IOSR Journal of Applied Physics (IOSR-JAP)
e-ISSN: 2278-4861.Volume 9, Issue 5 Ver. II (Sep. - Oct. 2017), PP 61-63
www.iosrjournals.org

X- Ray determination of thermal expansion of Iron Sulphide

[*]Mohammed Wahed Hussain, Mohammed Yousuf Hussain Ansari
Department of Physics Chaitanya Postgraduate College Warangal, Telengan Sate, India
Department of Physics Government Degree College Warangal, Telengan Sate, India
Corresponding Author: Mohammed Wahed Hussain

***Abstract**: Lattice constant of Iron Sulfide (FeS_2) was measured at various temperature by X – ray diffraction method. Slight nonlinearity in the temperature variation of lattice constant was observedat high temperature. The data were fitted to three term polynomial in the temperature range of 300K to 700K. $a_T = 5.4062 + 0.414 \times 10^{-4} T + 1.031 \times 10^{-8} T^2$. By Differentiating the equation we get the following equation for linear expansion as $\alpha = 7.64 \times 10^{-6}.+0.380 \times 10^{-8}$.Coefficient of expansion increases linearly with temperature in pyrite crystal.*

***Keynote**: X ray diffraction, Lattice Constant and Themal Expansion Coefficeint.*

Date of Submission: 21-08-2017 Date of acceptance: 23-09-2017

I. Introduction

The Iron Sulphide (FeS_2) is well known mineral known from centuries as a ignition material that gives spark when struckagainst. steel. In ancient Roman such materials are called as Pyrite. It is usually found in association with sulfides and oxides in quartz veins, sedimentary rock and metamorphic rock as well as in coal beds, as a replacement mineral in fossils. It is sometimes found in association with small quantities of gold. The metallic luster consist of pale brass yellow. It is also known as fool's gold.

The structure isface centred simple cubic with four molecule per unitcell. and was among the first crystal structure solved by X - ray diffraction. It belongs to the crystallographic space group *Pa*3 and is denoted by the Strukbericht notation C2.

The Unit cell is composed of Fe face centered cubic sub lattice into which S ions are embedded. The pyrite structure is also used by other compounds MX_2 of transition metals M and Chalcogens X = 0,S,Se and Te. Also certain elements with *X* standing for P, As and Sb etc. are known to adopt the pyrite structure.

In the first bonding sphere the Fe atoms are surrounded by six S atoms as nearest neighbors, .the material is diamagnetic semiconductor with a band gap of 0.95 ev. The Fe ion should be considered in low spin divalent state as suggested by Mossbaur spectroscopy.

The positions of *X* ions in the pyrite structure may be derived from the Fluorite structure. The disulphides of Fe, Ni, and Co form crystals with cubic structure known as pyrite. Its space group is Pa_3. These crystals are insoluble in water occurs as mineral and are stable over a high teperature range.

Pyrite group has attracted considerable attention in recent years. Number of properties has been investigated in detail over a wide range of temperature. Some measurements have been made earlier but they cover limited range of temperatures.

Experimental

A mineral crystal was available. It was ground to a fine powder. A complete diffractogram was obtained for the sample; it did not show up any phase other than the pyrite phase. The same sample was used for further photographic work at elevated temperatures. Copper radiation is not suitable for this substance. Diffraction photographs of good quality were obtained with Fe radiation. Although the quality of the photographs was good, very long exposure time was necessary because of the weak power from the iron target tube. Seven photographs were obtained in the temperature range 300-650 K.

The values of the lattice constant of iron sulphide obtained at different elevated temperatures are given in table-1. They are also shown in figure-1. There is a very slight nonlinearity in the temperature variation of the lattice constant. The data were fitted to a three-term polynomial in temperature; the following equation was obtained.

$a_T = 5.4062 + 0.414 \times 10^{-4}{}_T + 1.031 \times 10^{-8} T^2$

where a_T is the lattice constant in A and T is the temperature in K. by differentiation of the above equation, the following equation is obtained for the coefficient of linear expansion.

$\alpha = 7.64 \times 10^{-6} + 0.380 \times 10^{-8}{}_T$

The values of the coefficient of expansion calculated from this equation at some elevated temperatures are given in table-1 along with results from other investigations.

Gordon (1951) and Menary (1955) reported value of 5.4179 and 5.417 A for the lattice constant at room temperature. Straumanis et al., (1964) obtained values of 5.4174 and 5.4189 A for the lattice constant for a neutral sample and a synthetic sample respectively. Chrystal (1965) obtained a value of 5.4180 A at room temperature. The value obtained in the present work is 5.4195 A which is close to the value obtained by Straumanis et al.

Sharma (1951) obtained a value of 8.64 x 10^{-6} K^{-1} for the coefficient of linear expansion of iron sulphide at room temperature. Straumanis et al, (1964) give a range of values 8.3-9.65 (10^{-6} K^{-1}). Chrystal (1965) obtained a value of 9.07 x 10^{-6} K^{-1} at room temperature. A value of 8.78 x 10^{-6} K^{-1} has been obtained in the present work which is consistent with the earlier values.

The temperature variation of thermal expansion is shown in figure-2. Limited data at low temperature are available from the work of Valentiner and Wallot (1915).

The present results form a smooth continuation of the low temperature data. The present results are in fair agreement with the results obtained by Chrystal (1965). There is considerable difference between the results obtained by Sharma (1951) and those in the present work as well as in the work of Chrystal (1965). Sharma (1951) observed a nonlinear temperature variation and his values at elevated temperature are much higher than those obtained by Chrystal and in the present work.

Table-1 Values of lattice constant (a) of iron pyrites at elevated temperatures

Temperature (K)	**a (A)**	**Temperature (K)**	**a (A)**
305	5.4195	523	5.4305
376	5.4231	579	5.4337
425	5.4257	636	5.4356
476	5.4284	-	-

Table-2 Values of the coefficient of thermal expansion (α) of iron pyrites at elevated temperatures

Temperature (K)	**α (10^{-6} K^{-1})**		
	Present work	**Sharma (1951)**	**Chrystal (1965)**
300	8.78	8.64	9.07
350	8.97	9.22	9.31
400	9.16	9.85	9.61
450	9.35	10.01	9.90
500	9.54	11.23	10.19
550	9.73	11.99	10.48
600	9.92	12.78	10.77
650	10.11	13.32	11.03
700	10.30	14.50	11.35

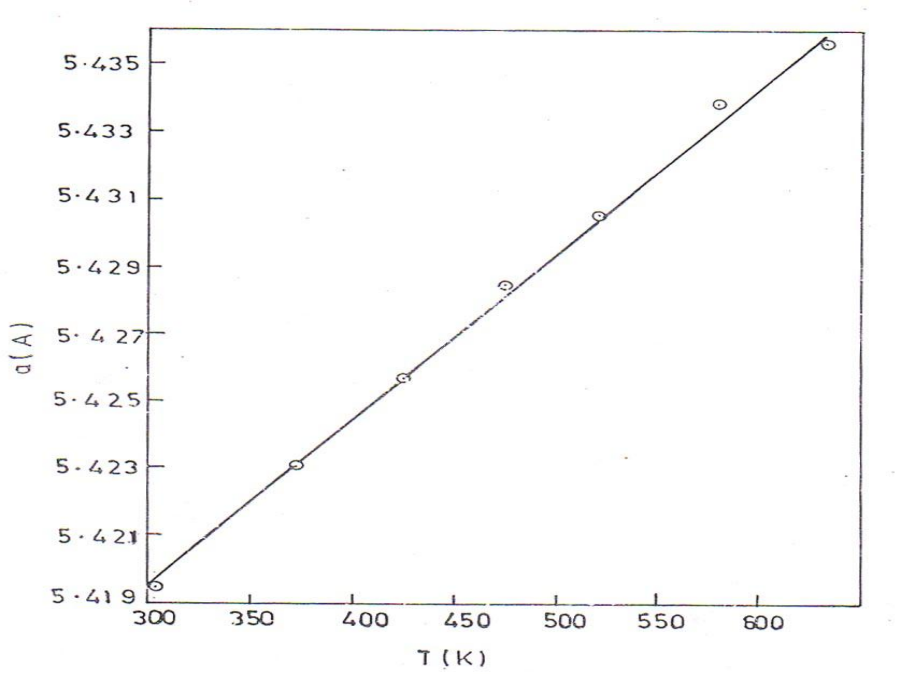

Figure 1: Temperature variation of lattice constant of FeS_2

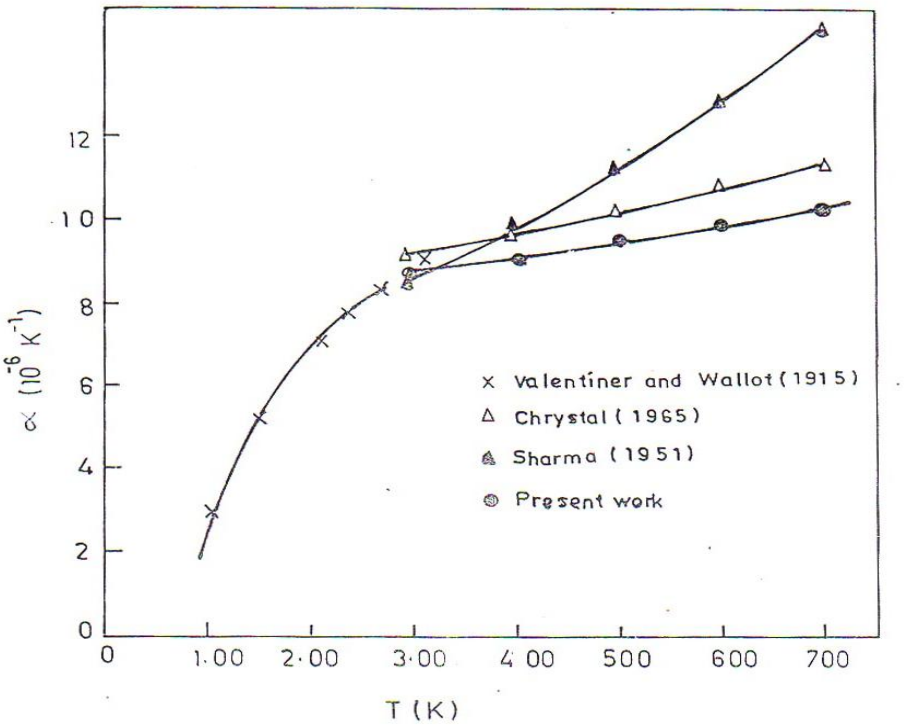

Figure 2: Temperature variation of thermal expansion of FeS_2

Acknowledgements

The authors are grateful to Dr.D B Sirdeshmukh for the encouragement and inspiring guidance throughout the career.

References

[1] Chrystal R S B (1965) Trans. Farad. Soc. 512, 1811
[2] Gordon (1951)Amer. Miner. 36, 918
[3] Menrarry J W (1955)Acta Cryst8, 840
[4] Sharma S S (1951)Proc. Ind. Acad. of Sci. 341, 72
[5] Stramaumanis M E, Armstrong G Cand Chan S (1964) Amer. Min . 49, 206

IOSR Journal of Applied Physics (IOSR-JAP) is UGC approved Journal with Sl. No. 5010, Journal no. 49054.

Mohammed Wahed Hussain. "X- Ray determination of thermal expansion of Iron Sulphide." IOSR Journal of Applied Physics (IOSR-JAP), vol. 9, no. 5, 2017, pp. 61–63.