our investigation of meteorites at the Daresbury SRS is continuing and future work will include EXAFS and powder diffraction studies of various chondritic meteorites, Brownlee (and other) particles and 'synthetic' dusts. Since EXAFS probes the local environment of specific species in the solid state this work will ultimately throw light on the likely nucleation and crystallization characteristics of cosmic (including interstellar) dusts.

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