

## Magnetic Properties of Fe<sub>2</sub>P Single Crystal

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The magnetic properties of hexagonal Fe<sub>2</sub>P single crystal are studied by the measurements of magnetization, susceptibility, thermal expansion and electrical resistivity along the principal crystallographic axes. It is found that the saturation magnetization per molecule and the Curie temperature are  $2.94 \mu_B$  and 208.6 K, respectively, and the anisotropy constant  $K_1$  is  $2.32 \times 10^7$  erg/cm<sup>3</sup> at 4.2 K, which is considerably larger than the values in 3d-transition compounds. The thermal expansion and the electrical resistivity show discontinuous changes at the Curie temperature indicating that the ferromagnetic to paramagnetic transition of Fe<sub>2</sub>P is accompanied by the first-order transition due to magnetoelastic effects. The exchange striction obtained from the measurement of thermal expansion is discussed on the basis of the theory of Bean and Rodbell.

### §1. Introduction

The crystal structure of Fe<sub>2</sub>P compound was first investigated by Rundqvist and Jelinek<sup>1)</sup> and refined recently by Carlsson *et al.*<sup>2)</sup> This compound has a hexagonal structure with a space group  $D_{3h}^3$  ( $P\bar{6}2m$ ), in which P atoms form a channel lined along the direction of the *c* axis and there are two non-equivalent Fe-atom sites. One of the two, Fe<sub>I</sub>, is surrounded by four P-atoms which form a nearly cubic tetrahedron and the other is Fe<sub>II</sub> surrounded by five P-atoms which form a pyramid as shown in Fig. 1(a). The Fe<sub>2</sub>P structure is built up from

a hexagonal packing of these channel pairs as shown in Fig. 1(b).

Magnetic studies of Fe<sub>2</sub>P compound have been done by many investigators, but there are considerable disagreements in the magnetic properties. The ferromagnetic Curie temperature has been obtained as 306 K by Chiba,<sup>3)</sup> 266 K by Meyer and Cadeville,<sup>4)</sup> 266 K by Fruchart *et al.*,<sup>5)</sup> 226 K by Bellavance *et al.*<sup>6)</sup> and 214.5 K by Wäppling *et al.*<sup>7)</sup> The value of magnetic moment per formula unit has been measured as  $2.65 \mu_B$  by Meyer and Cadeville,<sup>4)</sup>  $2.70 \mu_B$  by Bellavance *et al.*<sup>6)</sup> and  $2.92 \mu_B$  by Lundgren *et al.*<sup>8)</sup> There are also some differences in the hyperfine field obtained by the Mössbauer effect experiment. The hyperfine fields at Fe<sub>I</sub> and Fe<sub>II</sub> at 77 K were reported, respectively, as 117 and 175 kOe by Sato *et al.*,<sup>9)</sup> 110 and 140 kOe by Bailey and Duncan<sup>10)</sup> and 109 and 172 kOe by Wäppling *et al.*<sup>11)</sup> These disagreements may suggest that the slight differences of impurities and stoichiometry have serious effects on the magnetic properties as described by Meyer and Cadeville.<sup>4)</sup> In the present paper, the measurements of magnetization, paramagnetic susceptibility, thermal expansion and electrical resistivity have been carried out on the single crystals prepared carefully to know intrinsic magnetic properties of Fe<sub>2</sub>P compound.

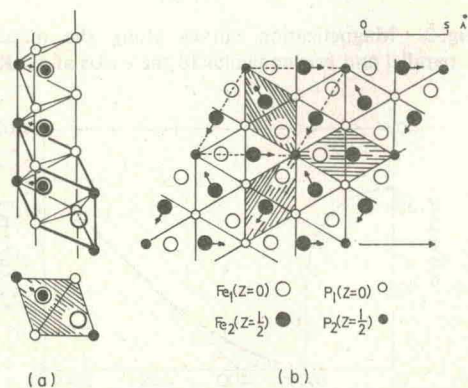


Fig. 1. Crystal structure of Fe<sub>2</sub>P. (a) Relationship of Pyramidal-site and tetrahedral-site atoms. (b) Arrangement of rhombo-hedra subcells.



## §2. Sample Preparation and Experimental Procedure

The compound was prepared by solid-vapor reaction. The mixture of the stoichiometric proportion of iron, 99.99% in purity of a powder form, and phosphorous, 99.999% in purity, was sealed in an evacuated quartz tube and then heated slowly up to 900°C for three days in a furnace and maintained at 900°C for two weeks and cooled in the furnace. The product was ground into powder, again sealed in a quartz tube with an argon atmosphere, melted at 1450°C for about 30 minutes and rapidly cooled in a water. The compound thus prepared was checked by X-ray diffraction to ascertain a single phase, and the deviations of stoichiometry in the ingot was not found with the test of the magnetic measurement of all the parts of the ingot. The single crystal was grown in an evacuated quartz tube by the thermal annealing of this ingot just below the eutectic point. From this crystal, a sphere-shaped specimen of 3 mm in diameter was prepared by the two-pipe lapidary method for the magnetic measurements. A cube specimen of  $7 \times 7 \times 7$  mm<sup>3</sup> with parallel surface to the *ab*, *bc* and *ac* planes was cut out for the measurements of thermal expansion. For the measurements of the electrical resistivity, the rectangular parallelepiped specimens of  $1 \times 1 \times 7$  mm<sup>3</sup> were cut out having the *c*- or *b*-axis direction along the longitudinal direction of the specimen. The magnetization of the single crystal was measured within an error of 1% by using a Foner-type vibrating-sample magnetometer in the applied field up to 50 kOe in the temperatures from 4.2 to 250 K. The paramagnetic susceptibility was measured within an error of 1% by using an automatic magnetic balance in the temperatures from room temperature to 700 K. The electrical resistance was measured by a standard four-probe method in the range from 77 K to 650 K with current reversal. As the current leads and potential probes the manganin wires of 0.2 mm in diameter were spot-welded on the specimen. The cross area of the specimen and the distance between the potential probes were measured with an accuracy of  $\pm 0.01$  mm. The measurements of thermal expansion were made by a dilatometer with an unbonded strain-gauge with an accuracy of  $\pm 5 \times 10^{-5}$

mm.<sup>12)</sup>

## §3. Results

Figure 2 shows the magnetization curves along the directions parallel and perpendicular to the *c* axis at 4.2 K. It is seen that the easy axis of magnetization is the *c* axis and the hexagonal anisotropy is very large. No magnetic anisotropy in the basal plane could be observed. The saturation magnetic moment is  $2.94 \mu_B$  per formula unit which is in good agreement with that obtained by Lundgren *et al.*<sup>8)</sup> This value is nearly equal to  $3.0 \mu_B$  which is the spin only value in the formal valences predicted by Goodenough.<sup>13)</sup>

Figure 3 shows the temperature dependence of saturation magnetic moment  $\sigma_g$  and inverse susceptibility  $\chi_g^{-1}$ . The temperature dependence of  $\sigma_g$  displays in accord with the Brillouin function for  $j = \frac{3}{2}$  rather than for  $j = \frac{1}{2}$  except for in the vicinity of the Curie temperature. The rapid decrease of moment in the vicinity of the Curie temperature is attributed to the fact that the ferromagnetic to paramagnetic transition

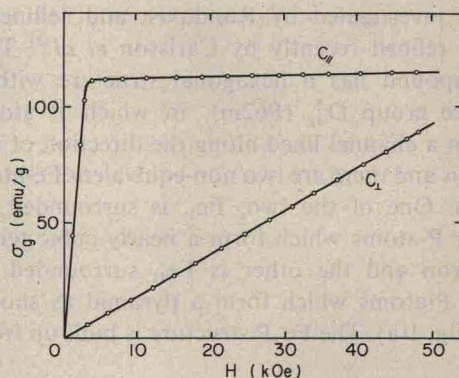


Fig. 2. Magnetization curves along the direction parallel and perpendicular to the *c* axis at 4.2 K.

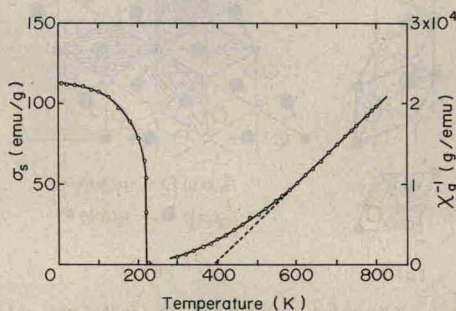


Fig. 3. Magnetic moment,  $\sigma_g$ , and inverse susceptibility,  $\chi_g^{-1}$ , plotted against temperature.