On the origin of apparently negative minimum susceptibilities of hematite single crystals calculated from low-field anisotropy of magnetic susceptibility

Josef Ježek[1], Martin Chadima[1,2], František Hrouda[1,2]

[1]Faculty of Sciences, Charles University, Albertov 6, CZ-128 43 Prague, Czech Republic
E-mail: jezek@natur.cuni.cz

[2]AGICO Ltd., Ječná 29a, Box 90, CZ-621 00 Brno, Czech Republic
E-mail: chadima@agico.cz; hrouda@agico.cz

[3] Institute of Geology, Academy of Sciences of Czech Republic, Prague, Czech Republic

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Introduction

As shown in the literature several times, the calculation of the anisotropy of magnetic susceptibility (AMS) of hematite single crystals using standard linear AMS theory (fitting tensor of 2^{nd} rank) reveals that the calculated minimum principal susceptibility is parallel to the crystallographic c-axis, but is negative, which has however evidently nothing to do with diamagnetism as found out through direct measurement of susceptibility along the principal directions.

The problem of negative minimum principal susceptibility can be split in two parts:

(1) How to represent single crystal AMS in such a case.

(2) How this phenomenon limits standard models of bulk (multi-crystal) AMS.

We investigate these two points, using susceptibility measured in symmetry planes of hematite crystal. We present our contribution in the original form, which was aimed as a poster.

Directional susceptibility

Tensor of magnetic susceptibility (**k**) is usually computed from a set of measurements by which magnetic field (red arrow in Fig. 1a) is applied in different directions. Response in this direction is represented by the directional susceptibility related to the susceptibility tensor as

$$k_d = d * \mathbf{k} * d' \qquad (1)$$

where **d** is vector of direction cosines.

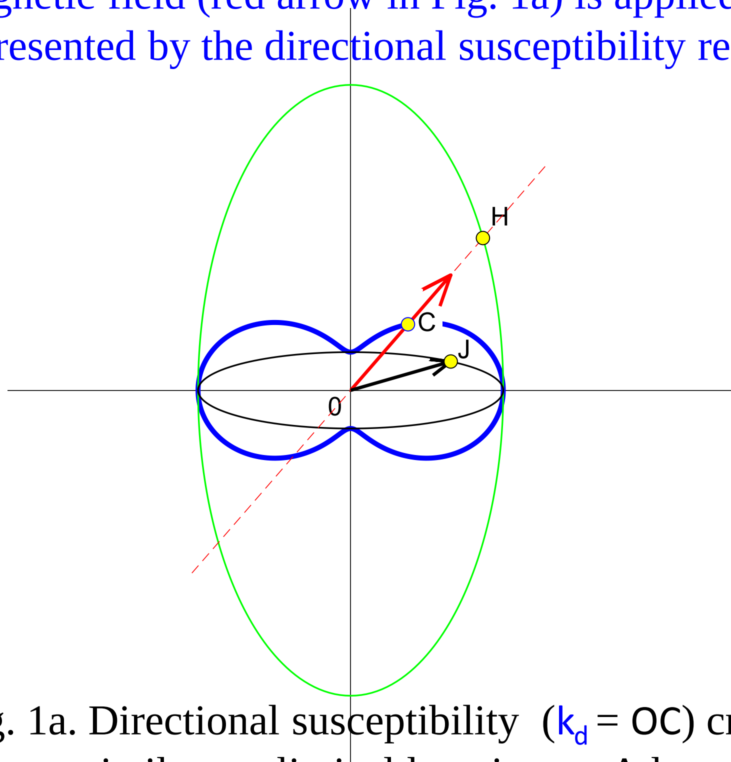
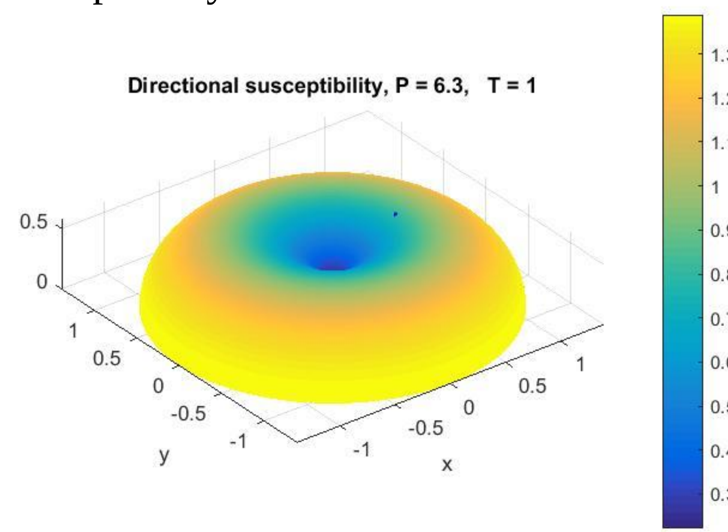


Fig. 1a. Directional susceptibility (k_d = OC) creates a curve similar to eliptical lemniscate. Adopted from Nagata (1961):

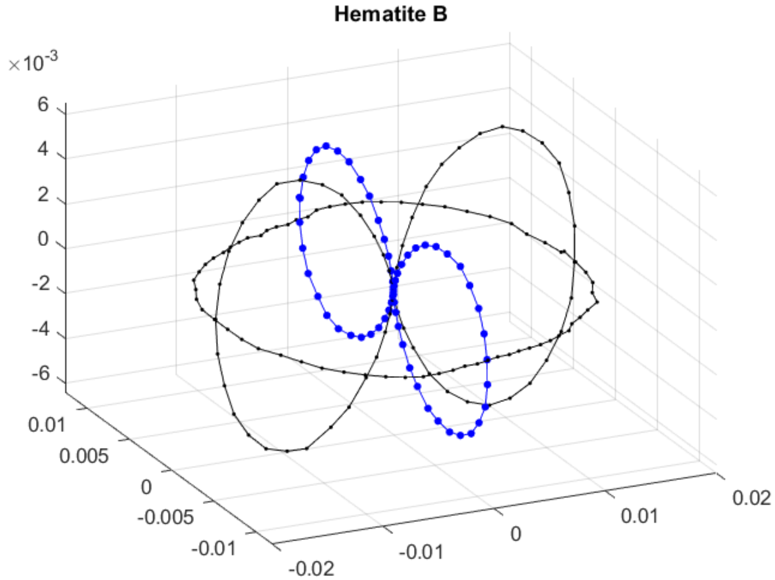
OH : direction of magnetic field H_{ex}.
OJ : anisotropic magnetization induced by H_{ex}.
OC : component of magnetization parallel to H_{ex} or the quantity measured by usual methods.

Assuming $|H_{ex}|=1$, OC is the susceptibility parallel to H_{ex}. Loci of H, where $OH=\frac{1}{\sqrt{OC}}$, represents the susceptibility ellipsoid (full line) and the loci of J (dotted line) is the magnitude ellipsoid.

Fig. 1b. Surface (upper part) of directional susceptibility.



Directional susceptibility of hematite measured in symmetry planes



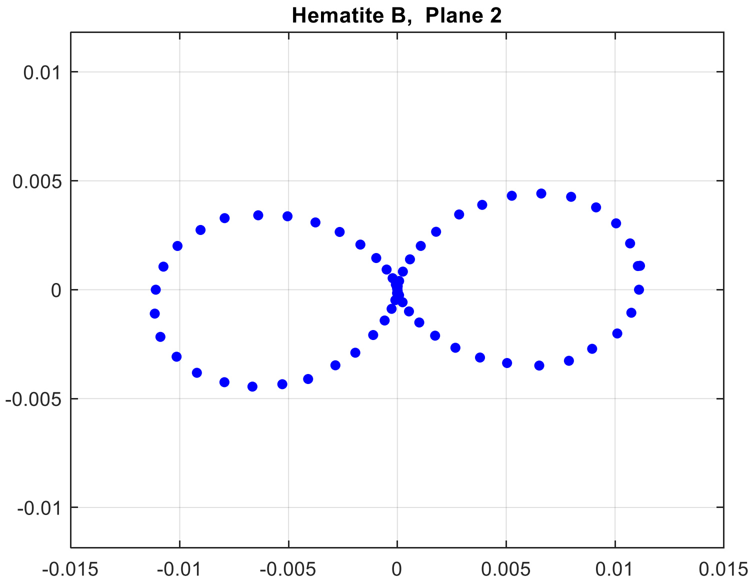


Fig. 2. Directional susceptibility measured in three mutually perpendicular planes of hematite (we shall investigate the blue one). Very small directional susceptibilities were measured in vertical direction, where minimum directional susceptibility is 2.56×10^{-5} (>0).

Fitting susceptibility tensor

Susceptibility tensor was fitted to measured directional susceptibilities. Its first eigenvector $\mathbf{e}_1$ is slightly deviated (ε_1=4.5°) from horizontal plane (due to imperfect arrangement of the measurement), and the maximum eigenvalue k_{max} = 0.011. Third eigenvector $\mathbf{e}_3$ is almost vertical.
The minimum eigenvalue that should serve as minimum principal grain susceptibility is negative, k_{min} = - 0.0006. The curve of directional susceptibilities back-computed from the fitted tensor is distorted near origin (Fig. 3a,b).

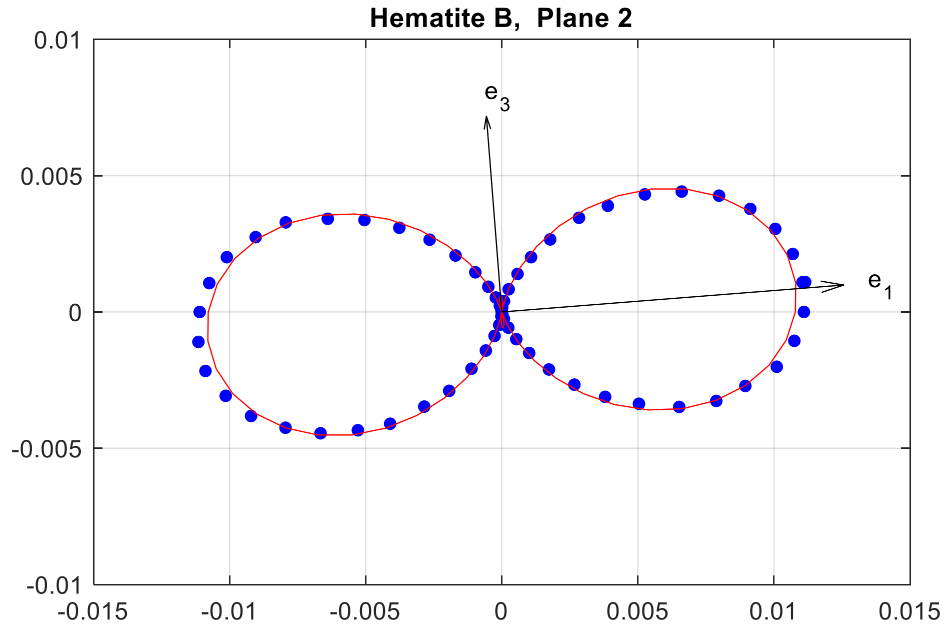


Fig. 3a. Directional susceptibilities measured (blue points) and back-computed (red curve) from the fitted tensor of susceptibility according to equation

$$k_d=[\cos\alpha, \sin\alpha]*k*[\cos\alpha, \sin\alpha]' \quad (2)$$

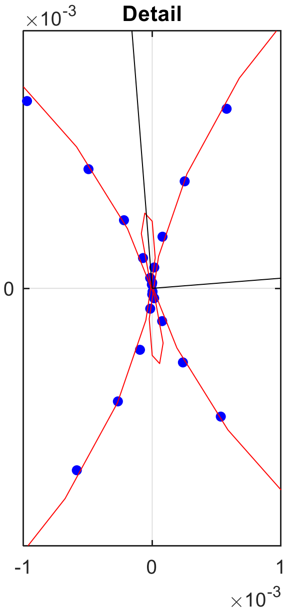


Fig. 3b. Detail. As a consequence of the negative eigenvalue, the curve of directional susceptibility overshoots through the origin to opposite halfspace.

Directional susceptibility corresponding to the fitted tensor

Directional susceptibilities back-computed from the fitted tensor of susceptibility and represented by lemniscate in Fig. 3 can be also expressed as a function of the angle (α) betwen given direction and horizontal plane

$k_d = k_{min} + (k_{max} - k_{min}) * (\cos(\alpha - \delta))^2$ (3)

where $\delta = \varepsilon_1$ (inclination of the first eigenvector).

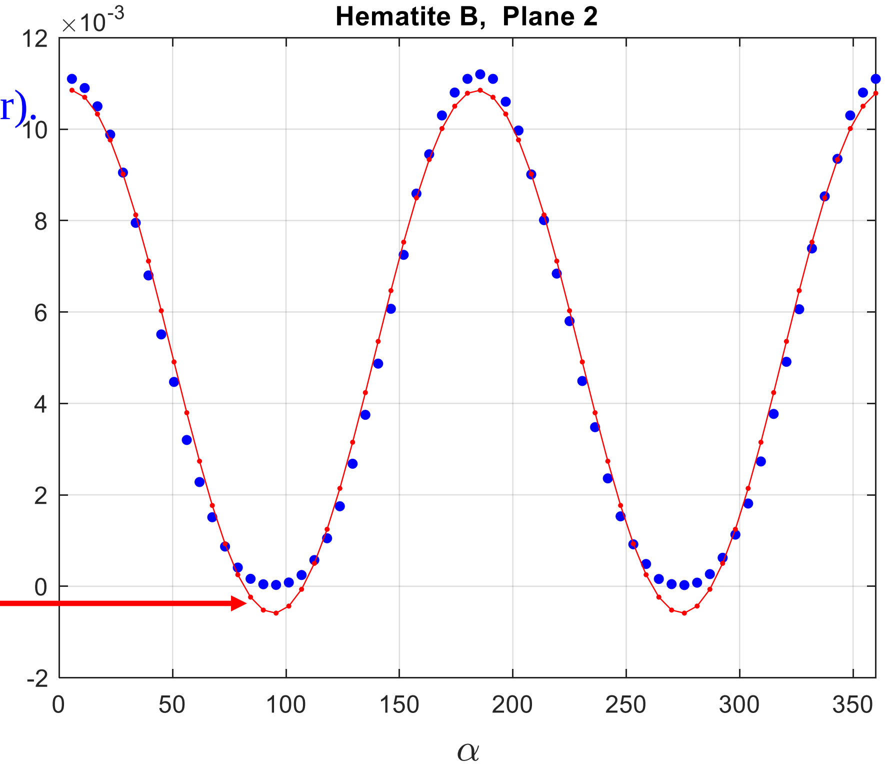


Fig. 4. Directional susceptibilities measured (blue points) and back-computed (red curve) from the tensor of susceptibility. Due to negative eigenvalue of the susceptibility tensor, the back-computed directional susceptibilities are negative for the angle α near 90° (vertical direction).

Non-tensorial expressions

Several expressions of hematite grain susceptibility are compared in Fig. 5.

The red curve in Fig. 5 corersponding to fitted tensor (the same as in Fig. 4) reveals insufficiency of tensor-description near minima and maxima of directional susceptibilities.

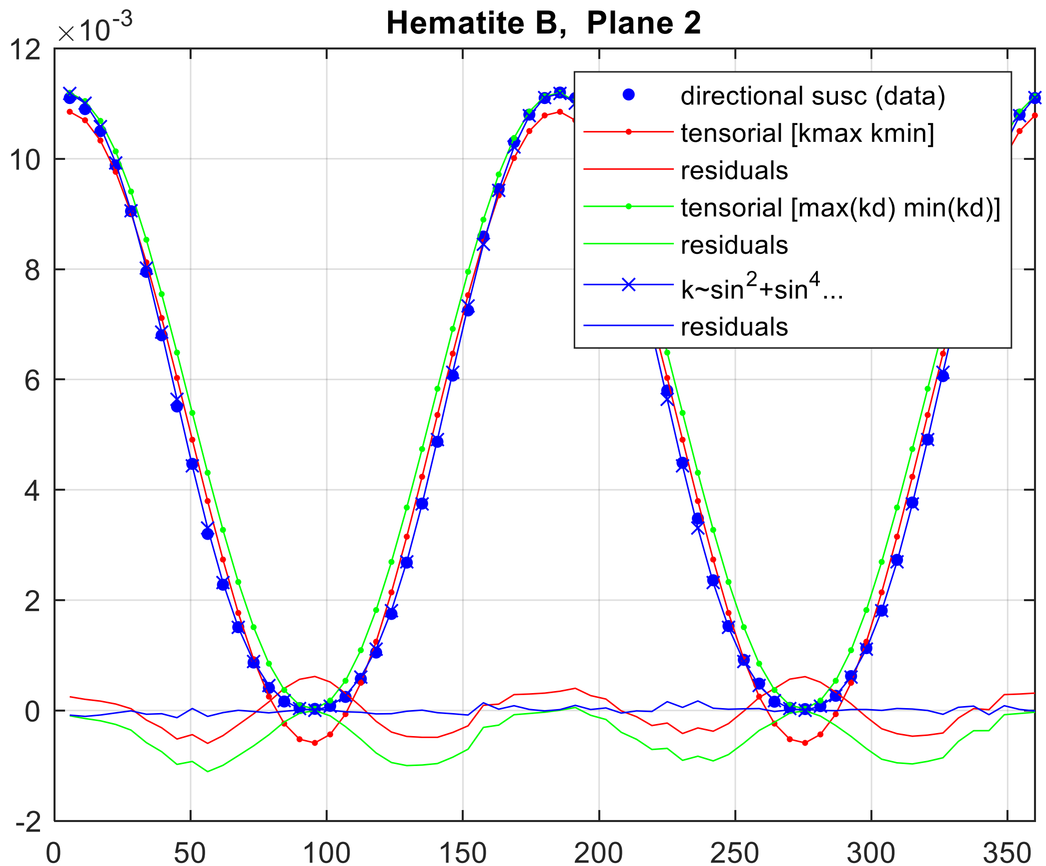
The green curve shows a naive experiment replacing k_{min} and k_{max} in the grain susceptibility tensor by minimum and maximum measured directional susceptibilities. This fits minimum and maximum exactly, but produces stronger residuals in between.

The blue curve represents a family of better fits that can be reached by power series involving even grades of cosine (or equivalently of sine)

$$k_d = a + b*(\cos(a-\delta))^2 + c*(\cos(a-\delta))^4 + \ldots \qquad (4)$$

First two terms correspond to previously examined tensorial representation. Involving more terms leads to non-tensorial expressions. They are all represented by the blue curve in Fig. 5 (they optically coincide).
Adding the 4th power term improves the fit substantially. Nevertheless, minimum susceptibility is still negative (a = -1.26e-4). With increasing power, the magnitude of minimum susceptibility decreases and it becomes positive by 8th power (a = 1.56e-6). This expression could be taken a proper model of hematite grain investigated.

Fig. 5. Different expressions of hematite susceptibility compared.



Fitting power series is justified by theory. But this more complex description of hematie grain cannot be expressed by a tensor of second rank and serve as an input in the already ellaborated models of bulk anisotropy.

How the (small) negative eigenvalues resulting from standard hematite crystal processing will influence the modelled bulk anisotropy?

Is there a simple correction of the grain susceptibility tensor convenient for fabric modelling?

Fabric modelling

We consider a measured sample containing oriented hematite grains. Bulk directional susceptibility in any direction is a sum of grain directional susceptibilities in that direction

$$k_{bd}(\alpha)=\Sigma k_{d,i}(\alpha) \qquad (5)$$

By measuring the sample, we obtain $k_{bd}(\alpha)$ in a number of directions α and then, by standard procedure, we fit the tensor of bulk magnetic susceptibility $\mathbf{k_b}$.

Fabric modelling is usually based on a sum of rotated grain tensors. For oblate uniaxial grains with principal susceptibilities $K_1 = K_2 > K_3$, tensor of modelled bulk susceptibility can be computed

$$\mathbf{k_{bM}} = K_2\mathbf{I} - (K_1-K_3)\mathbf{E} \qquad (6)$$

where $\mathbf{E}$ is orientation tensor of grain axes (poles to basal planes) and $\mathbf{I}$ is identity matrix (Ježek and Hrouda, 2002).

We can compare the fitted ($\mathbf{k_b}$) and modelled ($\mathbf{k_{bM}}$) bulk tensors or compare directional susceptibilities computed from these tensors (using eq. (1)) and the „true“ bulk directional susceptibilities $k_{bd}(\alpha)$. The latter is presented in Fig. 6.

Comparison of true and modeled directional susceptibilities

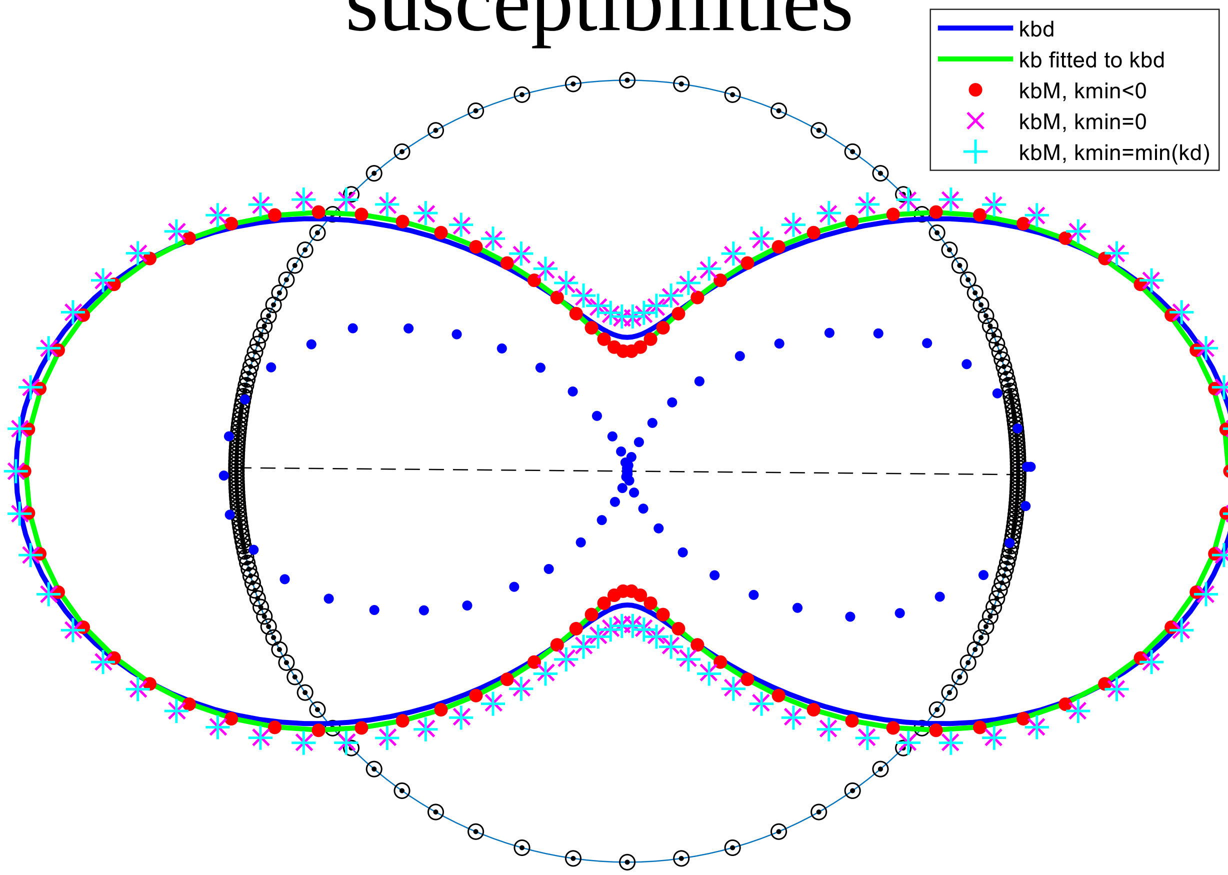


Fig. 6. Comparison of true and modelled bulk directional susceptibilities of a sample containing preferentially oriented hematite grains that have small negative minimum principal susceptibility. Scaling is arbitrary.

In Fig. 6, black dots on unit circle show preferred orientation of basal planes of hematite grains caused by vertical compression.

Each grain poses the same set of directional susceptibilities (as in Fig. 2). This is indicated by blue dots showing directional susceptibilities of a grain whose basal plane is oriented sub-horizontally. (Directional susceptibilities of other grains are rotated accordingly to grain orientation.)

Bulk directional susceptibility k_{bd} is plotted by blue curve. Due to preferred orientation, the curve is squeezed in vertical direction but not as much as grain directional susceptibility (blue dots).

Directional susceptibilities back-computed from the tensor of bulk susceptibility $\mathbf{k_b}$ create the green curve. This curve is close to the blue one, only in vertical direction, it tends more towards origin.

Coloured dots are directional susceptibilities computed from modelled bulk susceptibility $\mathbf{k_{bM}}$. This is done for several options of grain susceptibility tensor, differing by the choice of minimum principal susceptibility:

red … $K_1 = 0.011$ and $K_3 = -0.0006$ (as obtained by tensor fit of the original data, Fig. 3)

magenta … $K_1 = 0.011$ and $K_3 = 0$ (negative value replaced by zero)

cyan … $K_1 = 0.011$ and $K_3 = \min(\text{grain } k_d)$ (minimum measured directional susceptibility)

Results of the comparison and discussion

Red dots in Fig. 6 coincide with the green curve which means that fabric modelling based on the grain susceptibility tensor containing small negative minimum principal susceptibility (i.e., when we simply keep this value in the grain tensor) leads to result equivalent to fitting tensor in true directional susceptibilities of the sample (i.e., what we obtain by standard measurement).

Nevertheless, keeping the negative minimum grain susceptibility is unpleasant (creating a false feeling of diamagnetic behaviour of hematite in this direction). From this point of view, a replacement of the negative value by zero or by minimum grain directional susceptibility would be suitable. Fig. 6 shows such approach provides less accurate fit that keeps principal directions but decreases degree of fabric (P). By the intensity of preferred orientation shown in Fig. 6, P changes from approximately 5 to 4.

Important is that in fabric modelling, neither using the small negative grain susceptibility nor its replacement by zero or small positive value influences orientation of eigenvectors (lineation, foliation).

Comment: Fig. 6 indicates large value of modelled bulk fabric degree of anisotropy (PbM ~ 4 to 6) which corresponds to very large grain degree Pg. We can analyse it by means of eq. (6). We find

$$P_{bM} = [P_g(1 - E_{min}) + E_{min}]/[P_g(1 - E_{max}) + E_{max}] \qquad (7)$$

where E_{max} and E_{min} are eigenvalues of the orientation tensor of hematite poles. This relation is plotted in Fig. 7.

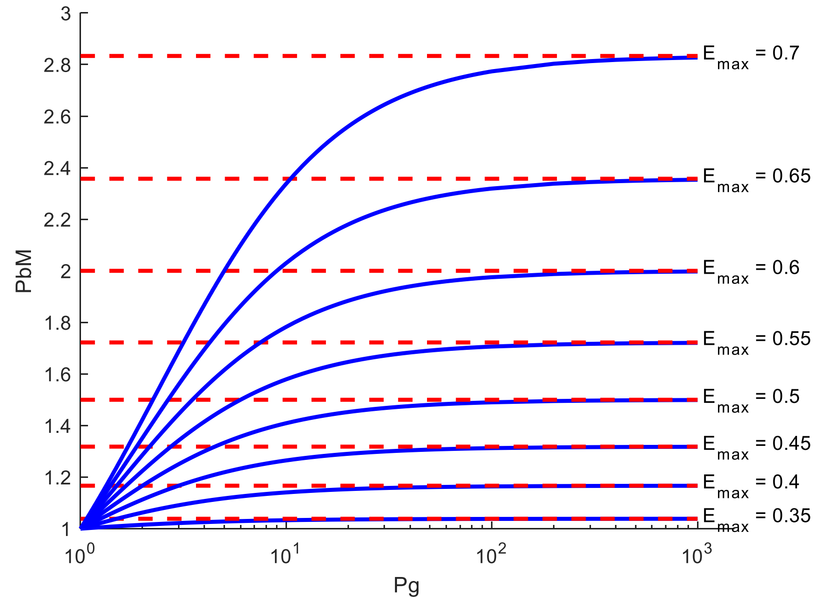


Fig.7 Equation (7) for different intensity of hematite poles preferred orientation.

When grain minimum susceptibility is very small (or equal to zero), the grain degree is large (or infinite) and the formula simplifies to

$$P_{bM} = (1 - E_{min})/(1 - E_{max}) \qquad (8)$$

This ratio is plotted in Fig. 7 by red broken line. For large Pg, the degree of bulk fabric is almost independent of Pg. It was observed already by Hrouda 1981 (Fig. 8).

Effects of Grain AMS and Preferred Orientation: a model

(Hrouda, 1981, JSG)

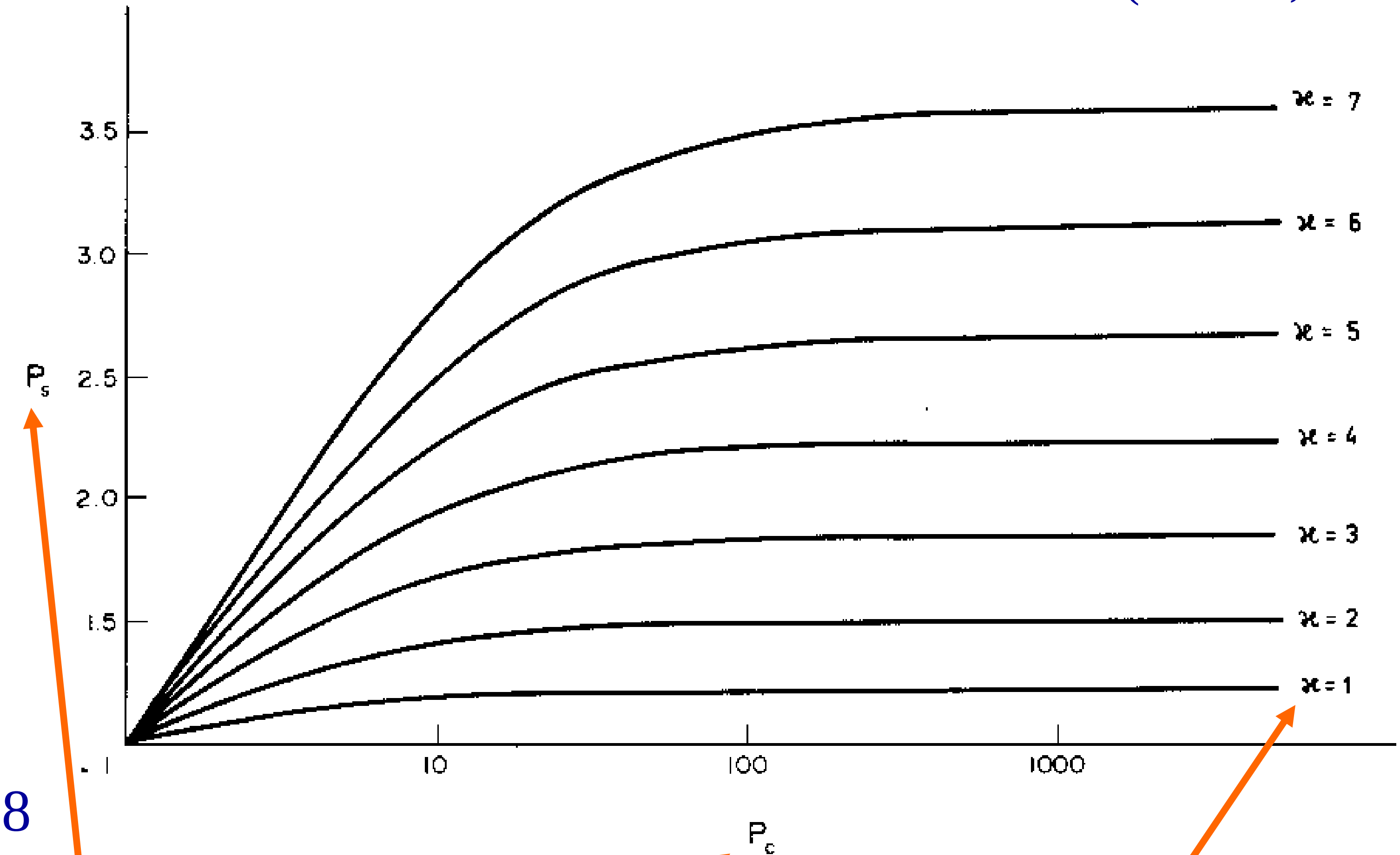


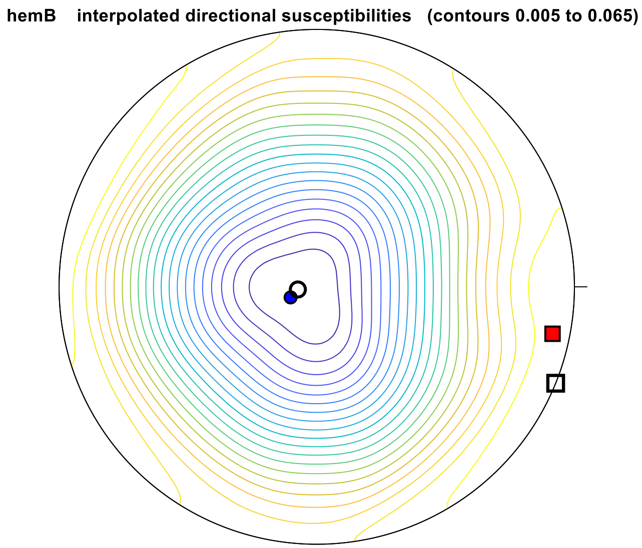
Fig. 8

Bulk degree of AMS, Grain degree of AMS, Concentration Parameter

If P_c>100, knowledge of its precise value plays no role in modelling.

Reconstruction of 3D directional susceptibility

Using data from all three planes, the surface of directional susceptibility was reconstructed. The result indicates that using full 3D data (that are currently measured by the authors of the contribution) should lead to analogous mathematical description as the one used above.



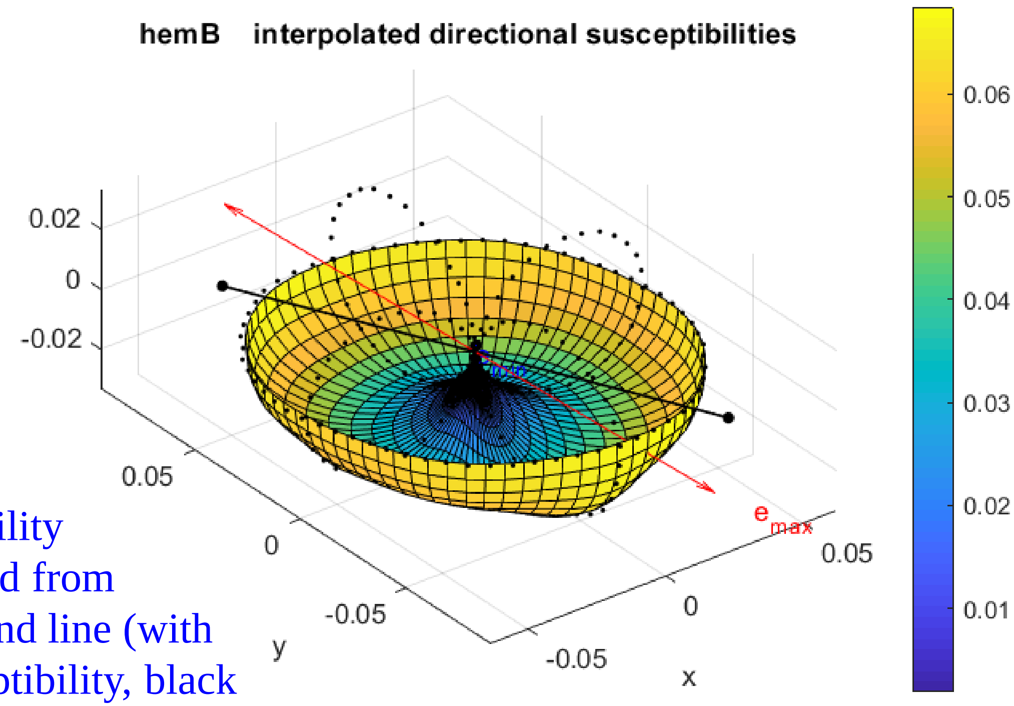


Fig. 9. Isolinies of directional susceptibility and its surface (lower part) reconstructed from all three measured planes. Red square and line (with arrows) show first eigenvector of susceptibility, black square and line indicates maxima of the surface of directional susceptibility

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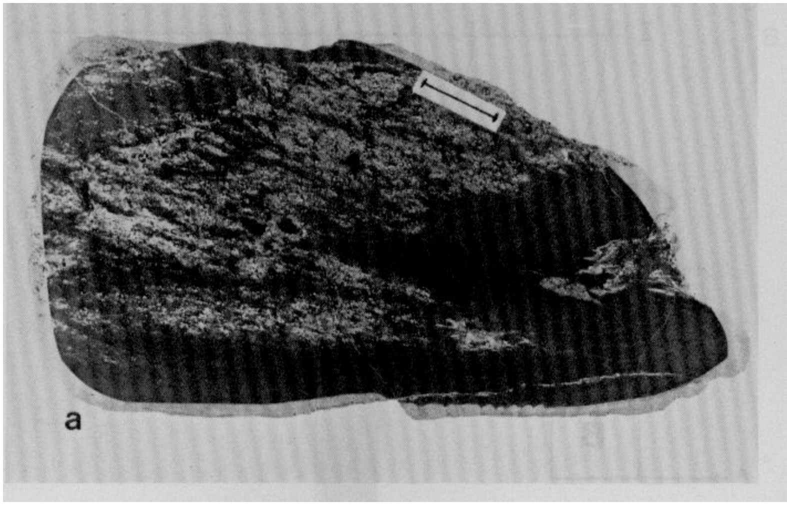
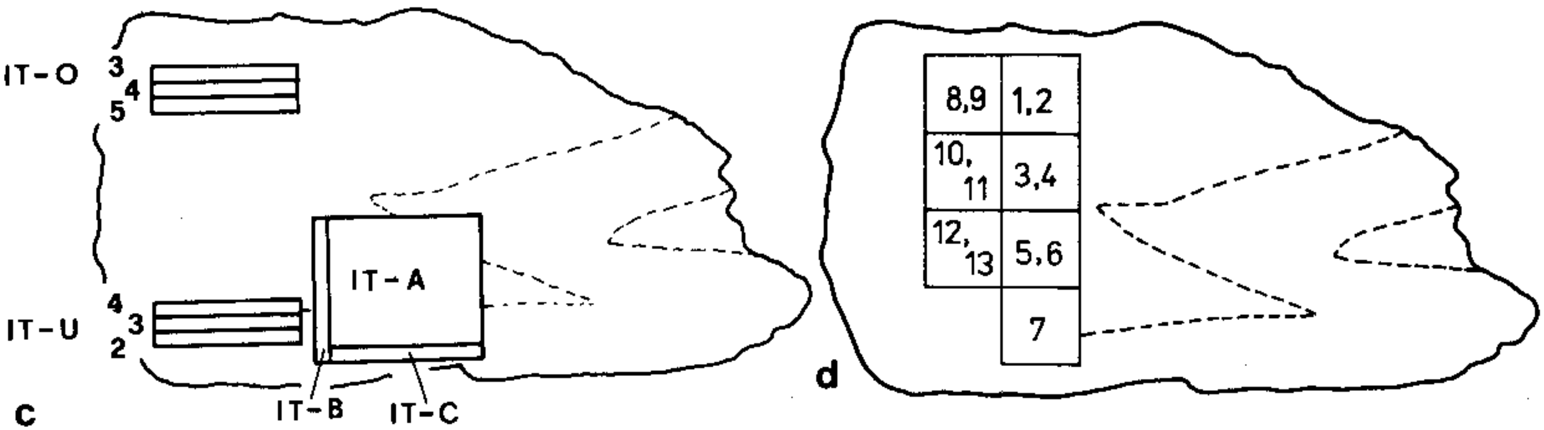
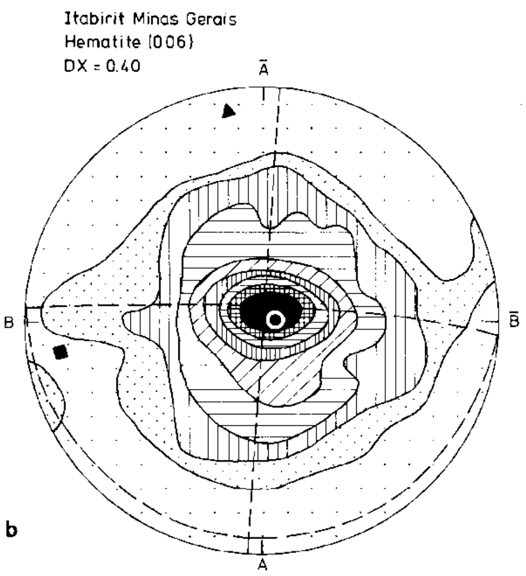
(Hrouda et al.,1985, J. Geophys.)

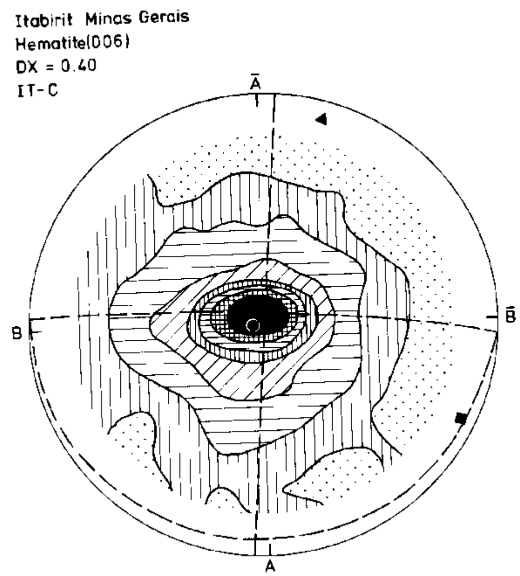


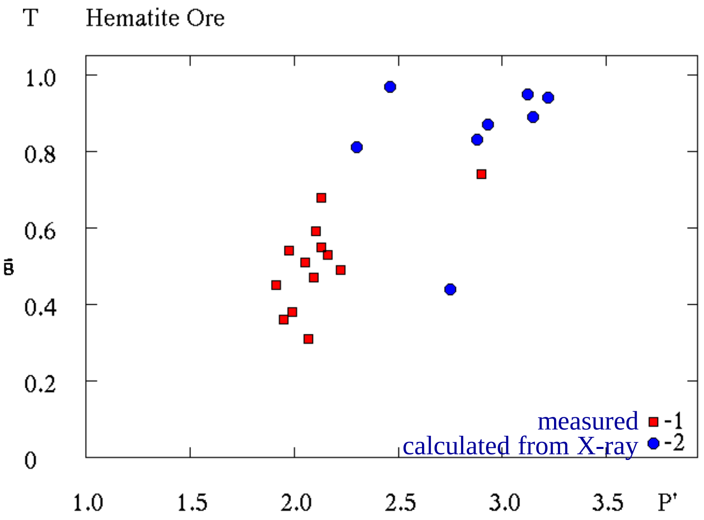
Reflected-light Microscopy
X-ray Pole Figure Goniometry
AMS



Theoretical and Measured AMS



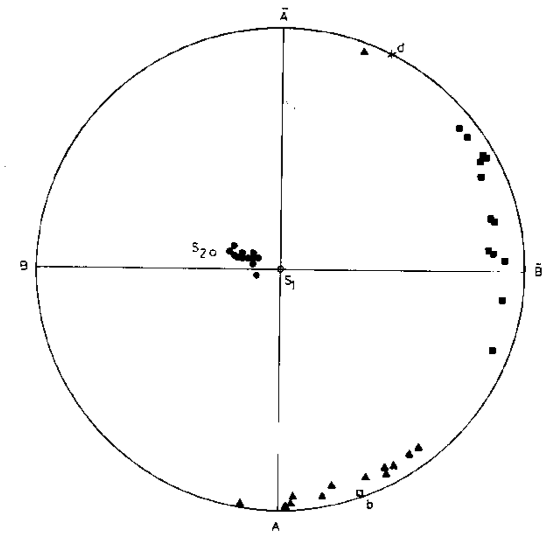




1. Measured principal susceptibilities are oriented in the same way as calculated theoretically from the c-axis pattern.

2. Measured degree of AMS and shape parameter are slightly lower than those calculated theoretically from c-axis pattern.

3. The above differences may result from the fact that the AMS and X-ray measurements were not executed on exactly the same specimens and the respective specimen volumes differed substantially (1 cm^3 vs. thin section).



Conclusion

Negative minimum susceptibility of hematite single crystal measured and calculated using standard AMS technique is an **artifact**.

It:

- does not invalidate standard models of magnetic fabric
- does not influence orientation of eigenvectors (lineation, foliation)
- can be replaced by zero or a small value > 0 in fabric modelling
- its replacement decreases, proportionally to intensity of preferred orientation, the parameter P
- in weak preferred orientation of grains this effect is not important