24.1-09 THE INFLUENCE OF THE DEGREE OF PERFECTION OF WEAK FERROMAGNETIC CRYSTALS ON MAGNETIZATION PROCESS. By V.G. Labushkin, V.V. Rudenko, E.R. Sarkissov, V.A. Sarkissyan, V.N. Seleznev, All-Union Research Institute of Physical-Technical & Radiotechnical Measurements, Moscow, U.S.S.R.

Magnetic Mössbauergraphy was used to study the surface magnetization process of weak ferromagnetic crystals $FeBO_3$ possessing different degrees of perfection which were evaluated by X-ray diffraction methods, that is, by the X-ray topography (the Lang method) and rocking curves method. The rocking curve width was 8" for one crystal and 80" for another. The experimental technique was similar to that described (Kovalenko et al., Pisma ZhETF (1977) 26, 92). Mössbauer diffraction intensity which depends on the spin direction of iron ions was studied as a function of magnetic field applied along the intersection line of two planes, the easy plane (III) and the scattering plane $(\vec{k}\ \vec{k}')$. The measurement data are shown in Figs. 1 & 2. It can be seen from the figures that the crystal possessing the greater number of defects (Fig. 2) has the higher anisotropy energy in the easy plane and takes the higher magnetic field H_1 to form a single-domain crystal. Besides, in this case the essentially higher field H_2 is required to turn the magnetization vector to the $\vec{H}$ orientation (Fig. 2), than in the case of more perfect crystal (Fig. 1).

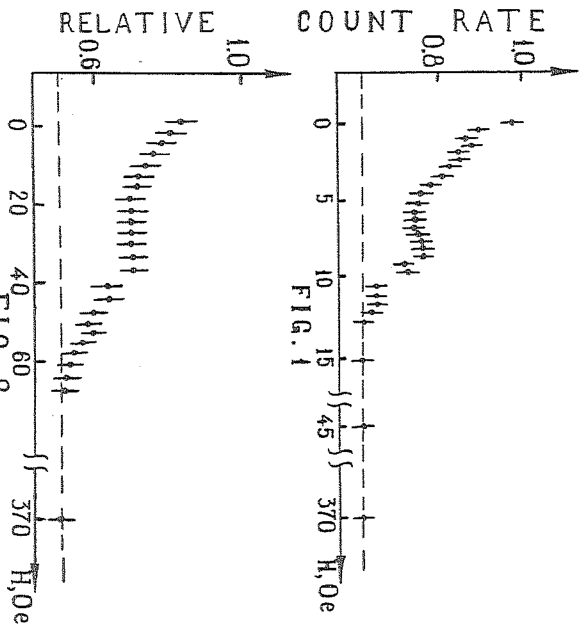

FIG. 2 FIG. 1

24.1-10 THE ESTIMATION OF POSITIVE AND NEGATIVE TRIPLETS VIA THE REPRESENTATION THEORY. By C. Giacovazzo, Ist. Mineralogia, Università, Bari, Italy; M. Camalli & R. Spagna, Ist. Strutturistica Chimica, C.N.R., C.P. 10 Monterotondo Stazione, Roma; M.C. Burla, A. Nunzi & G. Polidori, Ist. Mineralogia, Università, Perugia, Italy.

An important problem in the determination of crystal structure by direct methods is the recognizing of good triplets i.e., those for which $\cos(\phi_h+\phi_k-\phi_{h+k})\simeq 1$ and of bad triplets i.e. those for which $\cos(\phi_h+\phi_k-\phi_{h+k})\simeq -1$. A probabilistic theory has been used which exploits the information contained in the second representation of a triplet, that is to say in the special quintets

$$\Psi_5=\phi_h+\phi_k-\phi_{h+k}+\phi_l-\phi_l$$

and in the first representation of the special sextets

$$\Psi_6=\phi_h+\phi_k-\phi_{h+k}+\phi_l+\phi_p-\phi_{l+p}$$

The results are satisfactory. High probability values are frequently obtained which correctly indicate negative triplets. On the other hand the theory is able to improve the reliability of the triplet defined positive.

24.1-11 THE RESIDUAL FUNCTIONS R_2 AND R_2^N AS USED IN AUTOMATED X-RAY CRYSTALLOGRAPHY. By W. Van Havere and A.T.H. Lenstra, University of Antwerp (U.I.A.), Department of Chemistry, Universiteitsplein 1, B-2610 Wilrijk, Belgium.

In efforts to automate crystal structure analysis we use mathematical instead of chemical criteria.
An 'a priori' evaluation of the function, which discriminates between correct and incorrect models of the structure at hand, is of utmost importance. Residual functions, such as R_2 or R_2^N, appear to be useful in this context.

Until recently one could estimate $\langle R_2 \rangle$, the first moment of the unknown distribution $P(R_2)$. Using a new theoretical model we are able to evaluate also higher moments of the residual.

The validity of our mathematical model is demonstrated by the evaluation of R_2 for large completely correct or completely incorrect models in the space group P1. In these situations of mainly academic interest the coincidence between experiment and theory is surprisingly good.

In experimental situations a model of the structure looked for contains incorrect and correct atoms. The latter group consists of a set of positions known beforehand (e.g. from a Patterson map) and newly found positions (e.g. from a heavy-atom Fourier). New intensity distributions were developed to describe these practical situations. Again the moments of R_2 can be directly computed which means that R_2 remains a proper discriminator function.
We will demonstrate that in the evaluation of R_2 and related higher moments the space group symmetry is an important factor. Also, we will present some results pertinent to small structures, because structure size cannot be neglected as parameter in our statistical analysis.