Fe K-edge EXAFS and XANES of amorphous iron phosphate materials

G. Mountjoy, R. Apps, and G. Al-Hasni

School of Physical Sciences, University of Kent, Ingram Building, Canterbury CT27NH, U.K.

Amorphous iron phosphates are an interesting materials from several points of view: (i) lithium iron phosphate is an important battery material, and it has been reported that battery charging is improved if an amorphous layer is present [1]; (ii) iron phosphate glasses Fe_2O_3-P_2O_5 are suitable for nuclear waste immobilisation due to their high durability upon inclusion of sodium, i.e. Na_2O-Fe_2O_3-P_2O_5 [2], and (iii) some yeast cells use a biomineralisation pathway involving amorphous iron phosphate [3]. The iron environment in several amorphous iron phosphate materials has been studied using Fe K-edge EXAFS and XANES on beamline A1 at HASYLAB. The measurements were carried out in transmission mode, with samples prepared as pellets diluted with polymer. Figures 1 and 2 show EXAFS and XANES results for Na_2O-Fe_2O_3-P_2O_5 glasses with different sodium content. The results show that the coordination number of Fe is less than 6, and it decreases as the sodium content decreases. These EXAFS and XANES results are especially useful because precise information on the iron environment has been difficult to obtain from diffraction and ^{57}Fe Mossbauer spectroscopy. Further work is under way to develop accurate molecular dynamics models, e.g. see Figure 3. Such detailed structural information is ultimately required to properly understand and hence predict the useful properties of amorphous iron phosphate materials.

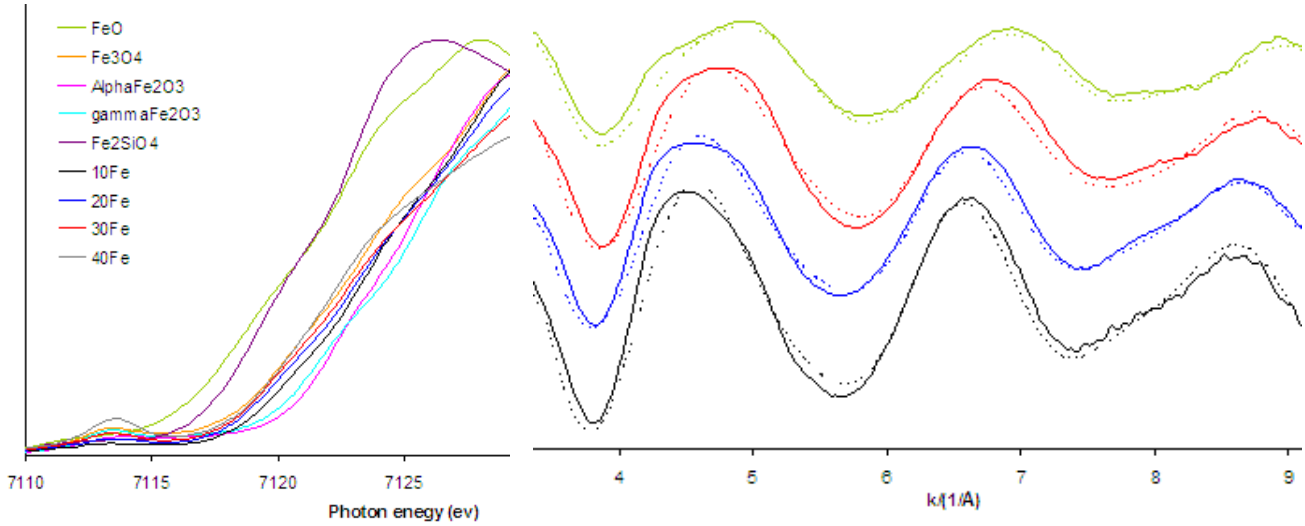

Figure 1 and 2: Fe K-edge EXAFS and XANES of (40-x)Na_2O-xFe_2O_3-60P_2O_5 glasses.

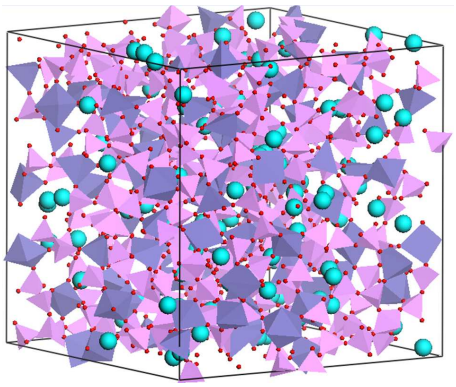

Figure 3: molecular dynamics model of 20Na_2O-20Fe_2O_3-60P_2O_5 glass (PO_4 are pink, FeO_n polyhedrons are grey and Na ions are blue).

References

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[3] W. He, W. Zhou, Y. Wang, X. Zhang, H.Zhao, Z. Li, S. Yan, Mater. Sci. Eng. C **29**, 1348 (2008)