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MARY KAISER WILLIAM

REACTOR AND NEUTRON PHYSICS DEPARTMENT ATOMIC ENERGY AUTHORITY, CAIRO

FROM

FACULTY OF GIRLS, AIN SHAMS UNIVERSITY, CAIRO EGYPT

1986

Theesa Advancers

Assistant Professor Dr. Yohia Abbos. Celia Abbos. Assistant Professor Dr. Evon Aziz Faras. Assistant Professor Dr. Ychia Abbos. 1-

2-

Approved

Head of Physics in . 14 A.Kency



Beside the present work in the thesis, the Candidate has attended and passed successfully post graduate for the partial fulfilment of the requirements of the degree of Master of Science in Physics during the academic year (1979-1980).

- 1. Electronics and Nuclear Physics
- 2. Solid State Physics and Radiology
- 3. A Special Course in Solid State Physics

Post Graduate Office

Ald A. Tole

Head of physics Delth

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ABSTRACT

The crystallographic and magnetic properties of the two ferrites samples $Ni_{1.5}$ Fe $Ti_{0.5}$ 04 and $^{Mg}_{1.5}$ Fe $Ti_{0.5}$ 04 have been studied by neutron diffraction.

The studied samples were chosen both for their importance in technology, and hence, the need for accurate knowledge of their crystallographic and magnetic parameters, and their role in clearing the fundamental properties of ferrites. To our knowledge no neutron diffraction studies was performed on these compounds.

The two compounds have the spinel structure and the two characteristic parameters of the spinel structure namely oxygen parameter and cation distribution of the individual cations between the tetrahedral (A) and octahedral (B) sites were determined from the comparison of the observed and calculated intensities of neutron diffraction diagrams taken for the two compounds, and using a least-squares computer program.

For the compound $\operatorname{Ni}_{1.5}$ Fe $\operatorname{Ti}_{0.5}$ \mathcal{C}_4 , it was found that the cation distribution in mainly determined by the site preference of the cations and the Ni^{2+} ions occupy the B-sites positions in the spinel structure while the Ti^{4+} ions were equally distributed between the A and B-sites positions. For the compound $\operatorname{Mg}_{1.5}$ Fe $\operatorname{Ti}_{0.5}$ O_4 , it was found that all the Ti^{4+} ions occupy the B-sites positions of the spinel structure. Using the determined lattice parameters and atomic positions the bond lengths in the unit cells were calculated.

Neutron diffraction measurements at high temperatures are used to determine the magnetic structures of the compounds under investigation. It was found that the compounds order ferrimagnetically under their Curie temperatures. To. The magnetic structures are Néel type with resultant magnetic moment equals to the difference of the magnetic moments of the tetrahedral (A) and octahedral (B) sublattices with complete parallism of ionic moments inside each sublattice. Relationships between structural and magnetic properties are discussed.

Introduction

The wide variety of magnetic materials can be rather sharply devided into two groups, the magnetically soft (easy to magnetize and demagnetize) and the magnetically hard (hard to magnetize and demagnetize). The destinguishing characteristics of the first group are the permeability and the magnetic loss factor, The permeability should be high and the losses low. Magnetically hard materials are made into permanent magnets, here a high coercivity is a primary requirement because a permanent magnet, once magnetized, must be able to resist the demagnetizing actions.

Ferrites which are soft magnetic materials have become firmly established as one of the most important classes of present day magnetic materials and are widely used in linear, digital and microwaves branches. (1,2)

Ferrites with high permeability and low losses are used for a wide range of applications in the field of carrier telephony, cores for inductors and transformers. The advantage of ferrites lies in their high

electrical resistivity; at least a million times of metals. This very large resistivity means that an applied alternating magnetic field will not induce eddy currents in a ferrite. This property makes ferrites almost ideal materials for high frequency applications.

Another class of application arose when it
was found possible to prepare spinel ferrites, such
as Mn Mg, Mn Cu and Li Ni ferrite, having
substantially rectangular hysteresis loops. The
main use of these materials is for memory cores.
These are very small toroids which are used in large
numbers as elements in rapid access data stores.

Another class of application is the microwave ferrites application which are used in wave guide isolators, switches, circulatores, modulators, etc.

By far the most important group of soft magnetic ferrites are those with cubic spinel structure.

, A.

Their composition is given by the formula $Me_3 C_4$, where Me are mostly a combination of several metal ions. The valency of the ions can vary between 1 and 5. The average valency should be 8/3.

The spinel structure which name originates from the mineral "spinel" Mg Al₂ O₄ has a cubic dense backing of oxygen ions. The metal ions, which are smaller than the oxygen ions, occupy part of the interstices. There are two types of interstices, tetrahedral or A-site which are surrounded by 4 oxygen ions, and octahedral or B-site surrounded by 6 oxygen ions.

The unit cell contains 32 oxygen ions, 8 A-sites and 16 B-sites. Usually the chemical composition is written as $Me^{2t} \left[Me_{2}^{37} \right]^{2-}$ where the ions on B-sites are given between the bracktes.

An important property of the spinel ferrites is the so-called cation distribution, i.e the distribution of the metallic ions over the A - and B-sites. The magnetic properties are related to the distribution of the cations in the lattice. Most cations distribution measurements are based on the resultant magnetic moments, which involve adopting a definite model for the magnetic structure. This demonstrates the advantage of distribution determination directly by x-ray diffraction and neutron diffraction. Each method has its limitation and is applicable only to certain systems. There are two reasons why it is often difficult to use x-ray diffraction in research on ferrites:

- 1. Most ferrites have cations that differ little in atomic number, so their scattering
 amplitudes are nearly equal but, for neutron diffraction the scattering amplitudes
 are significantly different.
- 2. Special methodes are necessary to determine exactly the oxygen parameter u with x-ray technique. Since the oxygen atoms make

only a relatively small contribution against the background of the reflections from the heavy atoms.

These difficulties are overcome automatically if neutron diffraction is used, since it gives not only the atomic structure but also the magnetic structure, since additional informations are obtainable from coherent magnetic scattering which contribute to the diffraction pattern at temperatures below the Curie point.

Among ferrimagnetic spinels, ferrites substituted with titanium are now becoming commerically important. Ferrites for high quality telephony filters are
required to have a low loss, a linear relationship between permeability and temperature and a stable value
of permeability over long period of time.

i.e a small disoccommodation. The addition of quadrivalent titanium ions, Ti⁴⁺. to manganese - zinc

ferrite as has been demonstrated by Stijntjes et al (3), shows considerable improvements in all these properties, which make it possible to reduce the size of an inductor whilst maintaining the same performance. A particular feature of the substitution of titanium is that the nature of disoccommodation process is modified giving pronounced improvements in the long term stability. This effect was described by Knowles et al (4).

The main purpose of the present work is to describe the use of neutron diffraction for studying two fer-rites having the composition

The crystallographic parameters, the distribution of different cations on the two sites and the oxygen parameter for the compounds under investigation are to be determined.