

Erratum: High field magnetization of FePS₃ [Phys. Rev. B **101, 024415 (2020)]**

 A. R. Wildes , F. Duc, F. Bourdarot, D. Lançon, M. K. Chan, F. Weickert, N. Harrison, V. Simonet, M. E. Zhitomirsky, M. V. Gvozdkova, T. Ziman , and H. M. Rønnow


(Received 19 December 2025; published 23 January 2026)

 DOI: [10.1103/ktqg-8ydq](https://doi.org/10.1103/ktqg-8ydq)

Errors have been discovered in the determination of the orientation of the crystal used for the experiments described in the original article. The experiments used parts cut along high-symmetry axes from a high-quality crystal of FePS₃. Subsequent neutron scattering experiments on the remaining crystal have established that the previously determined directions were incorrect.

Figure 1(a) shows the remaining crystal, which has a roughly right-angled-triangular shape. The subsamples used for the experiments were cut from the right and bottom sides of the crystal, corresponding to the hypotenuse and shortest side of the triangle, respectively. The orientations of these cuts were assumed to be correlated to the axes in the top right of the figure. Magnetization data were collected with high fields applied along the “*a*”, “*b*”, and “[110]” axes.

Careful alignment of the crystal for an experiment using the IN22 three-axis neutron scattering spectrometer at the Institut Laue-Langevin, Grenoble [1], showed that these axes were not the corresponding crystallographic axes for the sample. The corrected orientation required a clockwise rotation of the *ab* plane by 30° about the *c** axis. The bottom-right vector in Fig. 1(a) shows the *b* axis determined from the new experiment.

The relationship between the true crystal orientation and the applied field directions for the magnetization experiments is shown in Fig. 1(b). The figure shows the magnetic structure in the *ab* plane, consisting of ferromagnetic zigzag chains parallel to the *a* axis that are antiferromagnetically coupled along the *b* axis. The relationships between the initially stated in-plane applied field directions and the correct crystal orientation are described in Table I.

FePS₃ crystals are prone to the formation of twins due to stacking of the van der Waals layers. The twins correspond to a rotation of the *ab* planes by 120° about the *c** axis [2]. The crystal shown in Fig. 1(a) was previously determined to be almost completely detwinned. This was confirmed on IN22 by cooling the crystal to 80 K, below the Néel temperature of ~120 K, and searching for the 01½ and 01½ magnetic Bragg peaks in each of the three twin orientations. The data are shown in Fig. 1(c).

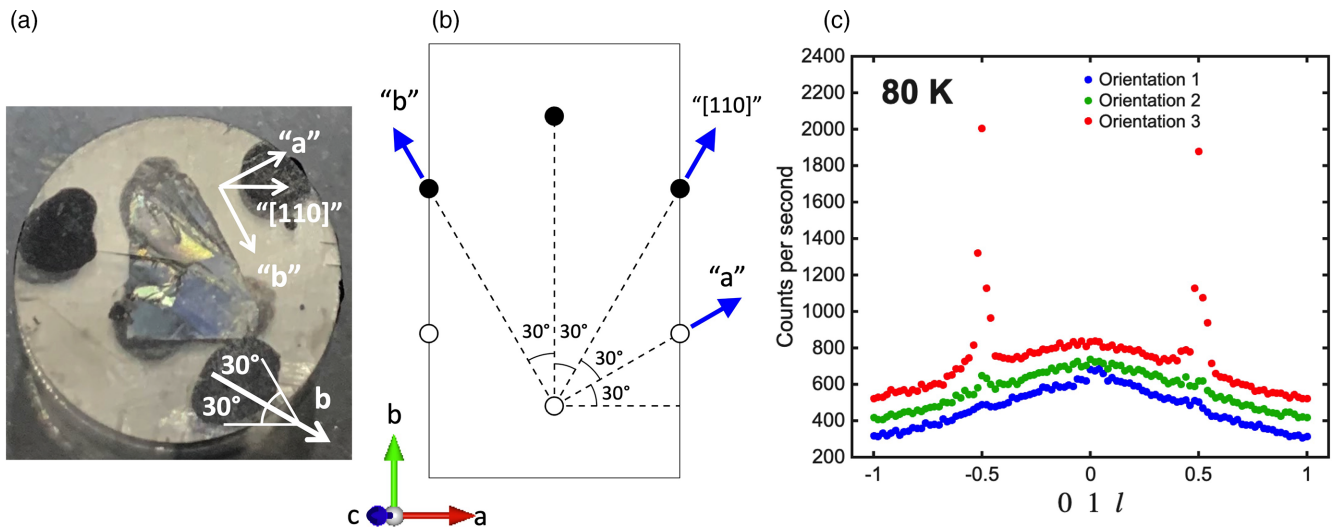


FIG. 1. (a) Remainder of the crystal used for the high-field magnetization experiments. The crystal is the lustrous right-angled-triangular object in the center of the photograph. The matte black blobs are glue used to mount the crystal. The axes labeled “*a*” and “*b*” show the initially assumed crystal orientation. The true *b* axis is shown in the bottom right. In both coordinate systems, the *c** axis is into the page. (b) The relationship between the magnetic structure of FePS₃ in the *ab* plane and the high-field directions for the magnetization experiments. Open and filled circles represent moments out of and into the page, respectively. (c) Neutron diffraction measurements at 80 K along the 01 $\bar{1}$ axis for the three possible 120° domains of the FePS₃ crystal in (a). The crystal axes were subsequently defined according to Orientation 3.

TABLE I. Conversion table between the originally stated field directions and the actual lattice directions determined in experiment [1].

Original directions	Correct directions
“ <i>a</i> ”	[310]
“ <i>b</i> ”	$[\bar{1}10]$
“[110]”	[110]

Only Orientation 3 shows strong magnetic Bragg peaks, identifying the dominant domain and establishing the *b* axis labeled in Fig. 1(a).

Inspection of Figs. 1(a) and 1(b) reveals a second error in the original article in that the “[110]” direction was wrongly designated as being 60° to the *b* axis. The [310] direction would have been the correct designation for the original axes definition. However, the incorrect designation coupled with the 30° error in the definition of the *a* and *b* axes results in the field being, in fact, correctly applied along the [110] axis. Consequently, only Fig. 5 from the original article needs correction, and the corrected version is shown in Fig. 2.

The identification of the correct axes has a minor impact on the discussion of the experimental results. As shown from Fig. 2 in this document and Figs. 6 and 7 in the original article, the magnetization data with high fields applied along $[\bar{1}10]$ and [110] show hysteretic behavior at 4 K with a metastable phase locking in for $H \gtrsim 40$ T. The results are qualitatively similar; however, the hysteresis is far more dramatic when the field is applied along the $[\bar{1}10]$ axis and appears to be coupled to a strong magnetostriction that caused the sample to self-delaminate. Figure 1(b) suggests that there should be no obvious difference between these two directions, both being parallel to antiferromagnetically correlated second-nearest neighbors. The observed difference may have been due to specific characteristics of the two subsamples used for the measurements, as they were cut from different parts of the crystal. The magnetization signal-to-background ratios for all the pulsed high-field measurements in Fig. 2 were relatively small due to the small subsample masses, which accounts for the apparent noise in the data and may also factor into the observed differences. However, an alternative explanation may come from the applied field direction relative to the *c* axis, which for the monoclinic structure of FePS_3 is at an angle of $\beta \sim 107^\circ$ to the *a* axis [3]. When subjected to pressures above 4 GPa, the compound undergoes a structural phase transition featuring a shear of the *ab* planes along the [100] direction resulting in $\beta \approx 90^\circ$ [4,5]. The crystal structure may thus be relatively elastic to shear distortions along [100]. Were a field applied along the {110} axes to result in a shear force parallel to the *a* axis, the $[\bar{1}10]$ field may drive a shear along $[\bar{1}00]$, increasing β in the opposite direction to the elastic shear and thus leading to greater magnetostriction.

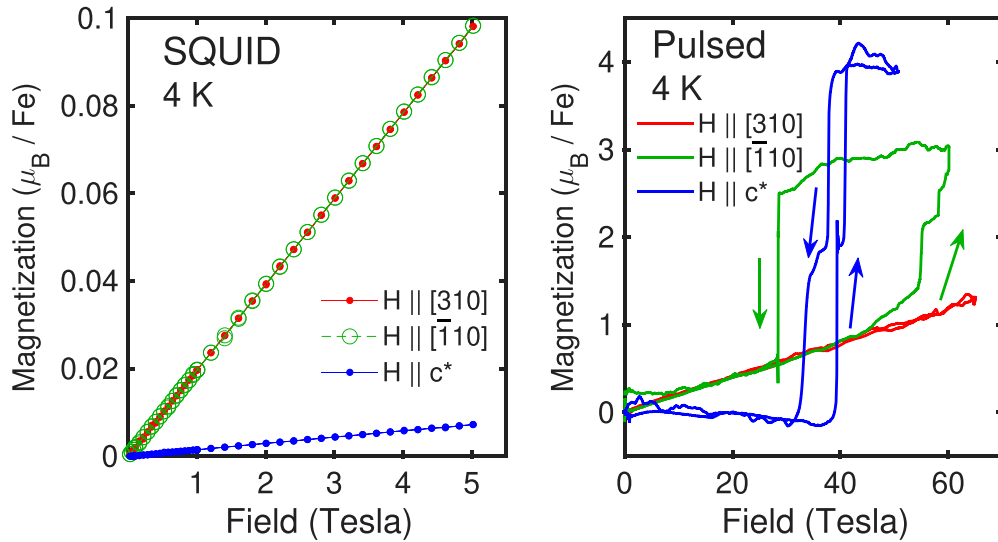


FIG. 2. Corrected Fig. 5 for the original article, showing the SQUID and pulsed-field magnetization measurements of FePS_3 at 4 K in a gaseous helium environment.

We thank the Institut Laue-Langevin for the allocation of beam time for Proposal No. 5-41-1209 [1].

DATA AVAILABILITY

The data that support the findings of this article are openly available [1], embargo periods may apply.

-
- [1] A. R. Wildes, N. Biniskos, F. Bourdarot, J. Brunat, M. J. Coak, S. Deng, F. Duc, J. Hernández, T. Moraine, and X. Zhang, The magnetic structure of the $M/M_{\text{sat}} = 1/2$ plateau in FePS_3 (2024), [10.5291/ILL-DATA.5-41-1209](#).
 - [2] C. Murayama, M. Okabe, D. Urushihara, T. Asaka, K. Fukuda, M. Isobe, K. Yamamoto, and Y. Matsushita, Crystallographic features related to a van der Waals coupling in the layered chalcogenide FePS_3 , [J. Appl. Phys. **120**, 142114 \(2016\)](#).
 - [3] G. Ouvrard, R. Brec, and J. Rouxel, Structural determination of some MPS_3 layered phases ($M = \text{Mn, Fe, Co, Ni}$ and Cd), [Mater. Res. Bull. **20**, 1181 \(1985\)](#).
 - [4] C. R. S. Haines, M. J. Coak, A. R. Wildes, G. I. Lampronti, C. Liu, P. Nahai-Williamson, H. Hamidov, D. Daisenberger, and S. S. Saxena, Pressure-induced electronic and structural phase evolution in the van der Waals compound FePS_3 , [Phys. Rev. Lett. **121**, 266801 \(2018\)](#).
 - [5] D. M. Jarvis, M. J. Coak, H. Hamidov, C. R. S. Haines, G. I. Lampronti, C. Liu, S. Deng, D. Daisenberger, D. R. Allan, M. R. Warren, *et al.*, Comparative structural evolution under pressure of powder and single crystals of the layered antiferromagnet FePS_3 , [Phys. Rev. B **107**, 054106 \(2023\)](#).