

Anisotropy of the cubic Fe_3S_4 induced in an electrostatic field

Abstract. A synthetic iron sulphide of spinel type became anisotropic when immersed in an electrostatic field. Analysis of the electron diffraction patterns observed from the Fe_3S_4 specimens showed that a preferred induction took place at about 313 K along the [111] axis in the crystal. This anisotropy became negligibly small over about 373 K.

An aqueous suspension of synthetic iron sulphide (Fe_3S_4 , space group: $\text{Fd}3\text{m}$, spinel structure, $a_0 = 9.87 \text{ \AA}$) was smeared on a smooth surface of mica lamina, about $3 \times 3 \times 0.1 \text{ mm}^3$ in size. The thickness of the sulphide layer deposited was about one micron. The specimen was then investigated in terms of electron diffraction. The disposition of the experiment is illustrated in figure 1. A monoenergetic electron beam served for charging up the

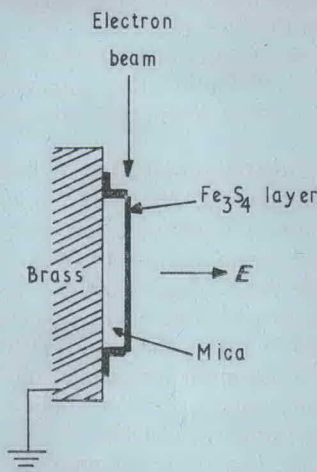


Figure 1. This shows the Fe_3S_4 layer deposited on a mica surface. A monoenergetic electron beam plays three roles, to charge up the mica layer, to heat the sulphide film and to undergo diffraction at it. E is the electrostatic field.

specimen with electrons (Yamaguchi 1966), for heating it by means of electron bombardment (Yamaguchi 1962), and for carrying out the diffraction experiments (Yamaguchi 1968).

The diffraction patterns observed are shown in figures 2 and 3, which correspond to the

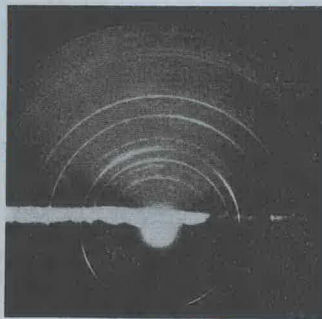


Figure 2. This shows the diffraction pattern from the sulphide specimen in figure 1. At a temperature of about 313 K. The reference pattern of gold is superimposed on the specimen pattern, and the (333) reflection from the sulphide shows a preferred displacement. Wavelength of the electrons: $0.0440 \text{ \AA}$ (75 kV), camera length: 50 cm.

Also included in the figures are the theoretically calculated values of Horner (1970), who used a L-J potential and summed ladder diagrams to all orders to produce ϵ_{sc} , and the results of experiments.

From the results several conclusions and comments can be made. Although ΔF changes the SCP ground state energy considerably (see figure 1) it produces very little change in the volume derivatives of the free energy (the SCP pressure and compressibility are not shown in figures 2 and 3 as their difference between the ISC values is so small that their inclusion would only detract from the clarity of the graphs). The pressure and compressibility are in relatively good agreement with experiment. We found that the compressibility curve calculated in this work lay virtually on top of the ^3He curve that was calculated in I using the L-J potential. For this reason that curve is not reproduced here. The SCP ground state energy is far too high. ΔF is of the right sign and magnitude to lower the energy and produce a value closer to Horner's (1970) result. It must be noted, however, that since ΔF is large compared with F_{sc} (nearly half its value at 18 cm^3) the original philosophy of ISC of treating it like a perturbation on the SCP free energy is questionable. The contribution of the next to the leading term of the second order theory, involving the fourth order force constant squared, might also be substantial. It is interesting to note, however, that this term is also likely to contribute a negative energy and lower the ISC ground state energy even more.

The use of the soft core Beck potential removed the computational difficulties involved in the hard core L-J potential calculations. Accurate numerical results could be obtained over the full volume range considered without recourse to ϵ_{sc} . Nevertheless the deep penetration of the SCP Gaussian wavefunction into the core of the repulsive part of the helium potential is physically unrealistic, and, we believe, is one of the major reasons for the very high value obtained for the ground state energy using SCP. SCP theories that include ϵ_{sc} (see for example Koehler 1967) lower the ground state energy considerably. These theories clearly contain greater anharmonicities than are involved in SCP alone and this is illustrated somewhat in the present work where higher order anharmonic terms have been included in SCP within the framework of ISC.

I wish to thank Professor G. K. Horton for suggesting the present work and for many helpful discussions concerning it. Acknowledgements are also due to Dr V. V. Goldman for use of his computer programme to calculate ΔF . I also wish to thank Dr G. C. Straty for drawing my attention to the experimental 18 cm^3 molar volume compressibility data. Financial support of the US Air Force Office of Scientific Research under grant No. AFOSR 68-1372 and the Rutgers Research Council under grant No. Quantum Crystals 07-2180 is also gratefully acknowledged.

Physics Department,
Rutgers University,
New Brunswick,
New Jersey, USA

G. G. CHELL†
5th May 1971

- BECK, D. E., 1968, *Mol. Phys.*, **14**, 311-5.
CHELL, G. G., 1970, *J. Phys. C: Solid St. Phys.*, **3**, 1861-5.
GLYDE, H. R., 1971, *Can. J. Phys.*, **49**, 761-75.
DUGDALE, J. S., and FRANCK, J. P., 1964, *Phil. Trans. R. Soc.*, **257**, 1-29.
GOLDMAN, V. V., HORTON, G. K., and KLEIN, M. L., 1968, *Phys. Rev. Lett.*, **21**, 1527-9.
HORNER, H., 1970, *Phys. Rev.*, **1**, A 1722-29.
KOEHLER, T. R., 1967, *Phys. Rev. Lett.*, **18**, 654-6.
STRATY, G. C., and ADAMS, E. D., 1968, *Phys. Rev.*, **169**, 323-40.

† Now at the Physics Department, Hicks Building, The University of Sheffield.