

MS41 P01

Crystal chemistry and magnetic properties of Cu_5FeS_4 (bornite): a Mössbauer study. M. Borgheresi^a, F. Di Benedetto^a, M. Romanelli^b, G.P. Bernardini^a, W. Lottermoser^c, G. Tippelt^c, G. Amthauer^c, ^a*Department of Earth Sciences and Natural History Museum, University of Florence, Italy.* ^b*Department of Chemistry, University of Florence, Italy.* ^c*Department of Materials Engineering and Physics, University of Salzburg, Austria.* E-mail: georg.amthauer@sbg.ac.at

Keywords: bornite, crystal chemistry, magnetism, Mössbauer

Cu_5FeS_4 (bornite) is an interesting compound because (i) it is one of the most important ore minerals for copper and (ii) it has special semiconducting and magnetic properties used in several high-tech materials, e.g. diluted magnetic semiconductors. Bornite occurs in three different polymorphs, i.e. high bornite (Fm3m), intermediate bornite (Fm3m), and low bornite (Pbca), connected by superstructure relationships. In high bornite, vacancies and metal-ions are completely disordered, in low bornite completely ordered.

Bornite orders antiferromagnetically at $T_N \sim 64$ K [1, 2, 3] and undergoes additional transitions at 35(3) K and 10 K [4]. Below 64 K, bornite is a collinear antiferromagnet with spins oriented parallel and antiparallel to the b-axis [1]. Concerning the crystal chemistry of bornite, major open questions still are (i) the valence state of Fe and Cu and (ii) the nature of the magnetic phase transitions at low temperatures which are not yet really understood.

The aim of the present investigation is to perform a Mössbauer study of bornite at temperatures below RT and by this (i) to contribute to the solution of the problem of site occupancy, valence state and chemical bonding of Fe in bornite and (ii) to obtain more informations on the phase transitions in the antiferromagnetic stability field. Results of this study will be reported at the conference.

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MS41 P02

Synthesis and structural studies of the ettringite group of minerals S. Cairns, and C. Wilson, *Department of Chemistry, University of Glasgow, Glasgow*; C. A. Kirk, *Department of Mineralogy, Natural History Museum, London.*

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Thaumasite ($\text{Ca}_6[\text{Si}(\text{OH})_6.12\text{H}_2\text{O}]_2(\text{SO}_4)_2(\text{CO}_3)_2$) and ettringite ($\text{Ca}_6\text{Al}_2(\text{SO}_4)_3(\text{OH})_{12}.26\text{H}_2\text{O}$) are members of the Ettringite group of minerals, with the general formula $\text{Ca}_6\text{X}_2(\text{SO}_4)_3(\text{OH})_{12}.26\text{H}_2\text{O}$, where X = Al, Cr, Fe, Mn, Si and the sulphate group can be substituted by carbonate or borate groups. Although the minerals are compositionally closely related, structurally they are different. Ettringite and Thaumasite¹ are the most important members of the

group as they form in cement pastes, mortars and concretes. They are formed by the action of sulfates on cement and concrete – the sulfate attack results in softening and disintegration of the cement matrix. This has major implications for the construction industry and further study into the structure of these compounds is required to address this issue.

The water structure and hydrogen bonding network in the Ettringite group of minerals are of particular interest, because they contain large amounts of water, approximately 40% by weight. It is clear from the importance of water structure to the integrity of these minerals that a detailed knowledge of the hydrogen positions in these structures is important to understanding the formation and stability of these minerals.

A systematic study of the structural chemistry of Ettringite, Thaumasite and their related phases is being undertaken using powder and single crystal x-ray diffraction, single crystal neutron diffraction, IR, TGA, DSC and SEM of both natural and synthetic samples². Although structural determinations have previously been carried out for several members of the Ettringite group, no systematic study has been carried out to investigate the structural relationships between them. A detailed phase diagram exploration is one of the aims of our programme, to include analysis of synthetic analogues of these mineral phases and investigations into potential solid solutions that may exist between different members of the Ettringite group.

The initial stages of a synthesis programme have begun, designed to provide single crystals of ettringite and new analogues of the ettringite family. It is my intention to report on the progress of both our synthetic programme and structural investigations into these minerals.

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MS41 P03

Influence of particle size on the thermal decomposition of calcite George E. Christidis^a, George Triantafyllou^a, ^a*Technical University of Crete, Department of Mineral Resources Engineering, 73100 Chania, Greece.* E-mail: christid@mred.tuc.gr

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Thermal decomposition of calcite has been studied thoroughly in the past due to its significance on the formation of lime. Lime and slaked lime are important synthetic industrial minerals, which are utilized in numerous industrial applications. In this study we examined the influence of crystal size on the thermal decomposition of calcite present in carbonate rocks from various places of Greece. The carbonate materials used are micritic limestones from Kefalonia (Lk) and Arta (La) areas with 18.5% and 3.2% porosity respectively and 4.1 μm and 1.5 μm mean grain size respectively, and marbles from Asfendou, Crete (Ma) and Naxos Island (Mn) each with 4% porosity and 335 μm and 656 μm mean grain size respectively [1]. The kinetics of thermal decomposition of calcite in the various materials was tested with Time-Temperature-Transformation (TTT) diagrams and isothermal curves obtained from TG analysis. The onset of the conversion of calcite to lime occurs at 640°C for all