**Frantsevich Institute for Problems of Materials Science of the National Academy of Sciences of Ukraine**

# Electronic structure of graphene nanosheets

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**The purpose of research:**

Study of the electronic structure evolution from starting carbon nanofibers material to graphene nanosheets.

**The task of the study:**

Obtain ultasoft X-ray emission C*K*α-bands of nanoscale carbon materials.

**Objects of research** - carbon nanofibers (CNF), oxidized graphene nanosheets (OGNSs) and graphene nanosheets (GNSs).

**The subject of study** - electronic structure of carbon nanostructured materials.

**Methods** - ultrasoft X-ray emission spectroscopy (USXES), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscopy (TEM).

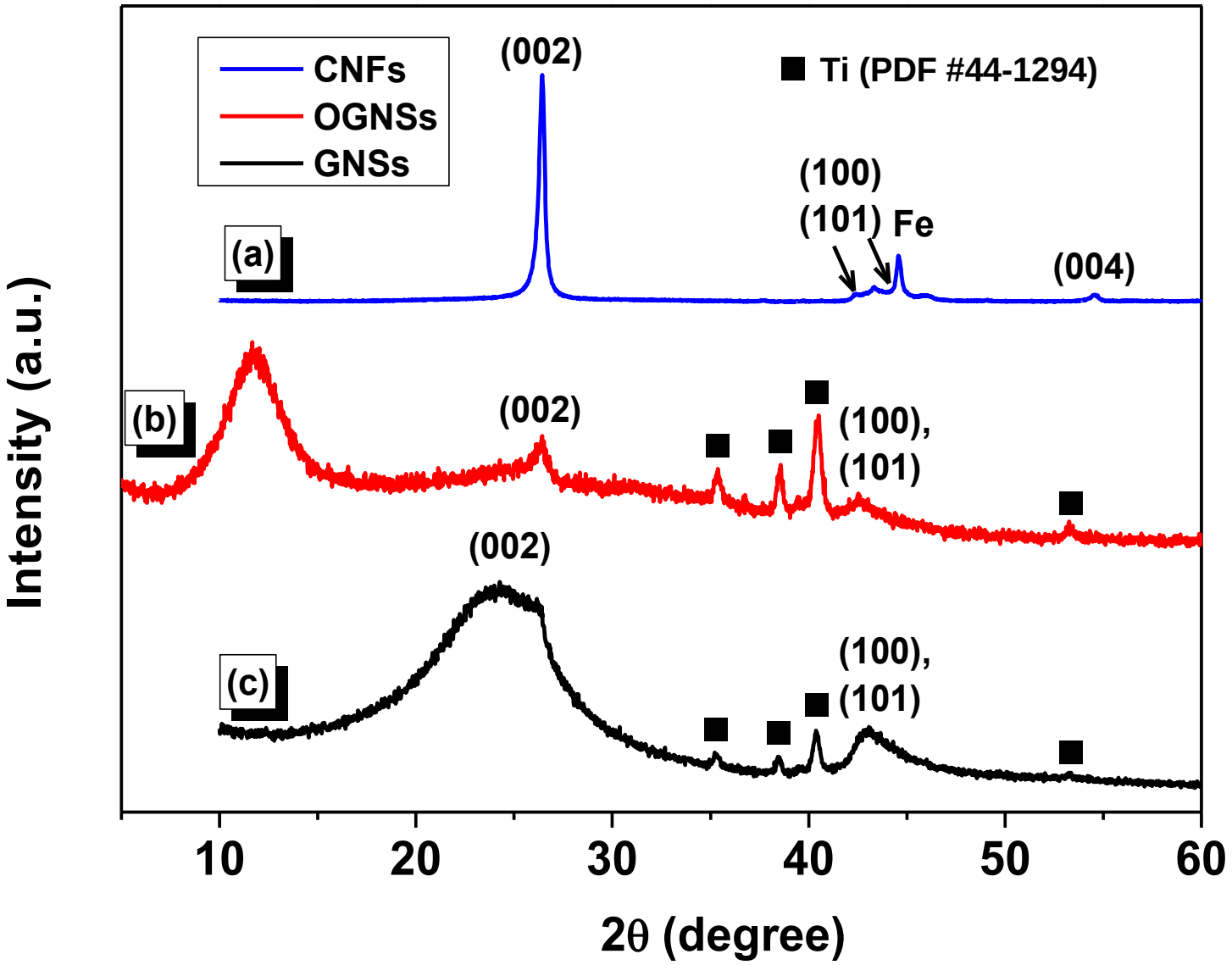


**Fig. 1** - The XRD patterns of (a) the starting CNF material, (b) OGNSs and (c) GNSs. (b)

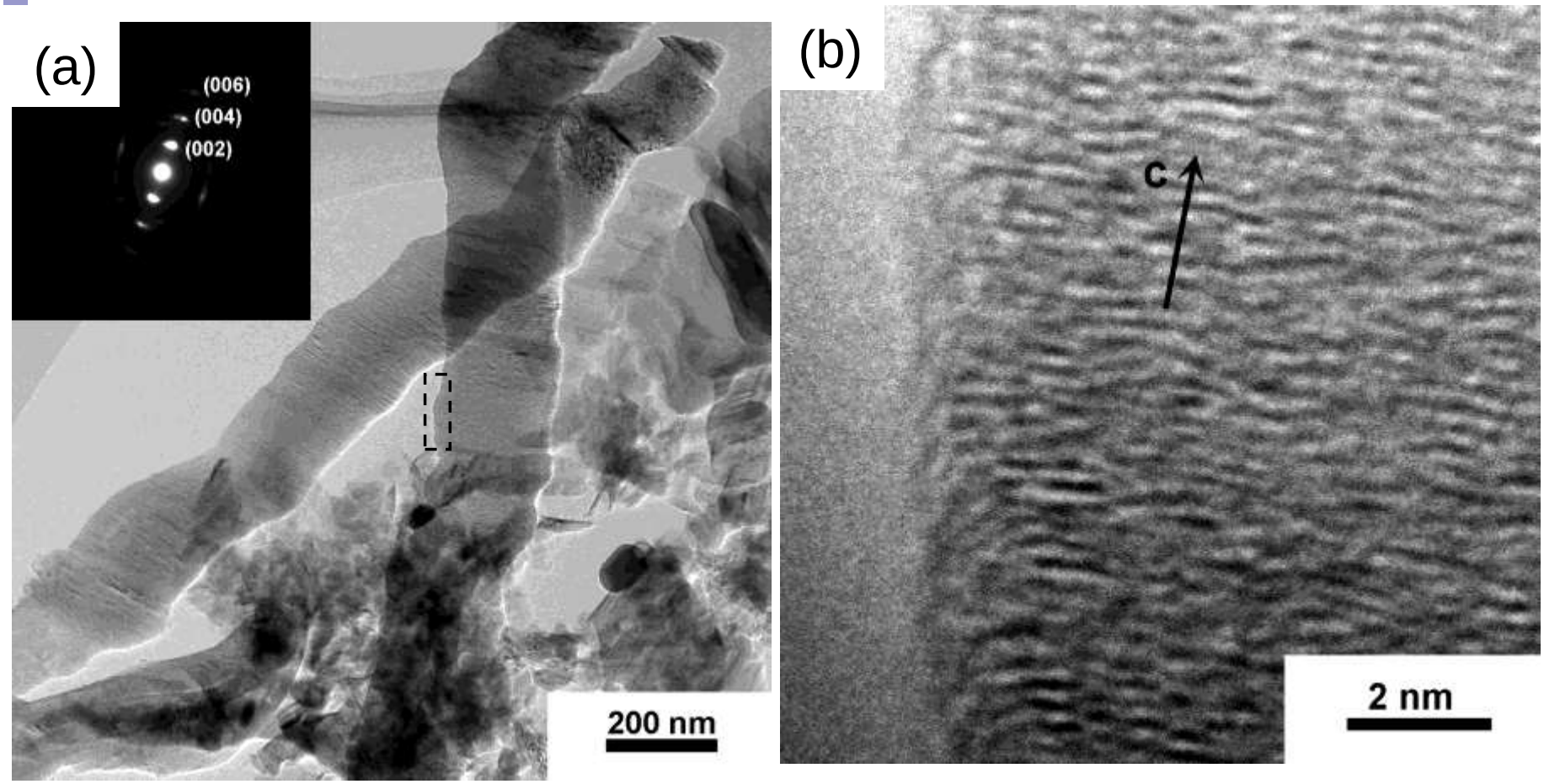


**Fig. 2** - (a) TEM image of the pristine CNF powder. (b) High-resolution TEM image of the rectangle marked in (a).

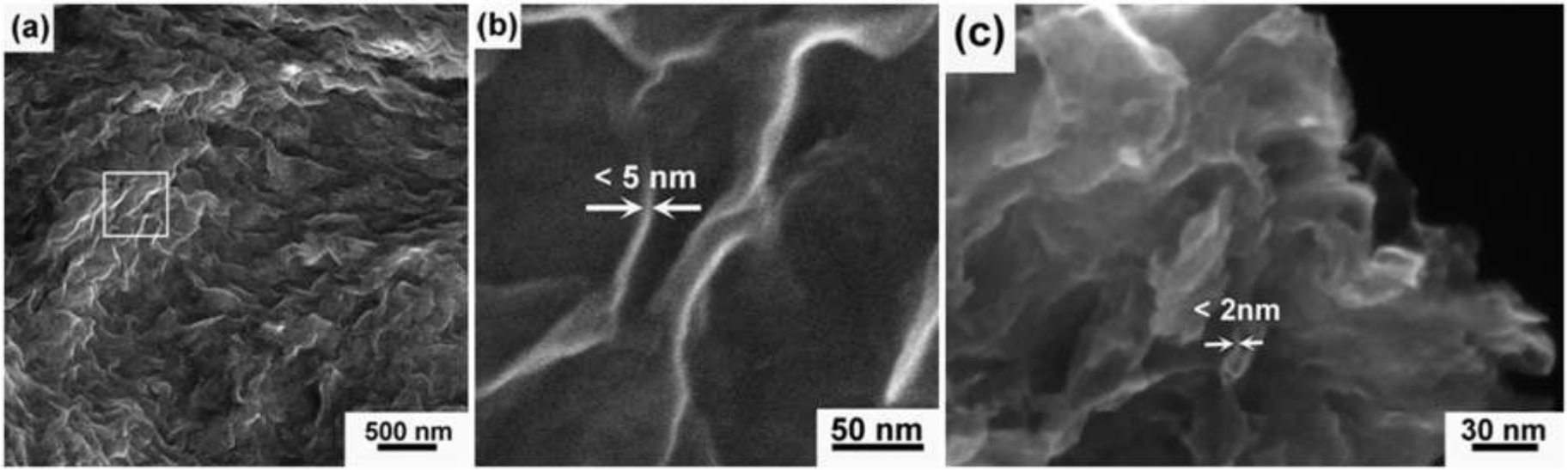


**Fig. 3 -** (a) SEM image of aggregated OGNSs. (b) SEM image of enlarged area surrounded by the rectangle in (a) of vertically oriented OGNS edges with a thickness less than 5 nm. (c) SEM image of GNSs produced via reduction of OGNSs with hydrazine hydrate. The GNSs are highly agglomerated, and the agglomeration has a fluffy curled morphology. A graphene nanosheet has a thickness at a curled edge less than 2 nm.

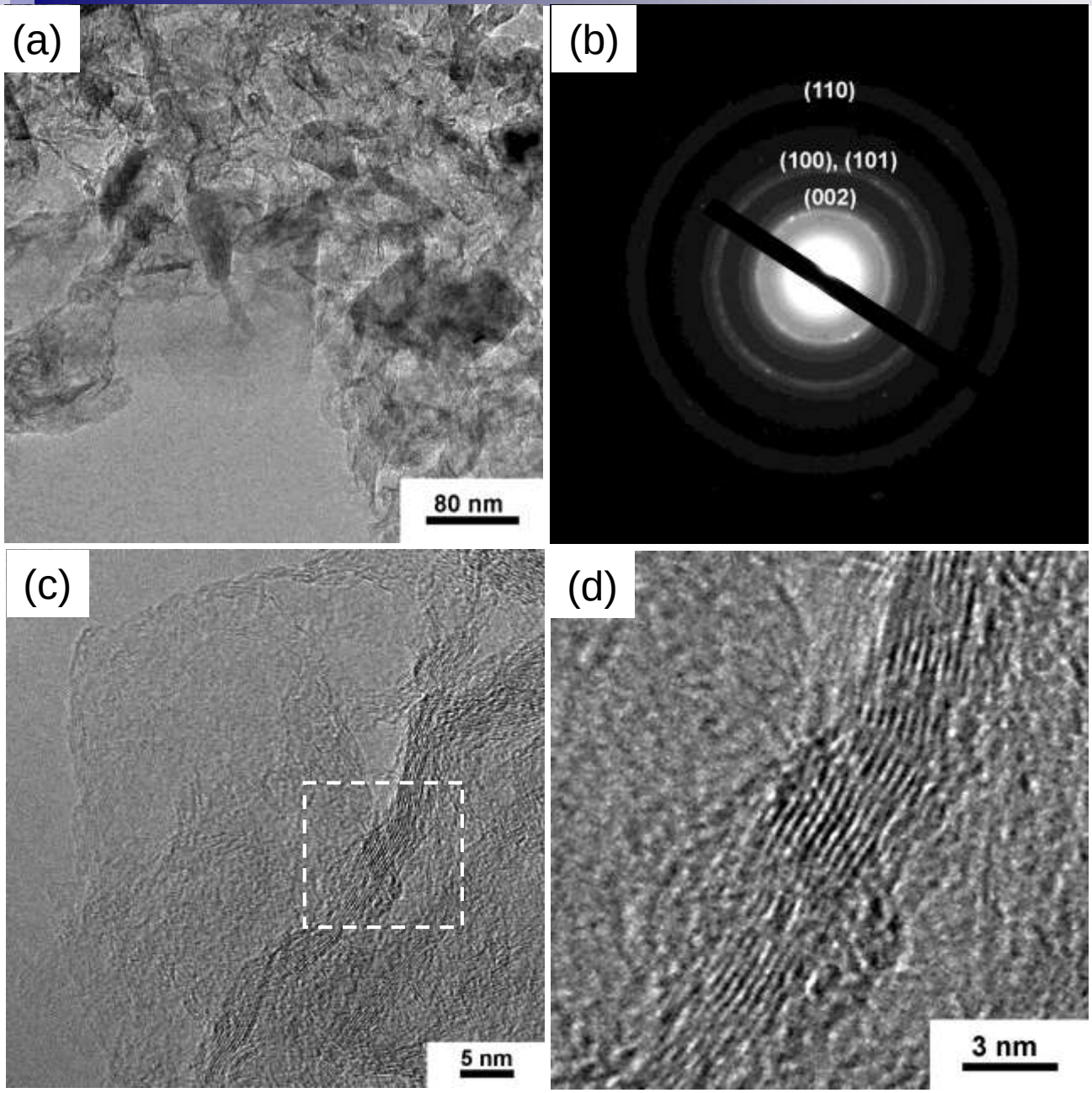


**Fig. 4 -** (a) TEM image of aggregated GNSs. (b) SAED pattern of the area in (a). (c) High-resolution TEM image of randomly selected area of GNSs. (d) The enlarged image of area surrounded by the rectangle in (c). Cross-section of graphene nanosheet in (d) shows the stacking of graphene layers.

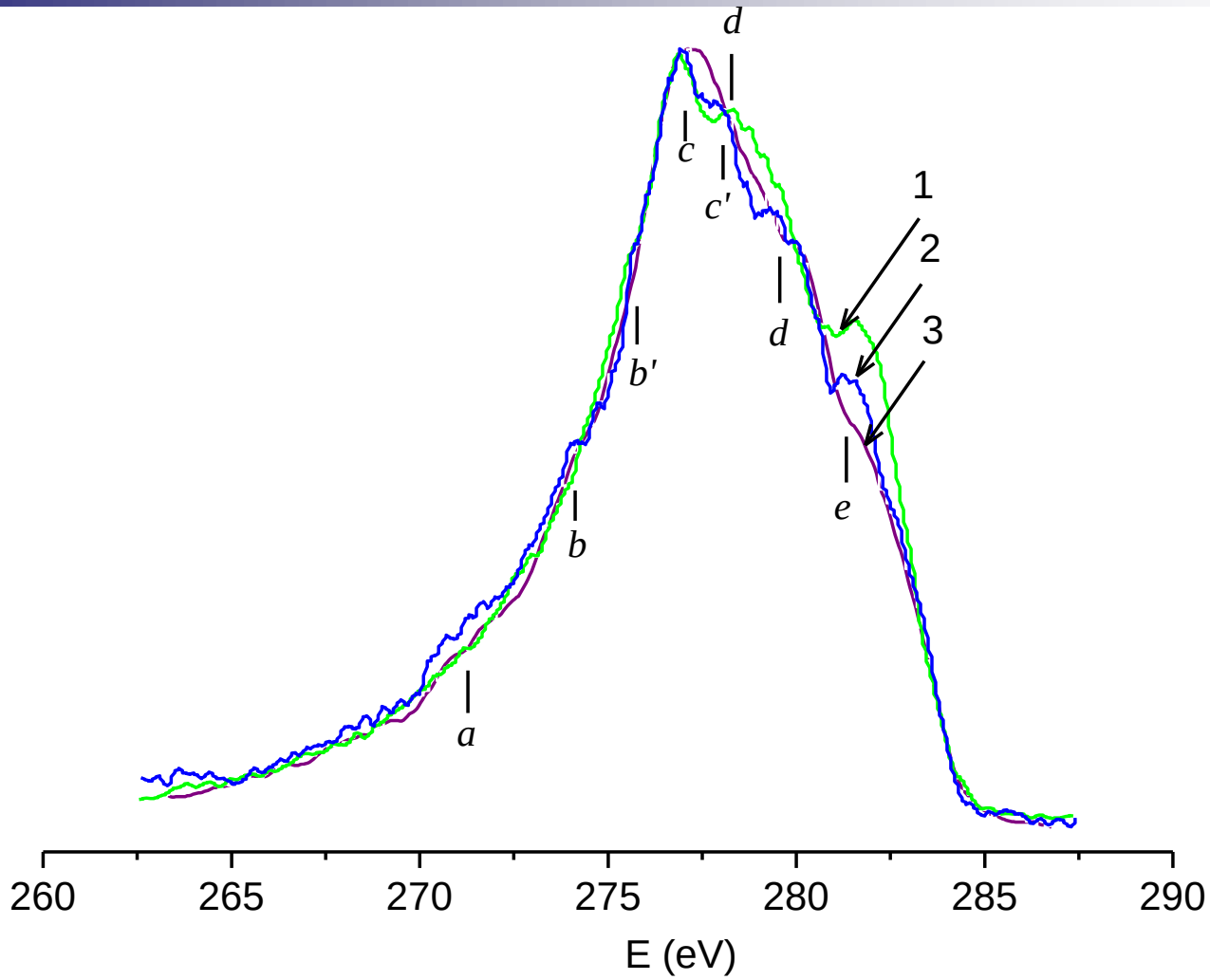


**Fig. 5** - The CKα-emission bands of the reference synthetic graphite (1), CNF (2) and nanofibres with a diameter of 30 nm (3).

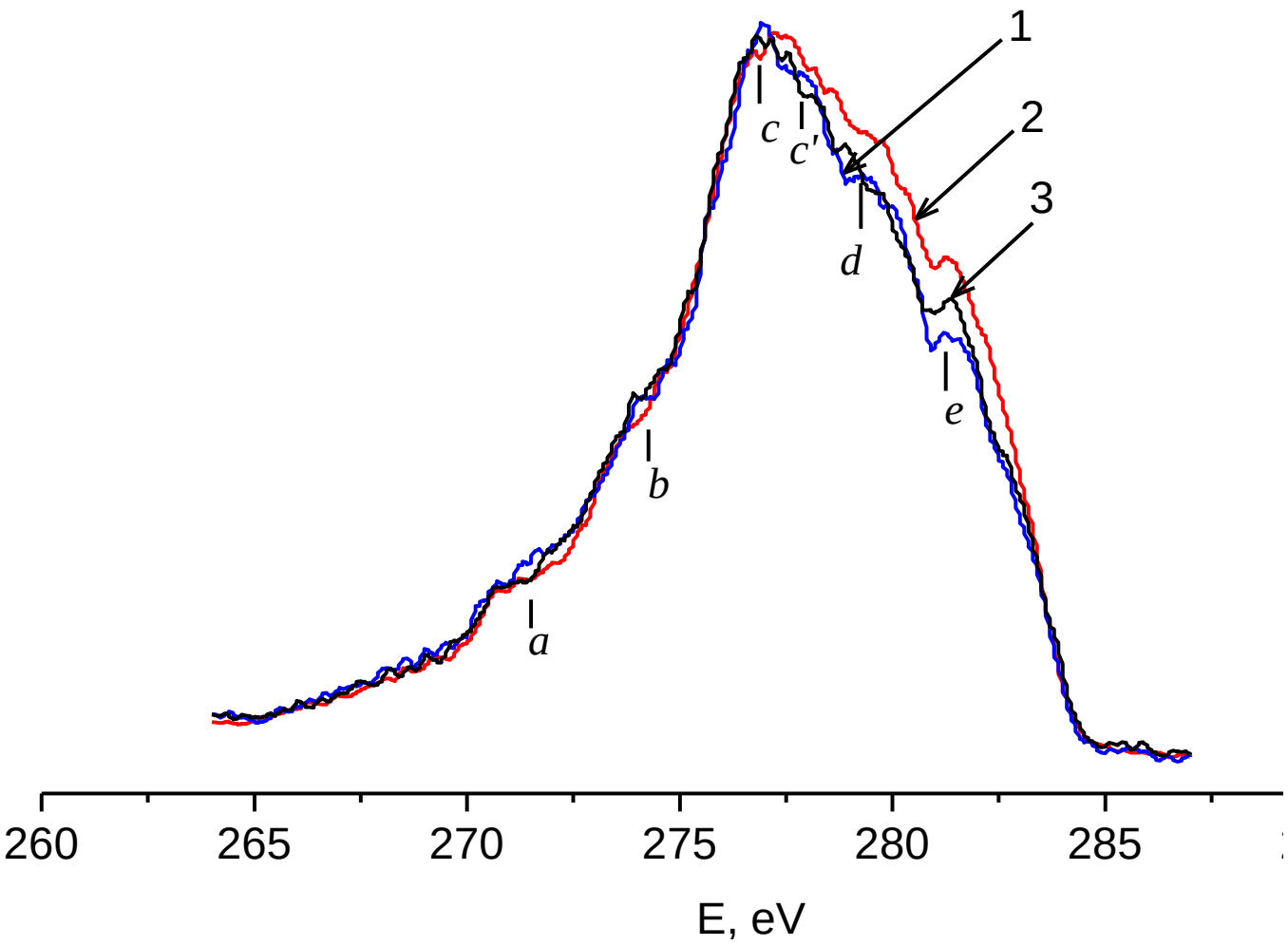


**Fig. 6** - The C$K_\alpha$-emission bands of: CNF (1), OGNSs (2) and GNSs (3).

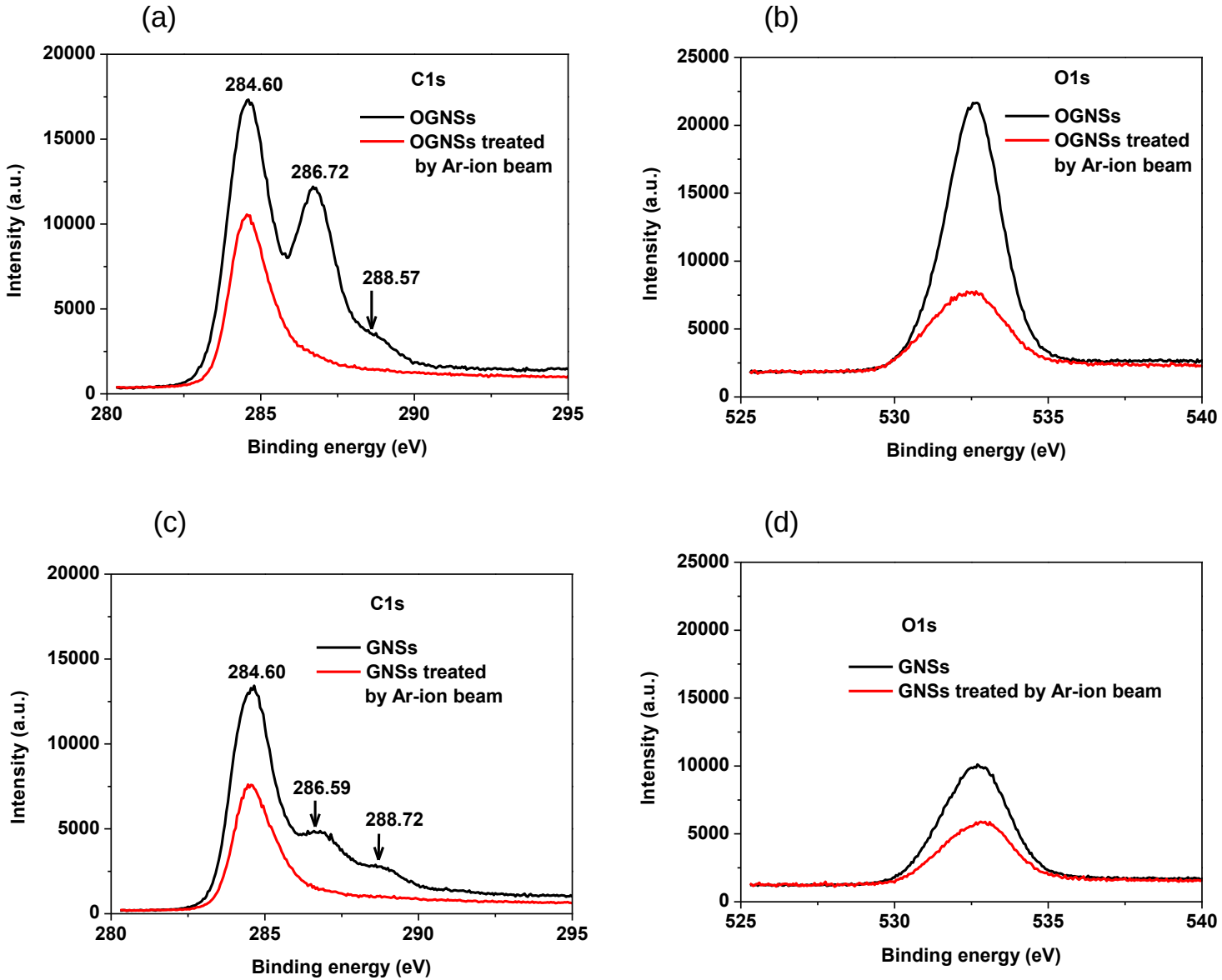


**Fig. 7** – C1*s* and O1*s*-XPS spectra of OGNSs (a and b) and GNSs (c and d) before and after treatment with an Ar-ion beam

# Conclusions

**1.** The effect of the degree of corrugation of the graphene nanosheets on the fine structure of the C*Kα*-emission bands was revealed owing to differences of π-subband intensities at different orientations of graphene layers. The intensity of the GNS C*K*α-band in the high-energy region was lower than that of the OGNS C*K*α-band. This is connected with a decrease in the distances between graphene layers from 0.75 nm to 0.337 nm, and an increase in the overlapping of misaligned π-orbitals between the corrugated GNSs.

**2.** Interaction of oxygen with electrons occupying carbon π-orbitals in the OGNSs leads to formation of attractive forces in the *c*-axis direction. As a result, the OGNSs become corrugated, with a curled morphology.

Thank you for attention