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To cite this version:

A. Govaert, C. Dauwe, J. de Sitter, E. de Grave. ON THE SURFACE CONTRIBUTION TO THE LINE PROFILE OF SMALL PARTICLES OF GOETHITE. Journal de Physique Colloques, 1976, 37 (C6), pp.C6-291-C6-292. 10.1051/jphyscol:1976659 . jpa-00216769

HAL Id: jpa-00216769

https://hal.science/jpa-00216769

Submitted on 4 Feb 2008

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JOURNAL DE PHYSIQUE *Colloque C6, supplément au n° 12, Tome 37, Décembre 1976, page C6-291*

ON THE SURFACE CONTRIBUTION TO THE LINE PROFILE OF SMALL PARTICLES OF GOETHITE

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Résumé. — Le principe de l'analyse des raies d'absorbtion Mössbauer dans le goethite est décrit. Leur forme asymétrique est due à deux contributions. La première provient de l'intérieur du grain et la deuxième est due à une diminution continue du champ hyperfin dans les couches de surface.

Abstract. — The principle for the analysis of the Mössbauer absorption lines in goethite is described.

The asymmetric broadening is due to two contributions. The first one arises from the core of the grain and the second one is due to a continuous decrease of the hyperfine field in the surface layers.

In figure 1 the Mössbauer spectra of two goethite samples are reproduced as a function of temperature. The spectrum of the sample from Ouenza (Algeria) shows asymetrically broadened lines over the whole temperature range. The room temperature spectrum of the sample from Horhausen (Germany) consists mainly of a superparamagnetic doublet, due to fast relaxation of the magnetic spin. Below 250 K we observe only a magnetically splitted spectrum.

The asymmetric broadening cannot be explained by the assumption of two discrete internal fields nor by relaxation of a completely coupled spin system. The asymmetric shapes can be satisfactorily described by superposition of two contributions [1]. The first one arises from the bulk part of the grain and causes a relatively sharp line, while the second is arising from the surface layers where the magnetic hyperfine field is continuously decreasing [2]. This decrease is described by convolution of a narrow Lorentzian line with one flank of a Gaussian distribution.

For the bulk contribution, we have chosen the Voigt profile [3], which was calculated to be the best fitting one to the outer lines of well crystallized goethite samples as those from Harz [2] and Loswithiel [4]. On this contribution we superposed the surface part in which only the Gaussian dispersion is variable. The Lorentzian width was taken equal to that from the bulk part. Further the relative amount of bulk and surface fractions is also varied.

In this way a set of theoretical profiles for the outer lines was calculated. From a comparison with the experimentally obtained profiles we can conclude :

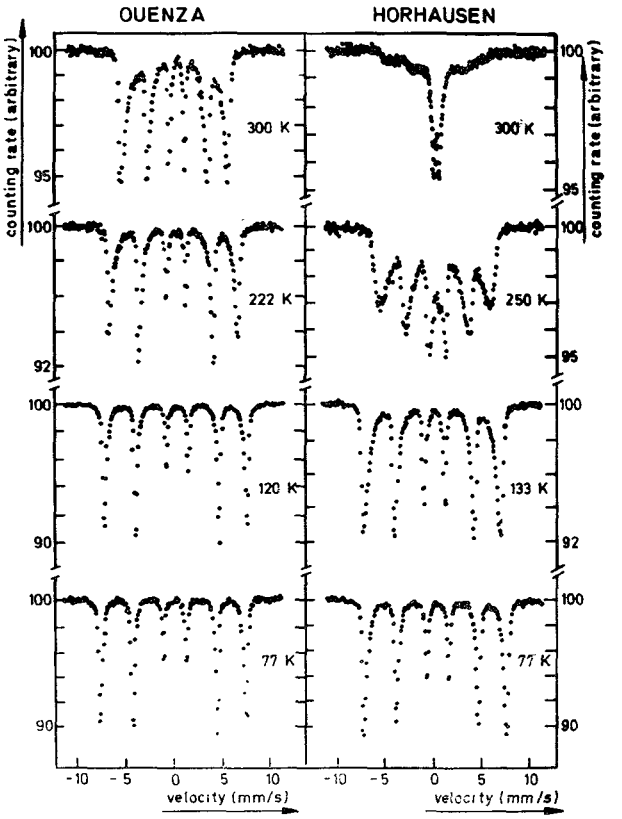

FIG. 1.

1) The magnetic hyperfine field as determined from the experimental peak position does not correspond to the bulk field especially at low bulk to surface ratio.

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Article published online by EDP Sciences and available at http://dx.doi.org/10.1051/jphyscol:1976659

2) The obtained relative amount of bulk to surface contribution as a function of decreasing temperature increases continuously which means that the number of decoupled outer layers decreases at lower temperature.

3) The dispersion σ_S of the field distribution decreases with decreasing temperature.

The authors wish to thank Prof. Dr. G. Robbrecht for his continuous interest and support of this work.

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