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A B S T R A C T S

*A.M. ZIATDINOV***EDGE π -ELECTRONIC STATES: THEORY, EXPERIMENT AND APPLICATIONS**

The review of the modern state on knowledge of the edge π -electronic states of sp^2 -hybridized honeycomb-like carbon nets is presented. The presence of such states in nanosize carbon structures was shown to result in the appearance of their essentially new physical and chemical properties. Some approaches to solving problems existing in nanotechnology of these promising materials are discussed.

Key words: π -electronic edge states, nanographene, nanographite, film structure, electronic structure, magnetic configuration, chemical activity

*N.S. SAENKO, A.M. ZIATDINOV***FERROMAGNETIC NANOCOMPOSITES BASED ON MULTI-WALLED CARBON NANO-TUBES PRODUCED BY METHANE CATALYTIC PYROLYSIS**

Research data on composition, structure and magnetic properties of carbon compounds produced by methane catalytic pyrolysis were presented. It was shown that they represent the ferromagnetic nanocomposites based on multi-walled carbon nano-tubes and magnetic nano-particles intercalated in them. The interpretation of revealed difference in electronic structure for carbon nanotubes and graphite near the Fermi level was proposed. It was revealed that the possible reason of increase in concentration of localized spins for the fluorinated nano-tubes is the formation of covalent bonds between fluorine and carbon atoms situated far from open ends of nano-tubes.

Key words: multi-walled carbon nano-tubes, magnetic nano-composites, electronic structure, chemical reaction, covalent bond, localized magnetic moments

*N.E. KORNIENKO, V.A. BRUSENTOV, E.L. PAVLENKO***RESONANT INCREASE IN SPLITTING AND VIBRATIONS SHIFTS AND BANDS INTENSITY GROWTH IN VIBRATIONAL SPECTRA OF DIFFERENT FULLERENES**

New non-linear quantum concepts on the influence of vibrational resonances sequences and strong vibrational-electronic interactions and unstable chemical structures are developed on the basis of vibrational spectroscopy and quantum chemical calculations of fullerenes $^{12}C_{60}$, $^{13}C_{12}C_{59}$, $^{13}C_2^{12}C_{58}$, BNC₅₈ et al., complexes with metal atoms $C_{60}M$. Increase in the splitting and frequency shifts of the vibrational bands, as well as the increase in the intensity of active and "dumb" vibrations in the resonance vibrations of $C_{60}Hg(3,7)$ ($2Hg(3)\approx Hg(7)$) was established which is due to the influence of the non-linear resonant interaction of vibrations.

Key words: fullerenes C_{60} , vibrational bands displacement and the splitting, vibrational resonance, vibration-electron interactions

Yu.A. KVASHNINA, A.G. KVASHNIN, T.P. SOROKINA, O.P. KVASHNINA, P.B. SOROKIN
MODEL OF ULTRAHARD FULLERITE. THEORETICAL INVESTIGATION

Using classical molecular dynamics method the new carbon nanocomposites based on polymerized fullerene and diamond were proposed and investigated. It was found that mechanical characteristics such as bulk modulus are in dependence on the size of fullerite, located into diamond shell. Bulk modulus of such materials is higher than bulk modulus of single crystal diamond in several times.

Key words: fullerite, diamond, bulk modulus, molecular dynamics.

A.G. KVASHNIN, O.P. KVASHNINA, T.P. SOROKINA, P.B. SOROKIN, W.E. BILLUPS
MODELING PHASE TRANSITION OF AMORPHOUS CARBON TO DIAMOND INDICED
WITH IONIZING RADIATION

Using classical molecular dynamics method the reason of formation of diamond clusters into the amorphous carbon under electron irradiation was studied. It was shown that activation barrier of transition of graphite cluster to diamond cluster takes place only in a case of clusters with size more than 14 nm, whereas smaller clusters could be obtained only by a chemical functionalization of graphitic materials which is in a good agreement with our experimental data.

Key words: DFT, graphene, diamond cluster, chemically induced phase transition

N.E. KORNIENKO, A.D. RUD, A.N. KIRICHENKO
SPECTROSCOPY OF DIAMOND-LIKE PHASES FORMATION IN ONION-LIKE CARBON

A structure of the D- and G-bands as well as the 2-nd order ones in vibrational spectra of onion-like carbon (OLC), produced by electrical discharge treatment of hydrocarbons and annealing of nanodiamonds was studied. Extra low-frequency D_k and G_k components of the fundamental bands coupled with the states at Brillouin zone boundary are revealed. A dual nature of the D-band in OLC, special characteristics of metastable diamond- and graphite-like states and anomalous shift of D- and G-bands was investigated. The occurrence of positive anharmonicity was shown to be the indicator of strong inner self-contraction of OLC.

Key words: onion-like carbon, vibrational D- and G-bands, self-contraction, diamond-like structure, positive anharmonicity

L.V. KASHKINA, O.P. STEBELEVA, E.A. PETRAKOVSKAYA, T.Yu. EMELYANOVA
STUDY OF DISPERSE WATER-COAL SYSTEMS BY H^1 NMR-TOMOGRAPHY ANALYSIS

The research results of coal-water fuel (CWF) based on the the Kansk-Achinsk brown coal and distilled water cavitation – activated in the hydrodynamic generator of rotor type are presented. Sedimentation properties were studied by rate measurement of particle precipitation and H^1 NMR-tomography. The cavitation treatment of dispersion medium was established to improve the rheological characteristics of CWF. The possibilities of the H^1 NMR-tomography analysis for the study of high concentrated coal-water suspensions were assessed.

Key words: cavitation technology, rheological models, sedimentation, suspensions, brown coal

N.M. BARBIN, M.R. SHAVALEEV, D.I. TARENTIEV, S.G. ALEXEEV
BEHAVIOR OF URANIUM AND CARBON AT RADIOACTIVE CARBON HEATING
IN NITROGEN ATMOSPHERE. THERMODYNAMIC MODELING

The article presents the results of thermodynamic modeling of radioactive graphite heating in the temperature range of 373-3373 K in a nitrogen atmosphere. Balances of distribution of radioactive carbon and uranium on phases were built.

Key words: thermodynamic modeling, radioactive graphite, uranium, heating (burning)

V.P. FILONENKO, I.P. ZIBROV, V.A. DAVYDOV, M.V. TRENKHIH
PHASE FORMATION IN B-C-N SYSTEM AT HIGH PRESSURES: STRUCTURE AND
CHARACTERISTICS OF HETERO-GRAPHENE AND HETERO-DIAMOND PARTICLES

The regularities of the formation of hetero-graphene and hetero-diamond phases were studied in the pressure range of 4–12 GPa at thermobaric treatment of mixtures of carbon nitride or melamine with boron. This paper presents some structural peculiarities and characteristics of individual particles with micro- and nano-dimensions. Synthesized BCN phases have a base lattice of boron nitride with homogeneously distributed carbon atoms. The phase transition to diamond-like phase does not require the use of catalysts.

Key words: high pressure, carbon nitride, melamine, boron, hetero-graphene phase, hetero-diamond phase

N.A. KALASHNIK, A.V. KALASHNIK, I.V. ARKHANGELSKIY, A.P. MALAKHO, S.G. IONOV
PHYSICAL-CHEMICAL PROPERTIES OF LOW-DENSITY CARBON MATERIALS OBTAINED
BY HEAT TREATMENT OF GRAPHITE FOILS IMPREGNATED WITH WATER SOLUTIONS

The mechanical and thermo physical properties of low-density carbon materials obtained by thermal decomposition of graphite foil impregnated with aqueous solutions of surfactants, boric or phosphoric acids were investigated. The introduction of fire retardant additives was shown to result in a significant shift of the

temperature of the oxidation start. Arrhenius parameters and reaction orders for reactions of thermal oxidation of the obtained carbon materials were calculated.

Key words: graphite foil, wetting angle, tensile strength, thermo gravimetric analysis, formal kinetics

**R.A. KHMELNITSKIY, V.A. DRAVIN, V.N. AMOSOV, N.B. RODIONOV, S.A. MESHCHANINOV,
R.N. RODIONOV, G.E. NEMTSEV, V.V. SARAIYKIN, S.A. EVLASHIN, E.V. ZAVEDEEV**

DIAMOND DETECTORS WITH THERMAL NEUTRON CONVERTERS BASED ON IMPLANTED ${}^6\text{Li}$

Diamond detectors with thermal neutron converters based on ${}^6\text{Li}$ isotope were created. Two types of detector contacts fabrication are considered: a) implantation of ${}^6\text{Li}^+$ ions directly into metal hetero-epitaxial iridium contact of diamond detector; b) contact is a graphitized layer formed as a result of ${}^6\text{Li}^+$ ion implantation into the diamond. Detectors were tested under d-d, d-t and Am-Be neutron source irradiation. The diamond detector was shown to operate as a radiometer of thermal neutrons.

Key words: diamond detector, thermal neutron converter, lithium ions implantation, contact

B.A. KULNITSKIY, I.A. PEREZHOGIN, V.D. BLANK POLYTYPES AND TWINS IN DIAMOND-LONSDALEITE SYSTEM

Under conditions of the high-temperature and high-pressure treatment of graphite we obtained a powder containing diamond and lonsdaleite (hexagonal diamond). The structure of the obtained material was studied by high resolution electron microscopy and EELS. 4H- and 6H-polytypes of diamond were observed. Incoherent twin boundaries within the diamond were studied. The lonsdaleite fragments located at different sides relatively to such borders can be considered as twin-oriented. In this case $(3-308)_{\text{hcp}}$ or $(-3304)_{\text{hcp}}$ can be the twinning planes of the lonsdaleite.

Key words: transmission electron microscope, diamond, lonsdaleite, stacking faults, high pressure

D.N. SMIRNOVA, N.N. SMIRNOV, T.F. YUDINA, A.P. ILYIN, N.Yu. BEYLINA

CHEMICAL MODIFICATION OF CARBON MATERIALS WITH ORGANIC ACIDS IN CLEANING PROCESS OF PHOSPHORIC ACID

A well-chosen process conditions of defluorination with the use of adsorption purification of phosphoric acid (EPA) allow not only remove objectionable content, fluorine, silicon, but also realize the selective extraction of scarce raw materials - rare earth elements (REE). Perspective direction of modification of carbon materials is the approach associated with the fixing on the surface functional centers by treatment with organic acids.

Key words: phosphoric acid, carbon material, organic acids

T.F. YUDINA, I.V. BRATKOV, T.V. ERSHOVA, N.N. SMIRNOV, N.Yu. BEYLINA

INFLUENCE OF CHARACTERISTICS OF NATURAL GRAFITE ON ITS ABILITY TO OXYDATION

In the work the study of effect of crystal parameters, ash and elemental composition of natural graphite of 4 different deposits on its ability to thermally expanding and corrosivity was carried out.

Key words: natural graphite, ash, oxidized graphite, thermally expanded graphite

V.N. TSELUIYKIN, A.A. KORESHKOVA

ELECTROCHEMICAL DEPOSITION OF ZINC-CARBON NANOTUBES COMPOSITE COATINGS

Composite electrochemical zinc carbon nano-tube coatings were obtained from alkali electrolyte in the pulse-reverse mode. The structure and tribological properties of these coatings were studied. The introduction of carbon nano-tubes into zinc plating was shown to reduce the friction coefficient of the coatings being formed.

Key words: composite electrochemical coatings, carbon nano-tubes, sliding friction coefficient, regression equation

**N.V. TIMOFEEVA, N.Yu. KUZNETSOVA, V.V. KRASNOV, A.S. RACHKOVSKIY, A.I. FINAENOV
ANODIC RECEIVING AND RE-OXIDATION OF GRAPHITE BISULFATE**

Ranges of potentials in which it is possible to obtain graphite bisulfate and its over oxidized forms in sulphuric acid solution with the anodic polarization and pre-molded dispersive graphite were revealed. The

properties of the synthesized compounds were determined. The obtaining possibility of thermally expanding graphite compounds with the desired characteristics was shown in a controlled mode.

Key words: pyrolytic and disperse graphite, anode synthesis, graphite bisulphate, over oxidized compounds, thermo-expanded graphite

S.L. ZABUD'KOV, M.V. MEDVEDEVA, I.N. FROLOV, A.I. FINAENOV

DEPENDENCE OF KINETICS OF ANODIC INTERCALATION OF GRAPHITE AND PROPERTIES OF OBTAINED COMPOUNDS ON COMPOSITION OF NITRATE ELECTROLYTES

In the article the influence of nitrate electrolyte and potentials of anodic treatment on the kinetics of the electrochemical intercalation and properties of the thermally expanding compounds are discussed.

Key words: thermal expanded graphite, graphite thermally expanding compounds, graphite nitrate, anode intercalation

A.L. MASLOV, N.I. POLUSHIN, M.S. OVCHINNIKOVA, I.Yu. KUCHINA

RESEARCH OF NANODIAMOND POWDER AND COMPOSITE ELECTROCHEMICAL COATINGS HARDENED WITH NANO-DISPERSED DIAMONDS

In given paper the complex studies of nano-sized diamond powder and composite nickel electrochemical coatings hardened with nano-diamonds were carried out. It is shown that nanodiamond powder consists of two phases: crystalline, and the corresponding phase of amorphous diamond. The introduction into the structure of the diamond nano-powders of nickel leads to a change in the topology of the surface of the composite electrochemical coating (CEP). The increase in nano-powder content to a certain concentration facilitates the grinding of nickel grain, and the presence of nanodiamonds in the structure can increase the microhardness of the CEP from 3.2 GPa to 6.4 GPa.

Key words: nano-diamonds, composite electrochemical coating, surface topology, microhardness, tensile strength

A.I. FINAENOV, N.Yu. KUZNETSOVA, S.L. ZABUD'KOV, V.V. KRASNOV, N.V. TIMOFEEVA

COAXIAL ELECTROLYZERS FOR CONTINUOUS ANODIC INTERCALATION OF DISPERSED GRAPHITE IN SULFURIC ACID

The results of measuring the electrical conductivity of mixture of graphite – 94 % of sulfuric acid are presented. The possibility of their use for the anodic synthesis of graphite bisulfate including continuous mode in coaxial electrolyzers of various modifications was shown.

Key words: graphite intercalation compounds, graphite bisulfate, thermally expanded graphite anode synthesis, continuous operation electrolyzers

S.A. URVANOV, N.V. KAZENNOV, E.A. ZHUKOVA, A.R. KARAEVA, V.Z. MORDKOVICH

REINFORCED COMPOSITE MATERIALS WITH APPLICATION OF ELASTOMERIC MATRIX BASED ON CARBON FIBER MODIFIED WITH CARBON NANO-TUBES

The studies on surface modification of carbon fiber based on poly-acrylonitrile with the use of protective interlayer from aluminum oxide were carried out. This protective interlayer was prepared with applying of hydroxide aluminum sol. Samples of composite material based on nano-tube modified with carbon fibers and silicone rubber were prepared with cold pressing. The influence of carbon nano-tubes on adhesion and thermo physical properties of composite materials was revealed.

Key words: composite, carbon fibers, carbon nano-tubes, elastomer, silicone rubber

L.F. SAFAROV, E.I. ANDREIYKOV, I.V. MOSKALEV

EFFECT OF COAL TAR PITCH MODIFICATION BY CO-PYROLYSIS WITH POLYCARBONATE AND OXIDATION ON COKES MICROSTRUCTURE

The microstructure of cokes obtained from the coal tar pitches modified by co-pyrolysis with polycarbonate and thermal oxidation was studied. An isotropic coke was obtained from the coal tar pitch modified by co-pyrolysis with polycarbonate.

Key words: coal tar pitch, polycarbonate, pyrolysis, thermal oxidation

S.V. PANIN, L.A. KORNIENKO, T. NGUEN SUAN, M.A. POLTARANIN, L.R. IVANOVA, S.V. SHILKO

**WEAR RESISTANCE OF COMPOSITES BASED ON SUPER HIGH MOLECULAR
POLYETHYLENE REINFORCED WITH DIFFERENT NATURE GRAPHITE**

Tribo-mechanical parameters of composites based on super high molecular polyethylene (SHMP) with carbon of different nature and dispersion were studied under conditions of dry friction, lubricating medium and abrasive wear. The introduction of industrial fillers (colloid graphite, carbon nano-fibers, pyrocarbon, treated schungite) decreases slightly the mechanical properties of compositions based on SHMP (yield point, breaking point). Wear resistance of compositions based on SHMP is increased by a factor of 2 at his filling with the 5 mass % of C and by a factor of 5.7 at his filling with the 0.5 mass % of nano-fibers. Graphite in various states plays the role of solid lubricant at tribo-coupling of composites based on SHMP and provides a high wear resistance at extreme conditions of operation, for example, at low temperatures and aggressive media.

Key words: super high molecular polyethylene, filler, graphite, wear resistance, over molecular structure

O.N. ABRAMOV, D.V. SIDOROV, T.L. APUKHTINA, V.A. KHRAMKOVA

PRODUCTION OF PITCH CARBON FIBERS BASED ON OIL ROW

Due to high specific parameters of stress-strain properties as well as workability in manufacturing and processing the carbon fibers hold a particular place among the reinforcing fibers for constructional purposes. On the set of engineering and economic parameters pitch (based on oilstock and coal-tar raw material), polyacrylonitrile and hydrated cellulose fibers are advanced carbon fibers. Discrete samples of oilstock based pitch carbon fiber were fabricated in SSC RF GNIChTEOS.

Key words: oil pyrolysis heavy resin, oil pitch, pitch fiber, carbon fiber, composites