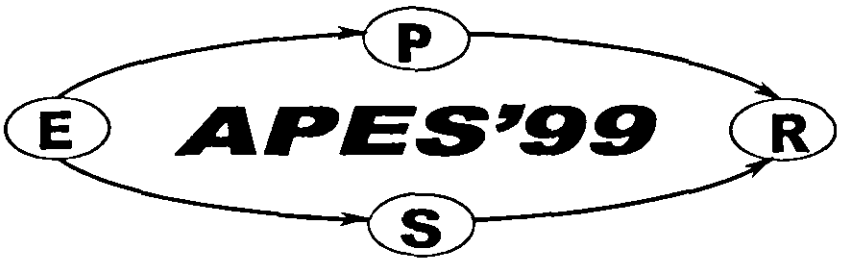
2nd Asia-Pacific EPR/ESR Symposium

PROCEEDINGS

(ABSTRACT)



Zhejiang University
October 31-November 4, 1999
Hangzhou China

CONDUCTION ESR AND $\alpha \leftrightarrow \beta$ PHASE TRANSFORMATIONS IN GRAPHITE INTERCALATION COMPOUNDS WITH NITRIC ACID

Nikolay M. MISHCHENKO and Albert M. ZIATDINOV

Institute of Chemistry, Far Eastern Branch of the Russian Academy of Sciences, 690022, Vladivostok, *RUSSIA*. E-mail: chemi@online.ru

The graphite intercalation compound (GIC) with nitric acid exists in two forms. When the ordinary form, α-$C_{5n}HNO_3$, is exposed to air or N_2 gas for an extended time period, the HNO_3 molecules, which stand essentially perpendicular to the graphite planes, reorient to lie nearly parallel, yielding the more dilute β-$C_{8n}HNO_3$ residue compound. Because synthesis of the residue compound is difficult and time consuming, most studies of HNO_3-GIC's have been confined to the α-type. In present work the results of Conduction ESR (CESR) and electroconductivity studies of $\alpha \square \beta$ phase transformations in HNO_3-GIC's are presented.

In α-$C_{10}HN0_3$ the CESR spectrum is axial with respect to the c-axis at all temperatures and is characterized by $g_{//} = 2.0023 \pm 0.0001$ and $g_{\perp} = 2.0028 \pm 0.0001$. At room temperature the line width at half height of the maximum peak height A (AH) is equal to 0,4 G and 0,42 G, respectively for H along and perpendicular to the c-axis. In β-$C_{24}HNO_3$ at all temperatures $g_{//} = 2.0024 \pm 0.0002$ and $g_{\perp} = 2.0028 \pm 0.0002$. At room temperature $\Delta H_{//}$ and $\Delta H_{\perp}$ are equal to 2,1 G and 2,5 G, respectively. In reintercaleted sample of α-$C_{10}HN0_3$ the CESR spectrum is characterized by same values of parameters, as in initial α-phase. The dependence of asymmetry parameter of the first derivative of the absorption line A/B (which is defined as the ratio of the maximum peak height (A) to the minimum peak height (B), both measured with respect to the zero line of the resonance derivative) on sample width (*l*) is presented in Fig. 1.

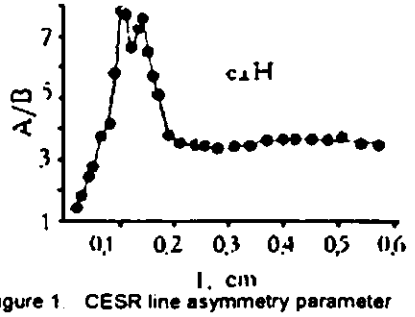


Figure 1. CESR line asymmetry parameter A/B (1) of β-$C_{24}HNO_3$ vers. sample width (*l*).

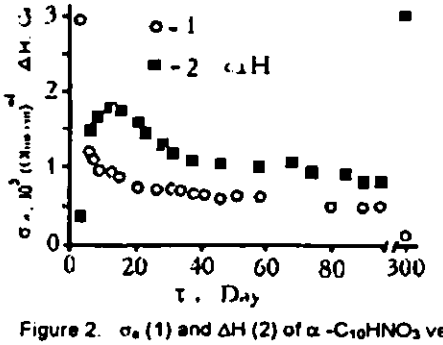


Figure 2. σ_a (1) and ΔH (2) of α -$C_{10}HNO_3$ vers exposure time inair.

At $\alpha \square \beta$ phase transformation of $C_{10}HN0_3$ the electroconductivity in basal plane (σ_a) monotonically decreases from $2.9 \cdot 10^5$ $(\Omega \cdot cm)^{-1}$ to $0.1 \cdot 10^5$ $(\Omega \cdot cm)^{-1}$ (Fig. 2). Herewith, changing a CESR linewidth does not correlated with change σ_a (Fig. 2). At reintercalation of $\beta C_{24}HNO_3$ the value of σ_a - conductivity does not change. The value of electroconductivity along the c-axis (σ_c) practically does not depend on HNO_3-GIC's modification. In all studied GIC phases at decreasing of temperature a CESR linewidth increases together with σ_a.

This work was supported by the Russian Foundation for Basic Research (NQ 97-03-33346a).