pressure-cell was loaded into a helium flow cryostate.

Analysis of the recorded data shows that $\text{Fe}_{17}\text{Te}$ is tetragonal with space group $P4/nmm$ at 80 K and $\approx0.45$ GPa. A commensurate antiferromagnetic monoclinic phase with propagation vector $k = (\frac{1}{2} 0 0 \frac{1}{2})$ was observed at $\pm 2$K and 0.44 GPa. The magnetic moments of iron of 1.74(7) BM were found to be parallel with the $b$-axis. The magnetic structure observed at $\pm 2$K and 0.44 GPa is closely related to the magnetic structure observed at ambient pressure and $T < 63$ K but with a reduced magnetic moment of iron [1]. The tetragonal $P4/nmm$ structure was preserved at a pressure of 1.15 GPa and 80 K. Cooling at this pressure revealed the existence of a new magnetic phase between 60 and $\approx 48$ K. The analysis of data recorded at 55 K shows that the magnetic phase is incommensurate with propagation vector $k = (0.445 0 0.486)$ was observed at $\pm 2$K and 1.15 GPa. The observed magnetic structure is closely related to the commensurate antiferromagnetic structure observed at $\pm 2$K and 0.44 GPa but with a sinusoidal modulation with an amplitude of 1.98(8) BM and it develops gradually upon cooling from 48 to 2 K.


Keywords: magnetic structure, neutron diffraction, high-pressure.

MS05.P32

Magnetic ionic liquids 1-ethyl- and 1-butyl-3-methylimidazolium tetrachloroferrate(III). Crystallization monitored by powder x-ray thermodiffraction


Ionic Liquids (ILs) are salts with melting points below 100ºC, i.e. they are liquids comprised entirely of cations and anions. ILs exhibit a unique set of physical properties that make them interesting for different applications: non-volatility, high thermal stability, wide liquid-state temperature range, good solvents for synthesis, etc. [1]. In addition, ILs containing transition metal complexes show very interesting magnetic properties [2]. It is known that the physicochemical properties of the ILs can be tailored by the selection of both cation and anion components, but the origins of their unique behavior are still relatively poorly understood [3]. Previous studies demonstrate that a correlation exists between the structure of the ILs in the solid and liquid states. Therefore the elucidation of the crystal structures of these compounds would provide a strong basis from which the ILs properties can be further rationalized. ILs display very complicated thermal and crystallization behavior, such as supercooling and glass formation, pre-melting or solid-solid phase transitions [4]. Usually, ILs thermal behavior studies have been performed by differential scanning calorimetry but, to our knowledge, no thermodiffraction studies have been reported yet.

One of the most prominent cation-type is the N,N'-diakylimidazolium. Their counterion may range from a simple halide to more sophisticated anions. We have investigated the thermal behavior of the magnetic room temperature ionic liquids (MRTIL) 1-ethyl-3-methylimidazolium tetrachloroferrate(III), EMIM[FeCl4], and 1-butyl-3-methylimidazolium tetrachloroferrate(III), BMIM[FeCl4], by using X-ray powder thermodiffraction and differential scanning calorimetry. EMIM[FeCl4] displays thermal polymorphism and exhibits reversible and irreversible solid-solid crystalline transitions with the formation of metastable phases. On the other side, for BMIM[FeCl4] homogeneous crystallization from the melt is inhibited and glass formation occurs on cooling. This amorphous solid crystallizes below room temperature by devitrification on heating from the cooled glassy state. Both systems show a very complex behavior with formation of metastable phases depending on the materials thermal histories. Acknowledgements: Spanish MICINN (MAT2006-01997, MAT2010-15094, MAT2008-06452-C04, and CSD2006-015, Consolider Ingenio 2010, “Factoría de Cristalización”) financial support and FEDER funding is acknowledged.


Keywords: ionic liquid, thermodiffraction, thermal polymorphism.

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Dynamic and crystallographic neutron studies of La$_{1-x}$Ba$_x$GaO$_{2+\delta}$: toward a better understanding of the proton diffusion in new fuel cell materials

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Fuel cells convert chemical energy directly to electrical energy cleanly and efficiently. A crucial part of a fuel cell is the electrolyte, a material that conducts ions. On the way towards practicable solutions, one of the biggest problems at the moment is the lack of stable and effective ion conductor at the desired intermediate temperature range (100-600°C). Solid oxide proton conductors present many advantages compared to the other candidates as they offer higher efficiency than conventional oxygen ion materials.

Novel oxide structures such as La$_{1-x}$Ba$_x$GaO$_{2+\delta}$ containing tetrahedral units and high proton and oxide ion conductivities have been shown to be potential candidates at intermediate temperatures [2,3]. Proton conductivity dominates in wet atmospheres below 700 °C, giving rise to as high protonic conductivity as $10^4$ S cm$^{-1}$ at 500°C [3,4]. In these systems water can be incorporated into the structure as protonic defects from humid atmospheres. However, despite the importance of proton conduction for energy applications, our understanding of the complex mechanisms driving the proton transport is still not well understood [1].

High-resolution neutron powder diffraction as well as quasi-elastic measurements will be presented to highlight our knowledge of the migration/diffusion of protons into the material and therefore understand the dynamic of the phenomenon.