The calculated values of the direct voltage drop on diodes were defined at current $2{,}264\times10^{-5}$ A because structure with area of 4 μm ×1 μm=4 μm^2 was simulated. The p-n-junction active region radius of diode as an device is 75 μm then diode active structure total area is $\pi\cdot(75)^2\approx$ 17671,5 (μm^2). The current value of $2{,}264\times10^{-5}$ A through device with area 4 μm^2 corresponds to one of 100 mA through device with area 17671,5 μm^2 at forward bias of diode p-n-junction. The current value of $2{,}264\times10^{-9}$ A through device with area 4 μm^2 corresponds to one of 10 μA through device with area 17671,5 μm^2 at reverse bias of diode p-n-junction.

Diode structure design parameters and electrical ones values received as a results of modeling are well matched with the experimental data.

CONCLUSION

The results of simulation of diode technological fabrication process and its electric characteristics for the cases of using next epitaxial film types: 1) 17.0SEPh2.0; 2) 25.0SEPh6.0; 3) 25.0SEPh20.0 are presented in this article. The calculation values of diode structure design parameters, threshold and breakdown characteristics and respective voltage values were received for three epitaxial film types. The calculated results are well matched with the experimental data.

REFERENCES

1. *Zee, S.* Physics of semiconductor Device: in 2 books / S. Zee., Vol. 1. M.: Peace. 1984. 456 p.
2. MOS-VLSI. Simulation of elements and technological processes/ P. Antonetty [and others]: Translation from English, M.: Radio and Communication. 1988. 490 p.
3. *http://www.synopsys.com.*

CW EPR STUDY OF NATURAL MONGOLIAN COALS

S. Munkhtsetseg[1], N. M. Lapchuk[2], N. A. Poklonski[2], N. I. Gorbachuk[2], Kh. Tsookhuu[1], G. Shilagardi[1], N. Tsogbadrakh[1], A. N. Oleshkevich[2]

[1]Department of Physics, School of Art and Science, National University of Mongolia, University Street, Ulaanbaatar, Mongolia, munkhtsetseg_s@num.edu.mn
[2]Department of Semiconductor and Nano-electronics, Faculty of Physics, Belarusian State University

CONTINUOUS WAVE ELECTRON PARAMAGNETIC RESONANCE (CW EPR) METHOD.

The cw EPR spectra were obtained in the solid state at room temperature (300 K) in glass tubes in a presence of air (I) and in a flow of nitrogen gas (II). The samples were in size of greater than 5 mm and weighted nearly 30 mg. Sample mass is measured on the Mettler Toledo AE 260 micro balance and size on SMZ-140 series Stereomicroscope with magnification range ×40. A Bruker Elexsys II E500 X-Band spectrometer was used operating at a frequency of 9.8 GHz, with a 100 KHz modulation frequency, 0.01-0.1 mT modulation amplitude and ≤ 200 mW microwave power (200 mW at 0 dB attenuation). The spectrometer was equipped with a super high Q-factor resonator (ER 4122 SHQE) which has a cylindrical shape TE_{011} cavity. Modulation amplitude and time constant of EPR regis-

tration were chosen from well-known requirements for undistorted registration of the first derivative resonance absorption signal by magnetic induction.

EPR spectra of the studied coals were registered as the first derivative of the microwave absorption versus applied magnetic field. The parameters of the EPR spectra: g-factor, linewidth (ΔH_{pp}) and integral intensity (I_{pp}) were evaluated. g-factor was determined as $g=h\nu/\beta H_r$, where h is the Planck constant, β the Bohr magneton, ν the microwave frequency, and H_r is the resonance magnetic induction. The linewidth (ΔH_{pp}) was determined as the difference of field positions of maximum and minimum of the first derivative EPR spectrum. The integral intensity (I_{pp}) is the distance between maximum and minimum of the first derivative EPR spectrum. Coal free radicals or the integral intensities of the EPR signals were detected and quantified using the approximation: (*the derivative amplitude· ΔH_{pp}^2)/sample mass*. Simulation of CW EPR spectra was done using the Matlab package EasySpin [1].

SAMPLES

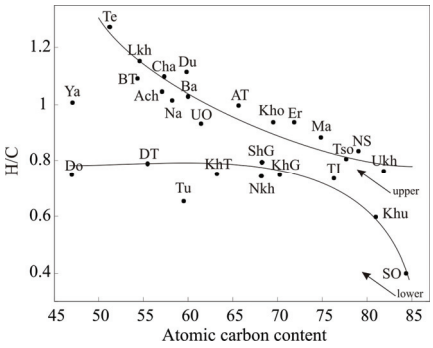

Fig. 1 Hydrogen atom contents (H/C in atomic unit) vs. carbon contents (in atomic unit)

The coals went under the determination of the elements C, H, N, O and S which has been carried out with instruments of the company LECO at the Micro Laboratory for Organic Chemistry (ETH, Zurich). The samples were digested first and the combustion products - carbon (CO_2), hydrogen (H_2O), sulfur (SO_2) and oxygen (CO_2) are analyzed quantitatively by infrared spectroscopy. Nitrogen (N_2) is determined by a thermal conductivity detector. These variables are measured in weight percent (wt. %) and are calculated in the air-dried (ad) base. Dependence between carbon content in studied coals and their atomic ratio of H/C is shown in figure 1. Due to this dependence the coals are grouped into upper and lower as following:

Upper group: Baganuur (Ba), Tevsh (Te), Aduunchuluun (Ad), Bayanteeg (BT), Yavar (Ya), Logiin-Khar (Lkh), Duvunt (Du), Chandgana (Cha), Maanit (Ma), Alagtogoo (AT), Ereen (Er), Ulaan-Ovoo (UO), Ukhaa-Khudag (Ukh), Tsagaan-Ovoo (Tso), Nariin-Sukhait (NS), Khotgor (Kho).

Lower group: Dov Tal (DT), Dovt (Do), Tugrug (Tu), Khar-Tarvagatai (KhT), Shariin-Gol (ShG), Tavantolgoi Seam I and IV (TI and TIV), Nuurtskhotgor (Nkh), Khushuut (Khu), Khuren-Gol (KhG), Saikhan-Ovoo (SO).

RESULTS AND DISCUSSION

Various EPR spectra of the studied coals were registered, e.g. symmetric or asymmetric, narrow and broad singlet. The EPR parameters of the spectra obtained in a flow of nitrogen gas are compared to the parameters in an air presence. The differences were observed in the EPR parameters such as line shape, peak-to-peak amplitude, line width and g-factor.

The coals have the same EPR line shape measured in the air and in the flow of nitrogen gas are Ya, UO, Te, Ma, Er, Lkh, Ad, KhT, Du, BT, Cha, Ba, AT and ShG. These coals are grouped as an upper level by the dependence of H/C ratio.

Symmetric signals in the air becomes asymmetric on coals Do, SO, UKh, Khu, Tu, NKh, NS, Tso, TI and TIV which are majority high rank and from the lower level.

Significant asymmetry, atypical signal shape with drastically descending in the centre has observed on the spectra of Kho and DT coals in both environments. The corresponding EPR spectra can be simulated as a spin with axial g-tenzors approximately (g_x=2.0062, g_y=2.0062, g_z=2.0063 for coal from Kho and g_x=2.0058, g_y=2.0058, g_z=2.0070 for DT).

Another effect from the oxygen presence on the EPR spectra is the interactions of coal with ambient oxygen, which broaden the EPR spectrum of coal. This can be true to the EPR spectra of the Khu, KhG, KhT, Nkh, Do, Du, Tso, Kho, TI, TIV, UKh, NS, ShG, UO, Tu, Cha, Lkh and Ad. The line width is not changed in Ya, DT, Er, Na, Te and AT coals and is broadened in the flow of nitrogen gas measurement of the other coals (Ma, BT, SO, Ba) that might have the formation of stable oxygen on the coals surface.

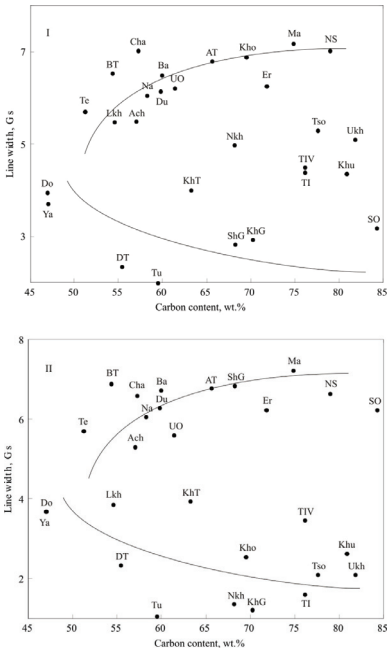

Fig. 2. CW EPR linewidth against coal carbon content I – in the air;
II – in the presence of nitrogen

EPR linewidth of whole signals was various, from 2.00 to 7.18 Gs in the presence of air measurement. In the flow of nitrogen gas measurement, the line width of the coals tends to narrow. The narrowest EPR line (ΔH=1.07 Gs) was registered from lignite coal Tu (carbon content of 59.41 wt. %) and the broadest (ΔH=7.23 Gs) was KhG coal with carbon content 70.14 wt. %. No linear dependence is observed between the linewidth of EPR signals and elements (hydrogen and oxygen) content of the studied coals. However, a tendency could be found in the plot of the line width against the carbon content. As shown in the figure 2 I and II two types of dependencies are cleared in both environments. The EPR line width less than 4 Gs coals have the tendency to decrease in the increase of the carbon content. These linewidth values are influenced by the oxygen presence (figure 2 I), particularly high rank coals such as Nkh, Tso, TI, TIV, Khu UKh and SO. Another type of coals has the line width greater than 5 Gs. The linewidth of these low rank coals is more stable in the presence of air measurement. On the basis of the H/C-values that for the coals with greater hydrogen content (≥ 5 wt.%) (Ma, Du, BT, NS, UO, Na, AT, Ad, Ba, Cha, Te, Er, LKh, ShG), the EPR linewidth is greater due to the hyperfine interaction between hydrogen and the spin centers.

It is likely the g-factor spread from 2.0015 to 2.0049 in the air ambient. In the flow of nitrogen gas g-factor of the most coals are shifted (lower or greater value). The variation of g-factor can be associated with free radicals of different nature in the coals. g-factor values

depend on two of elements (carbon and oxygen). g-factor is tended to decrease by the increase of carbon content in the studied coals. The oxygen effect can be easily eliminated by the flow of the nitrogen gas.

At the constant receiver gain and modulation amplitude the formulation: *(the derivative amplitude· $\Delta H_{pp}{}^2$)/sample mass* would be a proper measure of an EPR signal intensity. Therefore, the EPR signal intensity is increasing in the high content of carbon in the coals (figure 3). However, it was scattered in dependence on other elements (H, O, N and S) content of the studied coals. Changing measurement environment influences upon the peak-to-peak amplitude slightly in the coals. Increase on comparing air to nitrogen presence indicates the surface oxygen effect weakening. The considerable change can be seen only on coal SO that is significantly increased.

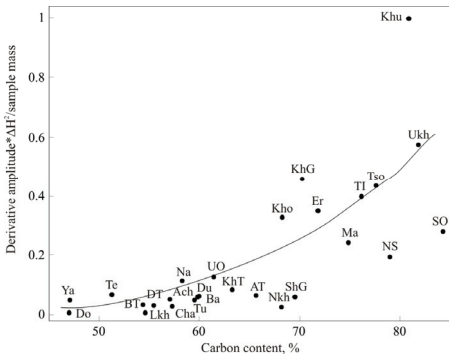

Fig. 3. Dependence of the peak-to-peak amplitude for the studied coals upon the carbon contents (wt.%)

As mentioned above the most of the cw EPR spectra of the studied coals are declined to asymmetry that can be from the complexity of the spin system. Therefore, complex character of the coal EPR spectrum is often visible at higher microwave powers, when some components partly saturated and the intensities of the others relatively increased. For this purposes, EPR microwave power saturation for each coal sample was measured. The dependence provides a measure of the interaction strength of the radical with the environment [2]. In both cases EPR spectra of the studied coals are saturated differently.

It is observed an extensive homogeneous saturation, exhibiting a maximum in the saturation curve, due to long relaxation times on coals from LK, Ad, Ma, Er, NS in the presence of air and UO, ShG, Do, LKh, Er, Ma, Ad deposits in the nitrogen gas flow. The second type of saturation curve with a leveling at lower power without any subsequent decrease in amplitude of the EPR signal for the coals from KhG, Khu, SO, Tu, TI, TIV, Nkh, UO, UKh, Do, AT, Kho in the air and Khu, Nkh, Tu, DT, TIV, Te and Ya in the nitrogen gas flow. An inhomogeneous saturation leveling causes the appearance of the narrow line overlapping on the broad line for the coals from KhG, Khu, Tu, Nkh, SO, TI, TIV, UO, UKh. Despite experimental environment, this phenomenon was observed on Khu, Tu, Nkh and TIV coals. A change in the EPR line of Kho and DT coals even at higher powers has not been observed. Therefore, asymmetry of these coals may be due to their specific structural nature such as an ash content, while the volatile matter of these coals are the lowest among the coals. A small degree of homogeneous saturation at the highest available power levels can be nearly true to the saturation curves of Ya, Na, KhT, Te, Du, Ba, Cha, ShG, BT, DT, Tso in the air and AT, Ba, Cha, Du, Na, KhT, BT, Tso, KhG, Kho, SO, UKh, TI, NS in the nitrogen gas flow measurement.

The saturation curve type is the same in two environments for the Tso coal, while the linewidth has changed significantly from nearly 5 Gs in the air to 2 Gs in the nitrogen gas environment. The environment change has not influenced on the saturation behavior of LKh, Ad, Ma, Er, BT, Du, Ba, Na and Cha who are from upper level. The linewidth of

these coals from first environment to second have no significant change and it is broad up to 7 Gs.

The saturation curve shows the one of components saturation character or broad (in the presence of air mostly) or narrow (in the flow of nitrogen gas mostly). The EPR spectra with two components in the coal has discussed in many of works [2, 3] that mainly attributed to two types of macerals (fusain and vitrain, respectively) in the coal. This is also proved by the dependences of atomic hydrogen-carbon ratio of the studied coals that particularly the lower group coals show the complexity in their EPR spectra. The narrow component is alleged to the presence of fusain (or inertinite) that is composed mainly of fusinite or carbonized woody plant tissue. One can also assign it to the coal spontaneous combustion since the same EPR property has observed on particular samples taken from the place where the coal self-inflammation center is. Broad component is attributed to the existence of vitrain in coal, which composed primarily of the maceral group vitrinite. Therefore, the observed absorption spectra in our case which regarded as two-components, the broad and narrow lines are attributed to the paramagnetic centres of vitrinite and inertinite, respectively. It is clear from the measurement results that the broad line is much more easily saturated, exposing a relatively weaker narrow line at high microwave power. The appearance of the narrow line is coal rank independent.

ACKNOWLEDGEMENT

Authors are very thankful to Prof. Gunnar Jeschke, who was given a possibility to do the measurements.

The work has been supported by F14MN009 project.

REFERENCE

1. Stefan Stoll, Arthur Schweiger // EasySpin: Simulating cw ESR spectra Biol. Magn. Reson. –2007. – V. 27. –P. 299–321.
2. *Silbernagel B.G.* Advanced electron paramagnetic resonance techniques for the study of coal structure / B.G. Silbernagel // Fuel. –1993. –V. 72. –N. 8. –P. 1219–1223.
3. *Retcofsky H.L.* Electron spin resonance in American coals / H.L. Retcofsky, J.M. Stark, R.A. Friedel // Anal.Chem. –1968. –Vol. 40 (11), –P. 1699–1704.

ADVANCED PULSE EPR STUDY OF NATURAL MONGOLIAN COALS

S. Munkhtsetseg[1], N. M. Lapchuk[2], N. A. Poklonski[2], N. I. Gorbachuk[2], Kh. Tsookhuu[1], G. Shilagardi[1], N. Tsogbadrakh[1], T. M. Lapchuk[2]

[1]Department of Physics, School of Art and Science, National University of Mongolia, University Street, Ulaanbaatar, Mongolia, munkhtsetseg_s@num.edu.mn
[2]Department of Semiconductor and Nano-electronics, Faculty of Physics, Belarusian State University

CONTINUOUS WAVE ELECTRON PARAMAGNETIC RESONANCE (CW EPR) METHOD

The continuous wave EPR spectra were obtained in the solid state at room temperature (300 K) in glass tubes in a presence of air (I) and in a flow of nitrogen gas (II). The samples were in size of greater than 5 mm and weighted nearly 30 mg. Sample mass is meas-