PS-10.03.14 USE OF OVERLAPPING REFLECTIONS IN DETERMINATION OF RETAINED AUSTENITE. By J. Garin and V. Martínez*, Universidad de Santiago, Casilla 10233, Santiago, Chile.

Determination of retained austenite in hardened steels is based on direct comparison of integrated intensities of high-angle reflections such as (200) and (220) of the face-centered-cubic austenitic phase, and (200) and (211) of the body-centered-tetragonal martensitic phase. In all cases care is taken in choosing diffraction lines to be measured, in order to avoid overlapping or closely adjacent lines from different phases.

This work describes the use of the stronger overlapped (111) and (110) peaks of austenite and martensite respectively. The mathematical separation of the peak profiles was based on the Pearson VII-type function (Naidu, S.Y.N. & Houska, C.R. (1982). J. Appl. Cryst. 15, 190-198), which is capable of describing a wide range of diffraction profiles.

Intensity data were collected at room temperature with a Philips vertical diffractometer equiped with a graphite diffracted-beam monochromator, using a normal Cu tube. Step scanning was performed with counting time of 20 s per point and 0.01° per step. A total of approximately 240 points per curve were collected for each sample.

The experimental results were further checked by use of NBS standard reference materials SRM 488, SRM 485a, SRM 486 and SRM 487, with 2.23, 4.70, 14.30 and 32.78 vol.% of austenite in ferrite respectively (Hicho, G.E. & Eaton, E.E. (1982). Adv. X-Ray Anal. 26, 137-140). In all of the investigated samples contents of austenite were within 2 % of the reference values.

The accuracy of the integrated intensities was then improved with the beneficial effects of higher precision in the calculation of the relative amount of retained austenite.

PS-10.03.15 INFLUENCE OF TEMPERATURE-DEPENDENT STATIC Fe-IONIC DISPLACEMENTS ON DIFFRACTION BY THE N-CONTAINING B.C.C.-Fe ORDERED INTERSTITIAL PHASES. By V. B. Molodkin, V. A. Tatarenko and C. L. Tsynman*, Department of Solid State Theory, Institute for Metal Physics, Kiev, Ukraine.

The diffraction by equilibrium alloy Fe—N is analysed on a model. The effect of both the presence of $n$ N-ions within $3^m$ octahedral interstices and a change of absolute temperature, $T$, on static displacements of $m$ solvent Fe-ions from $m$ "average"-lattice sites and on "average"-lattice periods of elastically-anisotropic host b.c.c. Fe-crystal is taken into account. So, within statistical thermodynamic methods (Khachaturyan A.G., 1974, Theory of Phase Transformations and Structure of Solid Solutions, Moscow: Nauka), an intensity of a spatial-fluctuation-dependent (diffuse) X-ray scattering, solely by static Fe-ionic displacements in completely-ordered $\alpha''$-Fe$_{16}$N$_2$-type tetragonal phase observed with diffraction wave vector $q=2\pi B+k$ at a host-crystal reciprocal-lattice point B below a temperature of disorder-order phase transformation, $I(q,T,C)\approx m^2 C^2 |f_N \exp(-iq\cdot h)-if_{Fe}qG(k)F(k)|^2 \delta_{k,k^j}$

where $C\equiv n/m$ is a relative concentration of N-atoms, $f_N$ and $f_{Fe}$ are atomic scattering factors of N and Fe respectively, $\delta_{k,k^j}$ is Kronecker's symbol. In the present work the values of $I(q)$ have been calculated without any assumptions about magnitudes of interionic (Fe—Fe and Fe—N) coupling parameters $G(k,T)$ and $F(k,T)$ (in off-stoichiometric interstitial $\alpha''$-type-phase with discrete ionic-crystalline structure containing

N-ions in one available interstitial sublattice, shifted with reference to Fe-lattice by vector h, for superstructural wave vectors $k^j$, matching up to the high-symmetry points $j=N_1,\ldots,N_s$ or $j=H$ in the first Brillouin zon ) other than that they can be adequately described by corresponding short-range "direct" interactions. The $I(q)$-versus-$T$ curves for intensities (in arbitrary reduced units) of superstructure reflections in reciprocal space for orientationally-ordered phase $\alpha''$-FeN$_c$ are shown in Figs. 1 ( $|q^N|=2\pi/a_0$, $|q^N|=\pi\sqrt{2}/a_0$), 2 ( $|q^N|=2\pi\sqrt{3}/a_0$, $|q^N|=\pi\sqrt{6}/a_0$) and 3 ( $|q^N|=2\pi\sqrt{5}/a_0$, $|q^N|=\pi\sqrt{10}/a_0$) by way of examples ($a_0$ is $\alpha$Fe-lattice parameter); their forms are intimately bound up with $k^j$ and $q^j=2\pi B+k^j$.

Fig. 1.

Fig. 2.

Fig. 3.
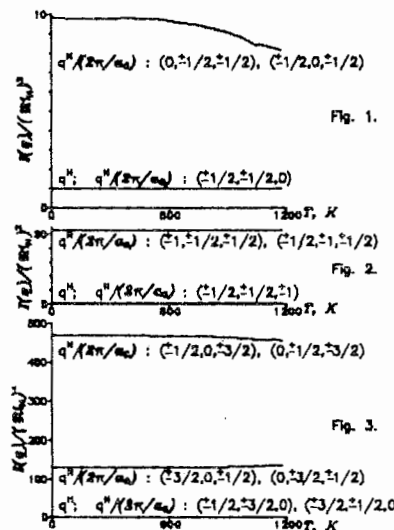
PS-10.03.16

## THE EFFECT OF STRUCTURE IN CIRCULAR DICHROISM INDUCED BY APPLIED ELECTRIC AND MAGNETIC FIELDS IN ALUMS DOPED WITH THE CR$^{3+}$ IONS.

By T. F. Veremeichik*, B. N. Grechushnikov, Z. B. Perekalina, A. Tinaev, I. A. Jakovleva, Institute of Crylstallography, Moscow, Russia.

For K-, NH4-alums doped with the Cr$^{3+}$ ions the effect of structure on local properties of the Cr$^{3+}$ ions and on their properties in the whole crystal were investigated under electric and magnetic fields. This is a research based on the circular dichroism (CD) spectra obtained by dichrograph, Raman, infrared, absorption spectra at 300, 100 K. The following calculations were made; the parameters of asymmetric part of crystal field, the frequencies of electron, electron-phonon transitions of the Cr$^{3+}$ ions, the rotational strengths of the CD bands. We found out that static and fluctuational parts of crystal field created by the structure and the local surrounding of the Cr$^{3+}$ ions compete in removing latent chiality in an individual Cr-cluster. On the other hand structure studies proved that chiral balance is removed for the sum of the Cr-clusters in unit cell under applied fields. The begining of the phase transitions under applied electric and magnetic fields were observed with intensity of the CD bands at $\approx$ 100 K.