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Analysis of Elastic constants and Lattice Parameters of Fe_2B from X-Ray Diffraction Technique

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***Abstract*— Elastic constants like Bulk modulus, Shear modulus and magnetic moment were calculated theoretically using the Birch–Murnaghan equations of state fitted into the equation of state. This data was compared with the experimental data Published by Chen B, Penwell D, Nguyen J H and Kruger M B 2004 *Solid State Commun.* The experimental data used for comparison was studied by using Energy - dispersive X-Ray diffraction technique, keeping the temperature constant. It is found that no phase transformation has taken place in this study of pressure change from 0 to 50 GPa. Lattice parameters were calculated using the already available data of D spacings .We noticed that the there is only a small variation in the pressure derivative of the bulk modulus, lattice parameters and the magnetic moments values. However the Young's modulus and shear modulus are as published by B Xiao et al, *A comparative study of Cr7C3, Fe3C and Fe2B in cast iron both from ab initio calculations and experiment.* The variation found in the bulk modulus is only due to the inconsistent pressure values in the experiment.**

***Keywords*— Iron Boride, Elastic constants, lattice parameters, high pressure, Theoretical analysis.**

I. Introduction

Iron Boride formed in the mircostructures of steel can alter the mechanical properties in a direct or indirect way. However the experimental data on mechanical properties of these compounds are limited. Hence the elastic constants are evaluated from the X-Ray diffraction of Fe_2B in this work. Metallic glasses which are used in various devices such as Electro-magnetic shielding plates, soft magnetic choke coils and high frequency power coils and medical equipment are made primarily from Iron Boron systems. Fe_2B is a primary component of this system and hence is the focus of this study.

Studies have shown that Energy - dispersive X-Ray diffraction under pressure variations of 0-50 Gpa do not cause a phase transformation of the crystal and hence the elastic constants such as bulk modulus and shear modulus remain constant [1]. The present work compares the experimental data already available with the theoretical data calculated by using equations (4), (5), (6), (7), (8) and (9)

II. Data Analysis

Fe_2B was subject to energy dispersive X-Ray diffraction at beam line X17C at the National Synchrotron Light Source (NSLS) at room temperature from 0-50 Gpa[1]. A liquid nitrogen cooled Ge detector with a 2θ of $15.008 \pm 0.02^{\circ}$ was used for collecting the data [1]. The nanostructure was studied using electron microscope imaging with the JEOL JSM7500FA cold Field Emission Gun Scanning Electron Microscope (FEGSEM)[1] . Fe2B under ambient conditions has a body centered tetragonal structure. It is ferromagnetic with the magnetic moment about 1.9Mb per Fe ion at 20K [1]. This experimental data concludes that the diffraction patterns at each pressure are similar to one another up to 50Gpa (fig.1) and hence we conclude that Fe2B did not undergo any phase transformations to another crystalline or amorphous phase.[1]

In their experiment, the following X-Ray diffraction lines were obtained from Fe2B at each pressure (Fig. 1): (121), (130), (400), (330), (123), (402), (332), (323) and (521). It is clear from the graph of figure 1 that the Bragg peaks shifted to higher energies as the pressure increased. [1]

Figure 1 and 2 are taken from [1].

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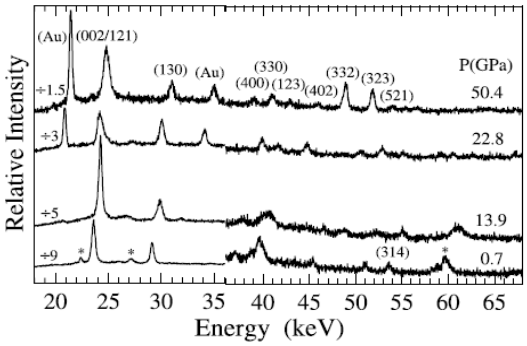

Fig. 1. Representative diffraction patterns at 0.7, 13.9, 22.8 and 50.4 GPa for quasi-hydrostatically compressed Fe_2B. The Bragg scattering peaks due to gold are marked with 'Au', while the peaks due to gasket are marked with asterisks and the peaks due to Fe_2B are labeled with the appropriate Miller indices. For clarity, the diffraction patterns in the ranges of 18–36 and 36–68 keV are presented in different scales.

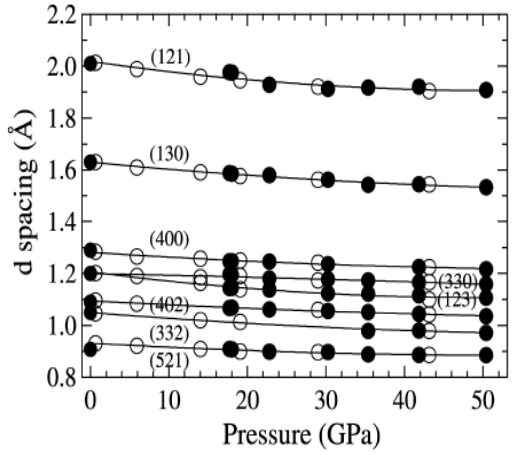

Fig. 2. Interplanar *d*-spacings as a function of pressure. The closed symbols indicate the data taken upon compression, while the open symbols are for the data taken upon decompression. The solid lines are guides. The (330) and (123) peaks overlap at low pressures, but separate with compression.

The above data in figure 2 was used to analyze and calculate the lattice parameters.

III. Theoretical Analysis

The Birch–Murnaghan equations of state was used to analyze the data

$$Fv = K[1\text{-}1.5(4\text{-}K`)fv] \quad (1)$$

Where negative of the Eulerian strain measure is fv and normalized pressure is denoted by F_v, F_v and f_v are defined as

$$fv=1/2[(V/Vo)^{2/3} - 1] \quad (2)$$

$$F_v=P[3f_v(1+2f_v)^{2.5}]^{-1} \quad (3)$$

Here, P is the pressure, V_0 represents the equilibrium lattice volume and V is the lattice volume at that pressure. Equation (1) (2) and (3) are taken from [1]. The Birch–Murnaghan equations of state are fitted into the solid state equation and therefrom equation (4) is obtained [2]. The bulk modulus (B_0), pressure derivative of B_0 and the equilibrium cell volume (V_0) for the corresponding crystal was obtained using equation (4) and (5)

$$E(V)= - 9/16B_0\ [((4 - B'_0)V_0{}^3/V^2) - ((14 - 3B'0)V_0^{7/3}/V^{4/3}) + ((16 - 3B'_0)V_0^{5/3}/V^{2/3})] + E_0 \quad (4)$$

$$P(V)=32B_0[(V_0/V)^{7/3}-(V_0/V)^{5/3}\times\{1 +3/4(B'_0- 4)[(V0/V)^{2/3}- 1]\} \quad (5)$$

Then from (4) and (5) the following equations are derived:

$$B_0 = [2(1 + v)/3(1 - 2v)]G \quad (6)$$

$$G = [1/(2(1 + v)])]E \quad (7)$$

Here B_0 is the bulk modulus and V_0 represents the equilibrium lattice volume B_0' is the pressure derivative of B_0 and E_0 is the equilibrium energy. Total energy E and pressure P are functions of cell volume V. G and E in expression (7) are shear modulus and young's modulus respectively. For a metal or a metallic bond dominated solid, a good approximation of this value equals 0.3. This assumption is valid in this case [2].The magnetic moment is calculated using the following equation [2].

$$\mu = \left| \int_{Eo}^{Ef} g(DOS, Spin\ up)\, dE - \int_{Eo}^{Ef} g(DOS, Spin\ down) dE \right| \mu_b \quad (8)$$

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In the above equation E is the energy and μ_b is the Bohr magnetron. The integral is calculated from the lowest energy level to the Fermi level for the specific orbital only. μ Refers to magnetic moment g(DOS, spin-up) and g(DOS, spin-down) represent the spin polarized density of state (DOS) for the up channel and the down channel respectively [2].

The lattice parameters were analyzed using the following equation.

$$1/d^2 = (h^2 + k^2) / a^2 + l^2 / c^2 \quad (9)$$

Here d refers to the d spacing, h, k, l are the miller indices and a and c are the lattice parameters. Since Fe_2B is has a tetragonal structure the length and breadth of the cube is equal and hence a=b. The d spacings were taken from figure 2 and fit into equation (9) and the results were obtained.

IV. Results

The calculated results of the shear modulus, Young's modulus, Bulk modulus, pressure derivative of the bulk modulus, and the magnetic moment are tabulated in Table1. Table 2 gives the published data of experimental and theoretical values which are compared with our calculated values. Table 3 gives the data of lattice parameters published by ICSD with the corresponding card number

TABLE I
AVAILABLE LATTICE PARAMETERS WITH THEIR ICSD CARD NUMBERS

ICSD Number	Lattice Parameters (A°)		
	a	b	c
16809	5.088	5.088	4.232

TABLE II
THE CALCULATED RESULTS OF THE BULK MODULUS, PRESSURE DERIVATIVE OF THE BULK MODULUS, SHEAR MODULUS, YOUNG'S MODULUS AND THE MAGNETIC MOMENT

Bulk modulus (Gpa)	Pressure derivative of Bulk modulus	Shear modulus (Gpa)	Young's modulus (Gpa)	Magnetic moment (μ_b)
331.54	4.56	150.32	395.43	2.06

TABLE III
THE CALCULATED RESULTS OF THE LATTICE PARAMETERS

Lattice Parameters (A°)		
a	b	c
5.06	5.06	4.22

The value of bulk modulus calculated significantly differs from the experimental values taken from [1]. This is due to the different methods of obtaining the bulk modulus as in [1]. The values of our work are same as the values in reference [2] with a slight difference in the Poisson ratio. Similarly the pressure derivative of bulk modulus is above 4 which tells us that the mechanical performance of Fe_2B will be greatly affected by pressure variation. As shown in figure 2. Because of this the bulk modulus also changes with variation in pressure and therefore there is a difference of values from [1]. The magnetic moment of Fe obtained is almost equal to that of [2] and different to that of [1] because only the 3rd orbital moment is calculated. If the orbitals of4p and 4s are also included then the moment will reduce considerably. The calculated values are almost the same as the values published by ICSD. There is an error of 0.5% in the a value and an error of 0.2% in the value of c . This error is very small and hence neglegible.

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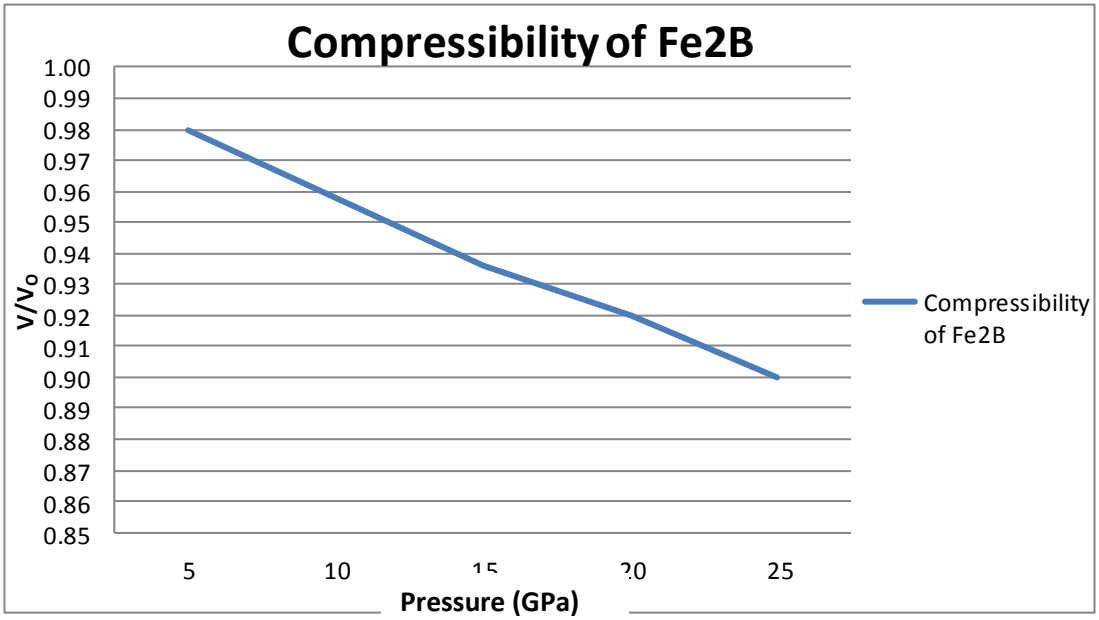
TABLE IV
THE PUBLISHED DATA EXPERIMENTALL AND THEORETICAL VALUES

Bulk modulus (Gpa)	Pressure derivative of Bulk modulus	Shear modulus (Gpa)	Young's modulus (Gpa)	Magnetic moment (μ_b)	References
164 ± 14 331.04	4.4 ± 0.5 4.44	--- 152.77	--- 397.22	1.90 2.02	[1] [2]



V. CONCLUSION

The elastic constants calculated are in good agreement with the published values in [2]. The variation found in bulk modulus from [1] is due to the change in the compressibility with the variation of pressure as shown in figure 2. As stated earlier the experimental evaluation of elastic constants are limited. Broadly these values may be easily calculated from the available X-Ray diffraction studies. The lattice parameters calculated are also in good agreement with the published values as there is a percentage error of 0.5% and 0.2% in the a and c values respectively .

The elastic constants may be further used to calculate the ultrasonic velocity. They can further be used to study the structure of the compound under investigation which is our future study.

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