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Shungite influence on the ITO-coatings basic features: mechanical, spectral, wetting parameters change

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Transparent conductive coatings (TCC)

ITO In_2O_3 (90%) + SnO_2 (10%) **Indium Tin Oxide**

Applications:
- Solar cells;
- Transparent electronics;
- Display technology.

Advantages:
- Best transmittance values;
- Best conductivity values;

Disadvantage:
- Very expensive.

Analogues
- **ZnO** Zinc Oxide;
- **AZO** Aluminum Zinc Oxide;

Physical parameters:
- Band gap 3.75 eV;
- Charge carrier mobility 35 $cm^2/V \cdot s$;
- Refractive index 1.97..2.06.

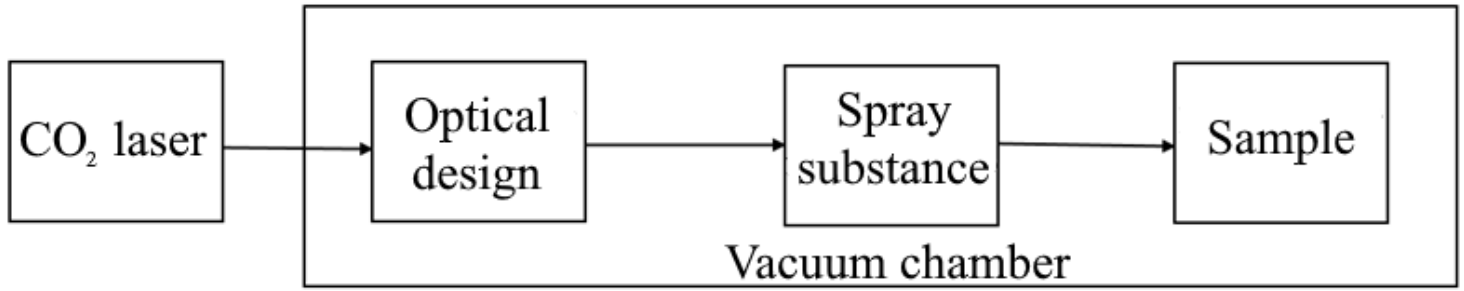
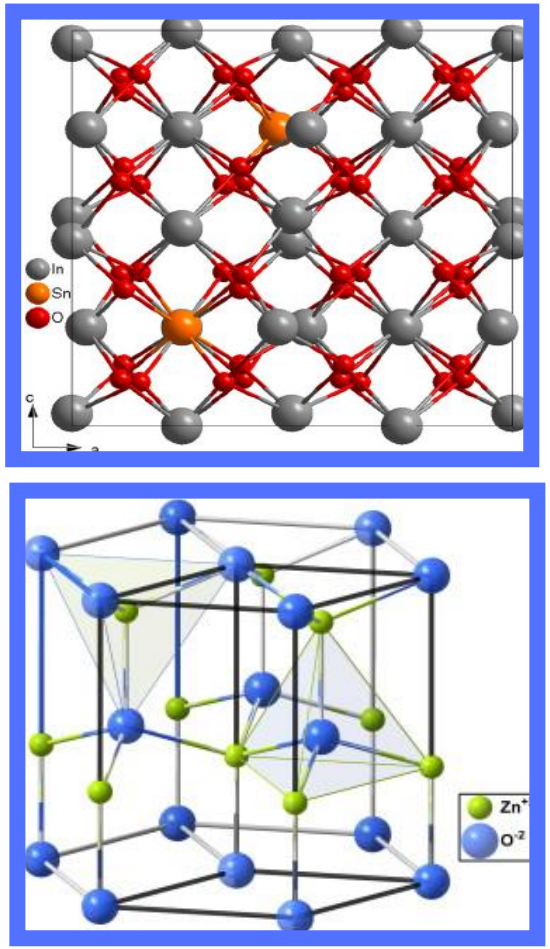


Figure 1 – Block diagram of the installation for the deposition of ITO films



[1]

[2]

Figure 2 - Models of ITO [1] and ZnO [2] structures

[1] Lovvik O. M., Diplas S., Romanyuk A., Ulyashin A.. Initial stages of ITO/Si interface formation: In situ x-ray photoelectron spectroscopy measurements upon magnetron sputtering and atomistic modelling using density functional theory // Journal of Applied Physics. 2014. – V. 115.
[2] Escudero R., Escamilla R.. Ferromagnetic Behavior of High Purity ZnO Nanoparticles // Solid State Communications. 2011. – V. 151. P. 97 – 101.

Shungite

Rock, the deposit of which is mainly concentrated in **Karelia** (region in the North-West of Russia).

Shungite nanoparticles are unique due to their:

- **Non-toxic** parameters;
- The ability to be **easily accepted from the earth's surface;**
- **Good refractive characteristics**.

How to improve the properties of TCC? → **Structuring with nanoparticles**

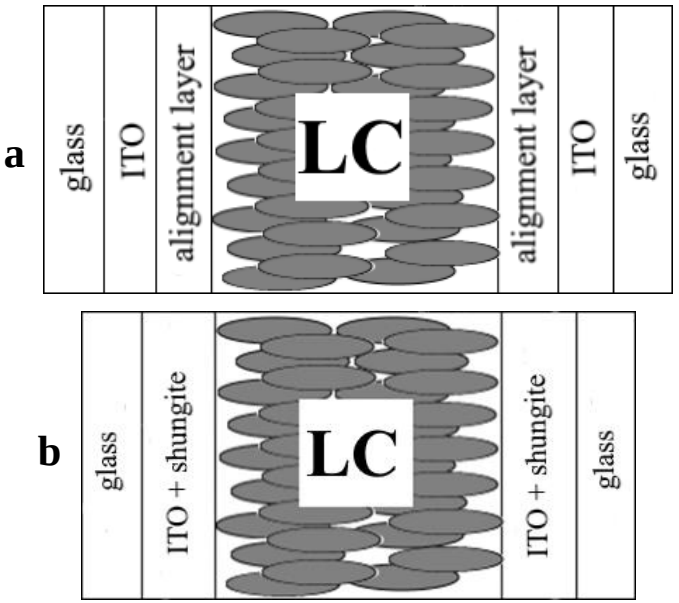


Figure 3 – Schematic representation of the simplest LC cell (a), LC with ITO modified with shungite (b)

Table 1 - The main components of shungite

Component	SiO_2	a-C	Al_2O_3	crystal H_2O	K_2O	Fe_2O_3	S	MgO
Mass composition, %	57	30	4	1.7	1.5	1.49	1.2	1.2

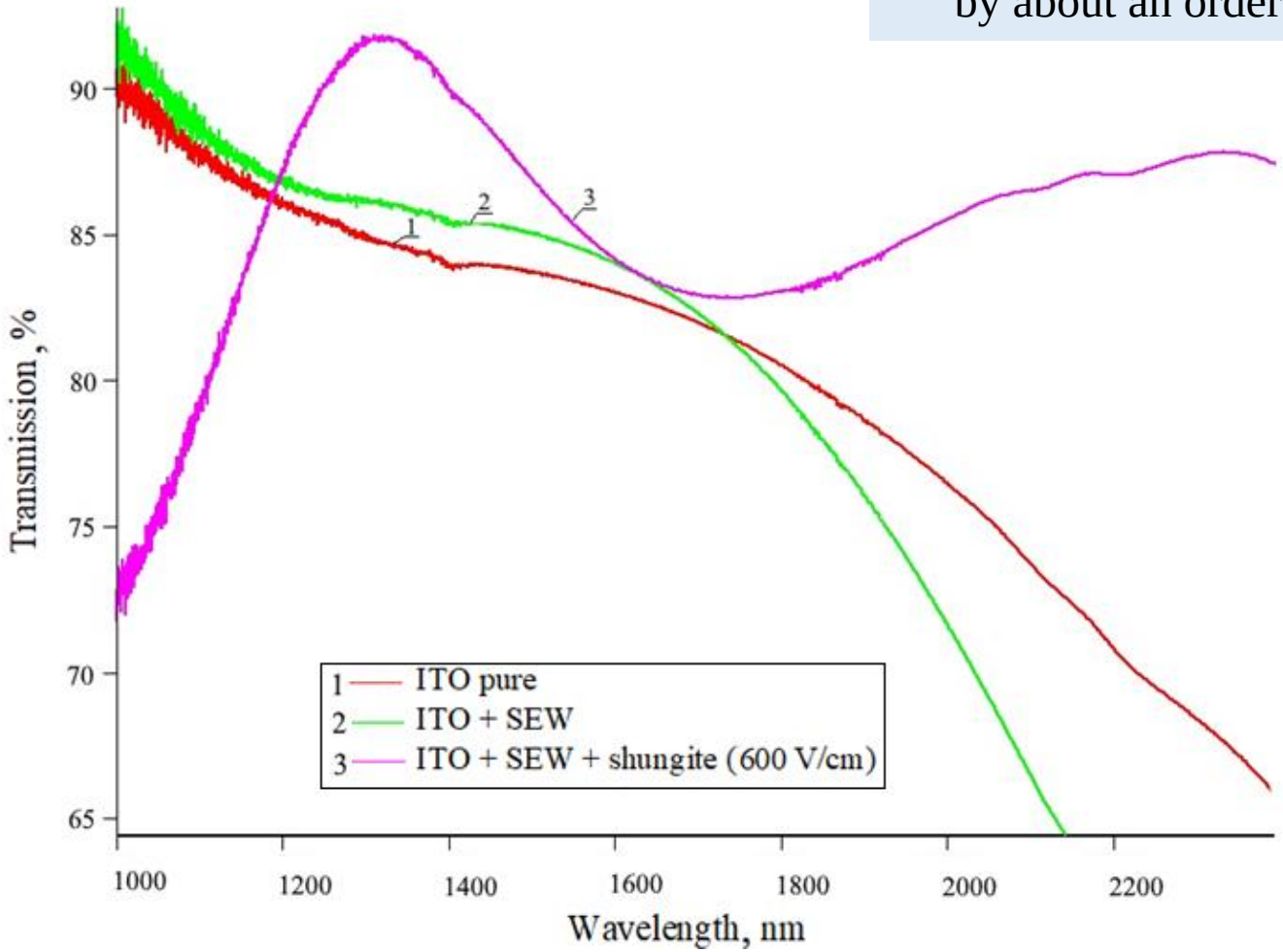
Transmission spectra

The shift of the transmission spectra by **40 nm** to the IR region indicates:

1. Changing the **band gap** E_g;
2. A change in the **mobility of charge carriers** by about an order of magnitude.

→ $E_{g\ (\text{pure ITO})}$ = 3.86 eV;
$E_{g\ (\text{ITO+shungite})}$ = 3.44 eV.

→ Future research



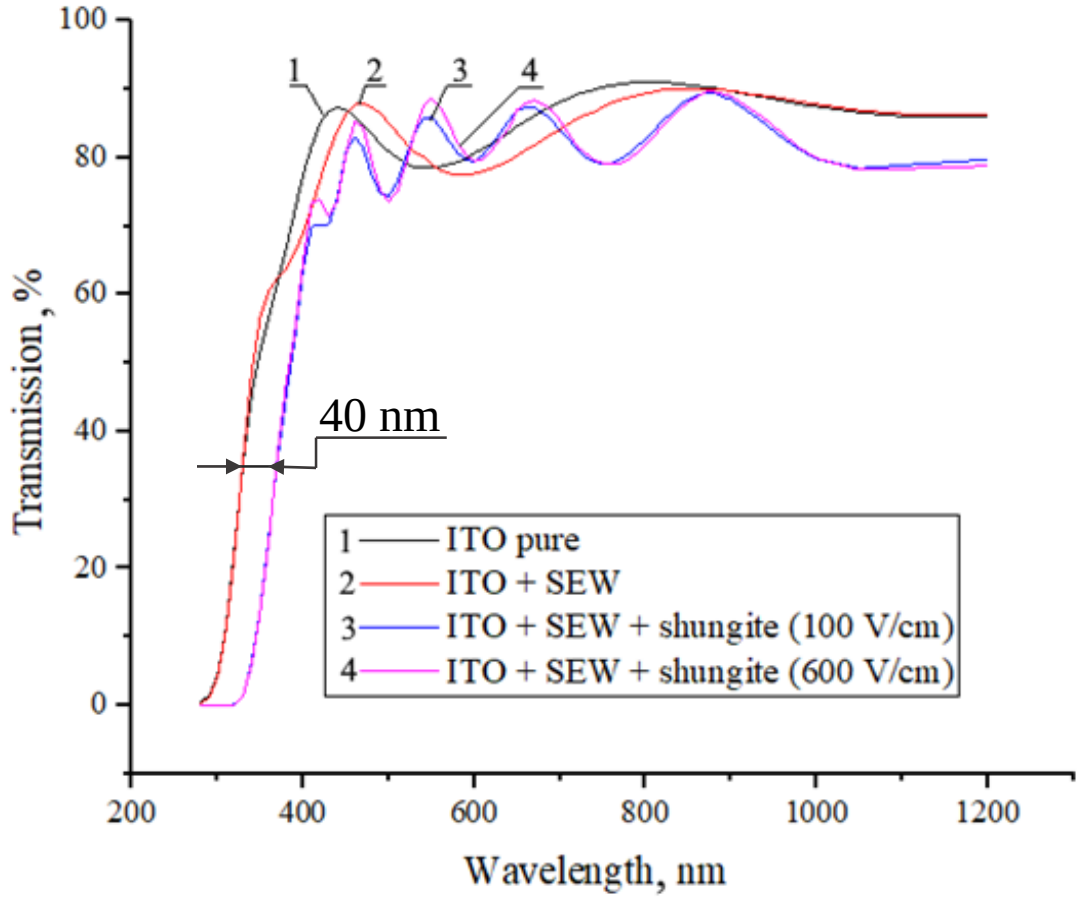


Figure 6 - Transmission spectra of the studied samples in the IR range (left) and the visible range (right)

Microhardness

Table 2 – Changes in the mechanical strength of ITO during structuring of CNTs and shungite

Sample	Microhardness, 10^9 Pa	Increase in microhardness compared to pure ITO	Reference
ITO	2.2 – 2.4	-	Present work
ITO+CNTs	4.2 – 4.8	In 2 times	[Toikka A. S., Kamanina N. V., Zubtcova Y. A. Carbon Nanotubes as Means to Optimizing the Operation of Liquid Crystal Cells// IEEE. 2020.]
ITO+shungite	8.0 – 20.0	In **3.6 – 8.3** times	Present work

Improvement in mechanical strength

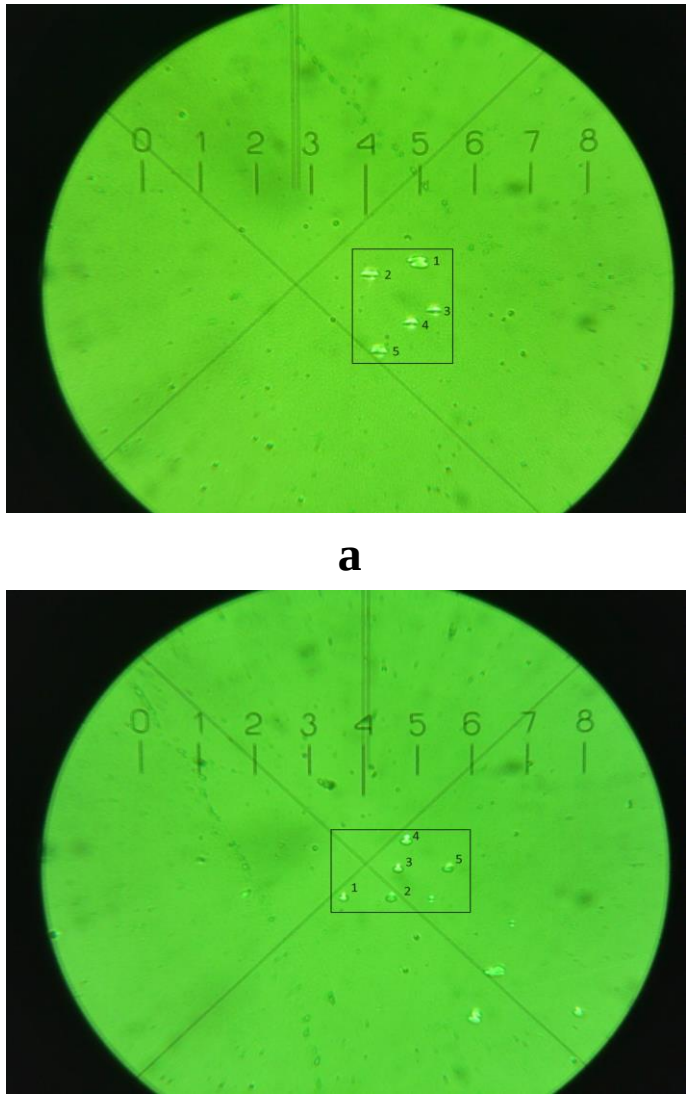


Figure 7 - Measurement of microhardness of the sample ITO+shungite:a - surface image at a load of 1 g; b - image of the surface at a load of 5 g

Wetting parameters

Table 3 – Contact angle and free surface energy

Sample	Θ_Y, °		Free surface energy, mJ/m^2		
	Water	Toluene	Polar	Dispersive	General
ITO pure	90.7	31.3	3.4	21.8	25.1
ITO+SEW	84.9	22	5.3	22.7	28.0
ITO+SEW + shungite (100 V/ccm)	63.4	27	12.4	19.3	31.7
ITO+SEW + shungite (600 V/cm)	**74.0**	9.3	11.5	21.0	32.6

The structure «ITO + shungite» is **hydrophilic**

Calculation of free surface energy:

$$\frac{\gamma_t(1+\cos\theta_Y)}{2\sqrt{\gamma_t^d}} = \sqrt{\gamma_e^p}\sqrt{\frac{\gamma_t^p}{\gamma_t^д}} + \gamma_e^d.$$

Θ_Y – Young's contact angle;
γ_t – surface tension;
γ_e – free surface energy;
γ^d – dispersion component;
γ^p – polar component.

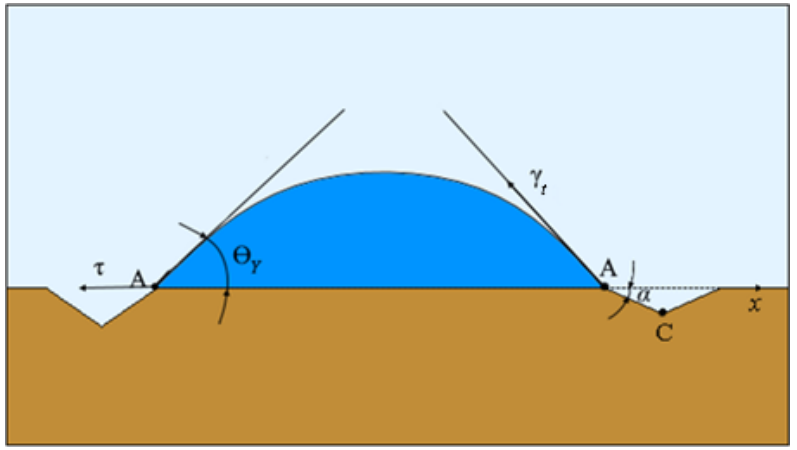


Figure 8 – Schematic representation of a liquid drop on a solid surface

Surface relief

Table 4 – Sample surface roughness

Sample	Roughness, nm					
	I order		II order		III order	
	Average	SD	Average	SD	Average	SD
ITO pure	18.0	10.6	11.6	4,7	4.4	1.7
ITO+SEW	27.6	15.5	13.4	2,6	7.6	6.4
ITO+SEW + shungite (100 V/cm)	**150.5**	87.8	**51.1**	9,8	**25.4**	5.4
ITO+SEW + shungite (600 V/cm)	**236.8**	150.2	**86.5**	13.1	**17.8**	4.4

Creating relief for the alignment layer

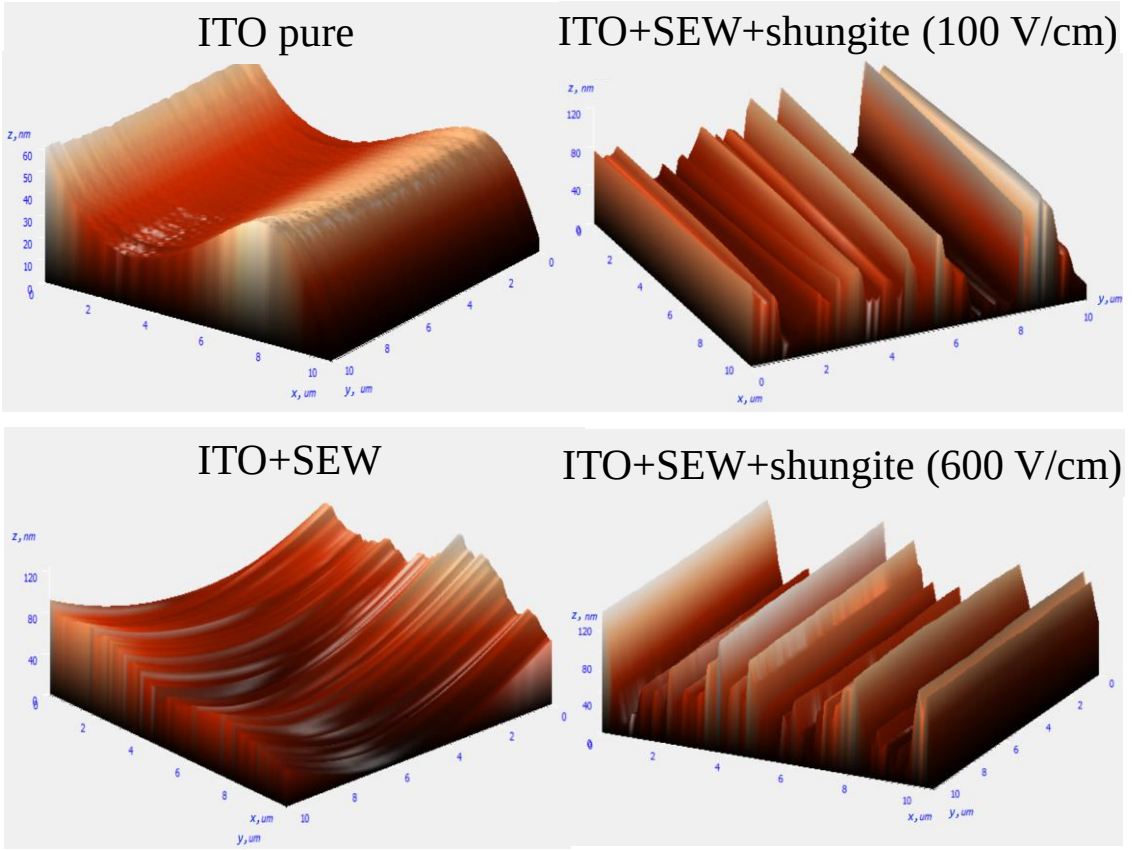


Figure 9 – Sample surface profiles

Conclusion

1. The "ITO + shungite" system has **prospects for use in devices operating in the IR range**. There is a shift of the transmission spectrum by 40 nm towards the IR range, a significant increase in the transmission in the IR range.

2. Structuring ITO with shungite can significantly **increase the mechanical strength**.

3. Samples with shungite have more **hydrophilic** behavior.

4. Structuring ITO with shungite, as well as subsequent surface treatment with an electromagnetic wave, allows you to create an **innovative relief for orienting liquid crystal molecule**s.

5. The **plans** include studying the process of increasing laser strength, changing the mobility of charge carriers and refractive properties by ellipsometry, as well as obtaining images using SEM and X-ray diffraction analysis.

Thank you for your attention!