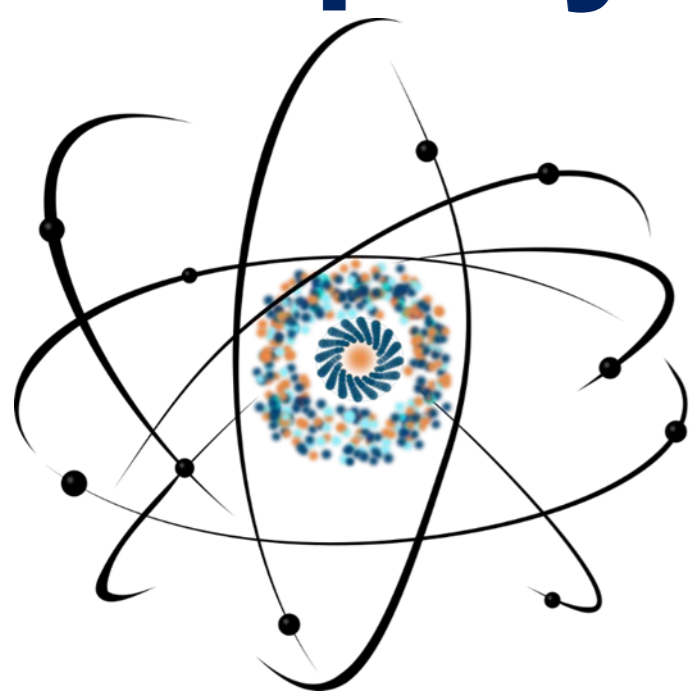


Chemical and electrochemical nanofabrication of polyaminothiazole/graphene oxide composites



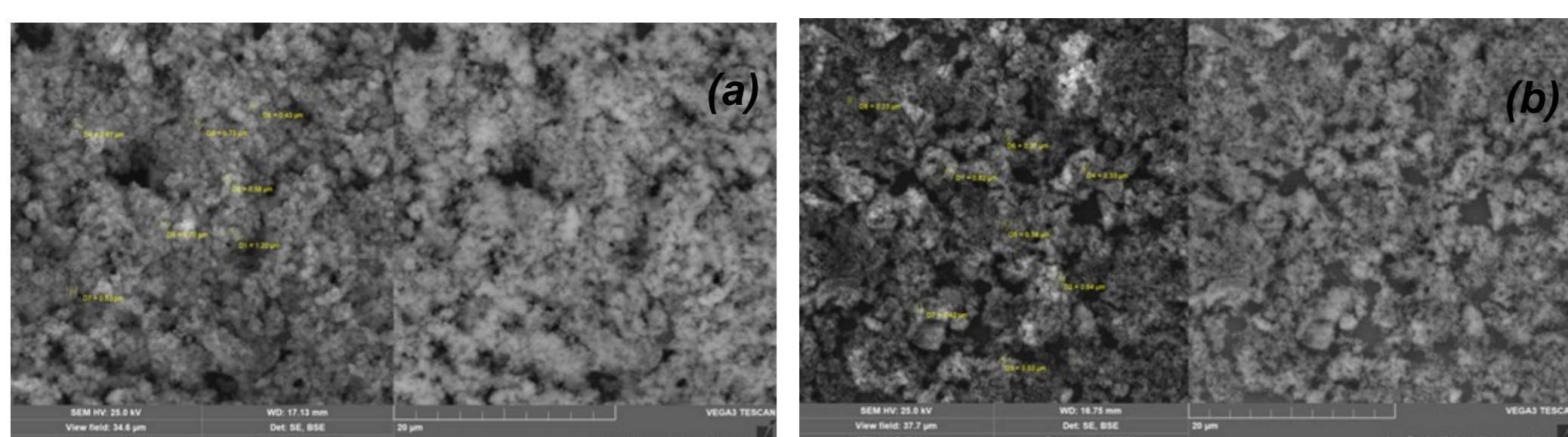
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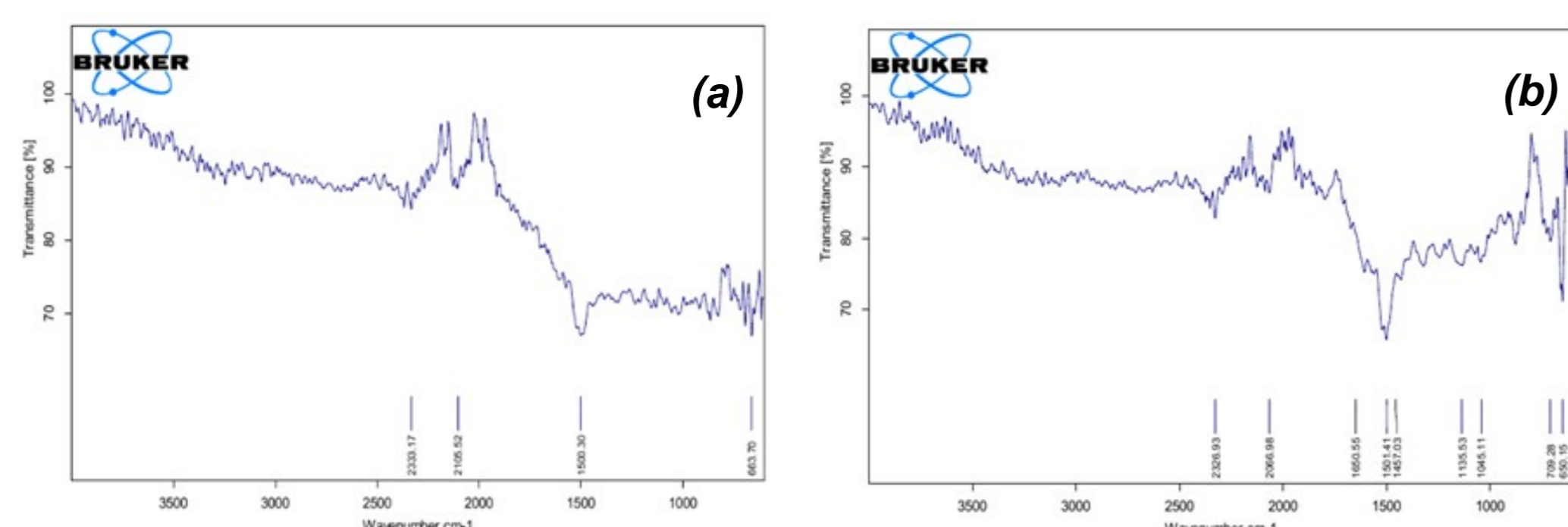
Conducting polymers (CP) are similar to metals and semiconductors due to their electrical and optical properties while preserving the useful properties of polymers – easy and inexpensive synthesis, elasticity, etc. Materials based on CP are versatile because their properties can be easily modified by surface functionalization and/or doping. One of little studied CP is poly(2-aminothiazole) (PAT), which contains S and N in a 5-membered thiazole ring. PAT has interesting sorption properties [1]. It is known that 2-aminothiazole is a biologically active compound with antimicrobial, antitumor properties [2]. In addition, graphene-based coatings functionalized with PAT have been reported to show potential applications in corrosion protection and antistatic coatings [3]. Therefore, optimizing the conditions for the synthesis and studying the physicochemical properties of PAT and its composites is a promising and actual task. In this work, we studied the conditions of chemical synthesis of PAT and its composites with graphene oxide (GO) in an aqueous solution under the action of inorganic oxidants, as well as electrochemical deposition on electrode surfaces of various natures – Pt and optically transparent SnO₂.

Chemical Synthesis



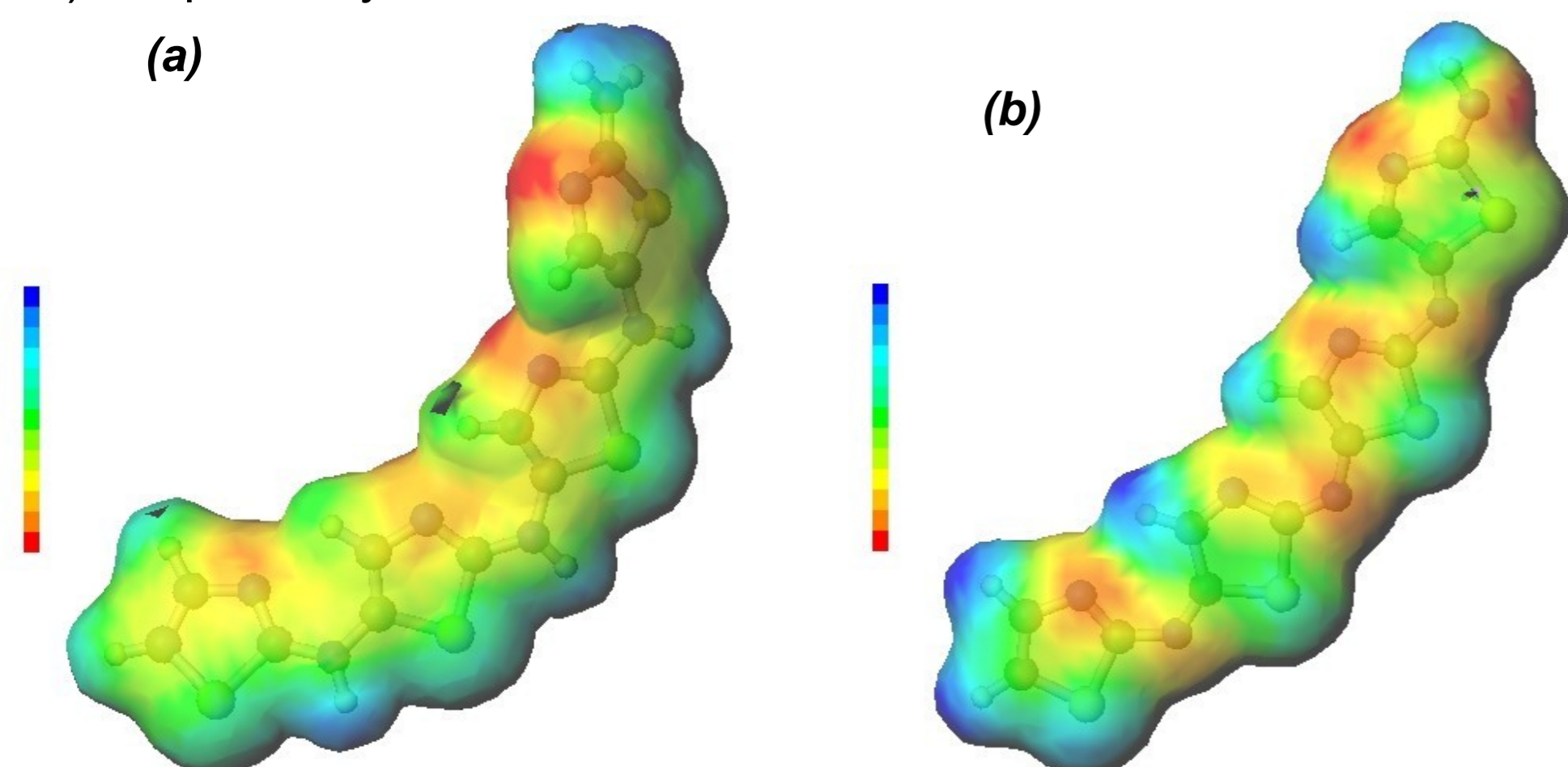
SEM images of PAT (a) and PAT/GO (b). Si substrate, magnification - 8000

The globular structure of obtained polymer with a globule size near 0.4-0.6 μm was shown by SEM. For PAT/GO the globules are smaller.



FT-IR spectra of PAT (a) and PAT-GO composite (b)

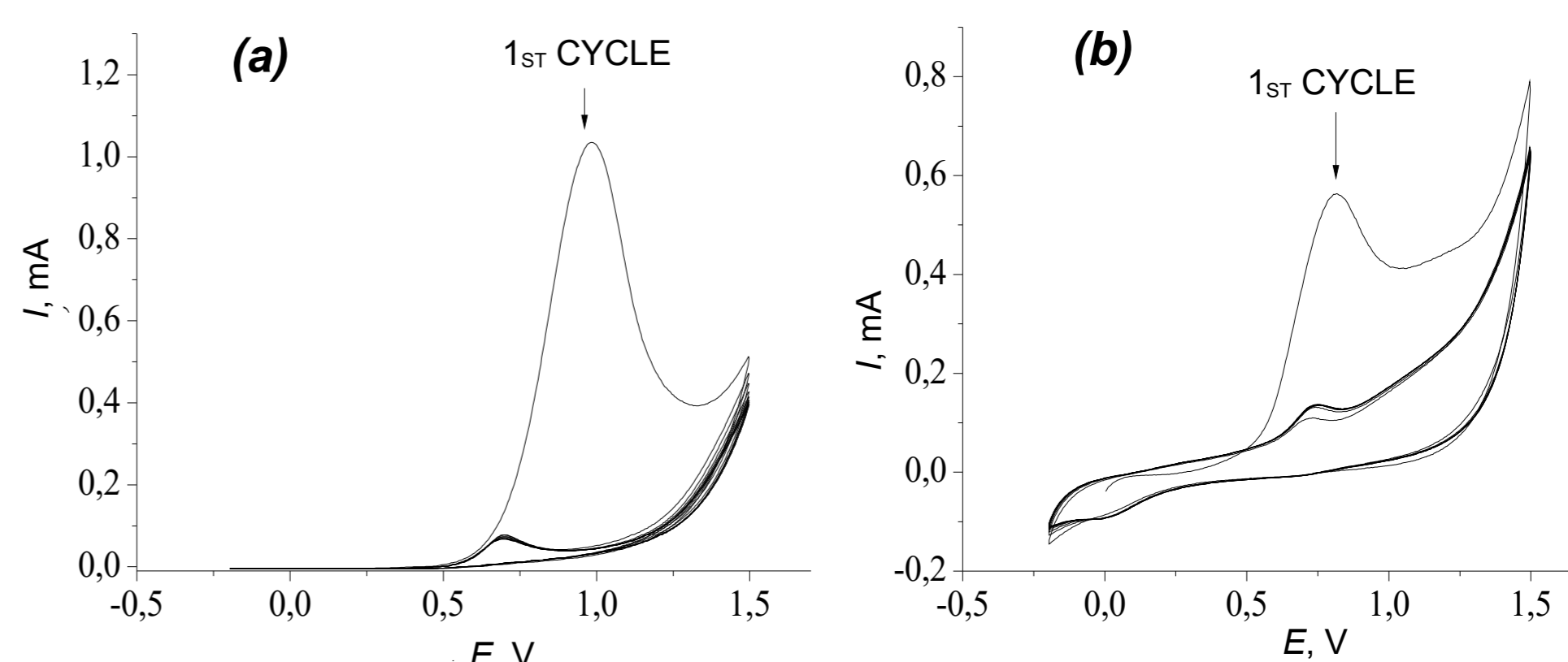
According to the FT-IR spectra of PAT and PAT/GO composite, the polymerization of aminothiazole occurs through the amino group, which is evidenced by the absence of characteristic signals in the region of 3000-3500 cm⁻¹. Absorption peaks at 2333 cm⁻¹, 2105 cm⁻¹, 1500 cm⁻¹, 664 cm⁻¹ are characteristic of PAT groups (CH-NH-CH), (C-N), (C=C), (C-S), respectively.



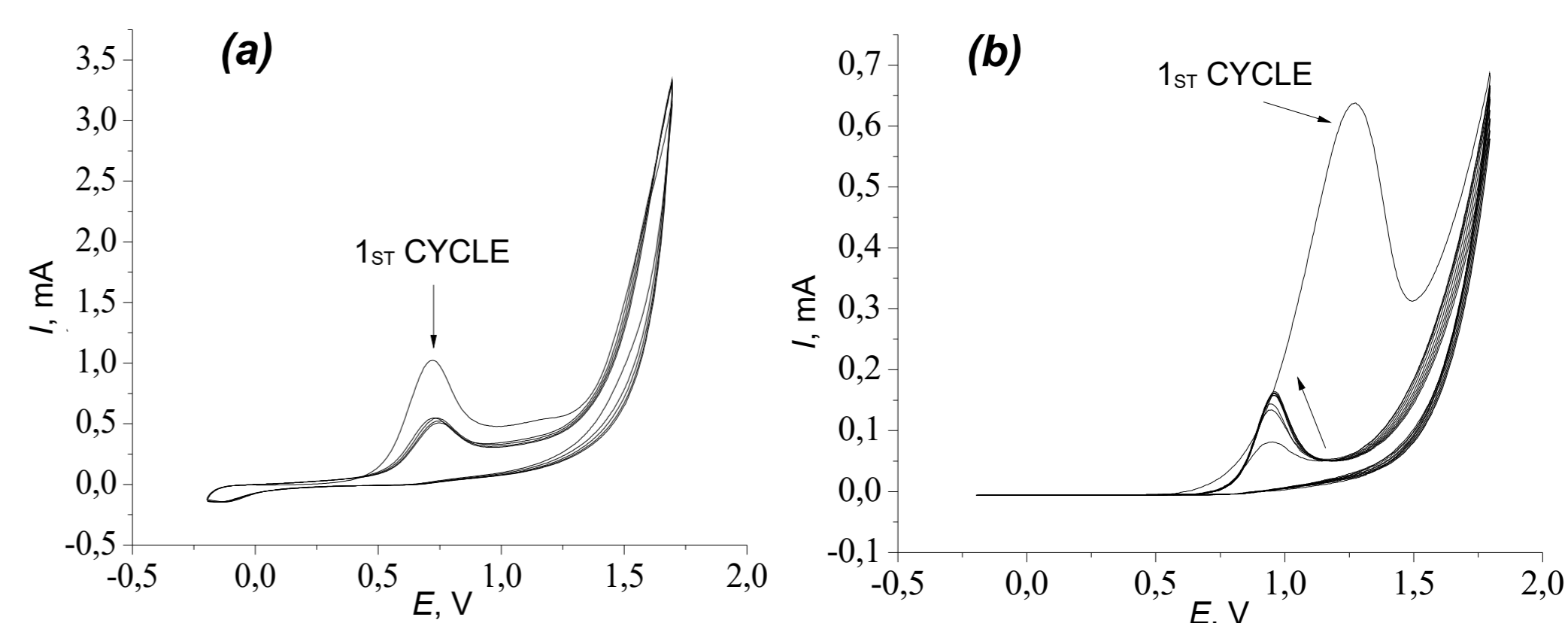
Molecular electrostatic potential maps of tetramer of 2-aminothiazole (a) and its imidothiazole form (b)

Quantum-chemical modeling of 2-aminothiazole (AT) molecules and its oligomers was carried out using the MOPAC 22.0.6 and the WINMOSTAR graphical interface, using the semi-empirical PM7 method. Conformational analysis of AT tetramer indicates that its macromolecule has the shape of a spiral, and S atoms and N-H groups are located on its outer side (Fig. 1a). In the case of the imidothiazole form of the AT tetramer, the oxidized macromolecule has a configuration close to the placement of atoms in one plane (Fig. 1b).

Electrochemical Deposition

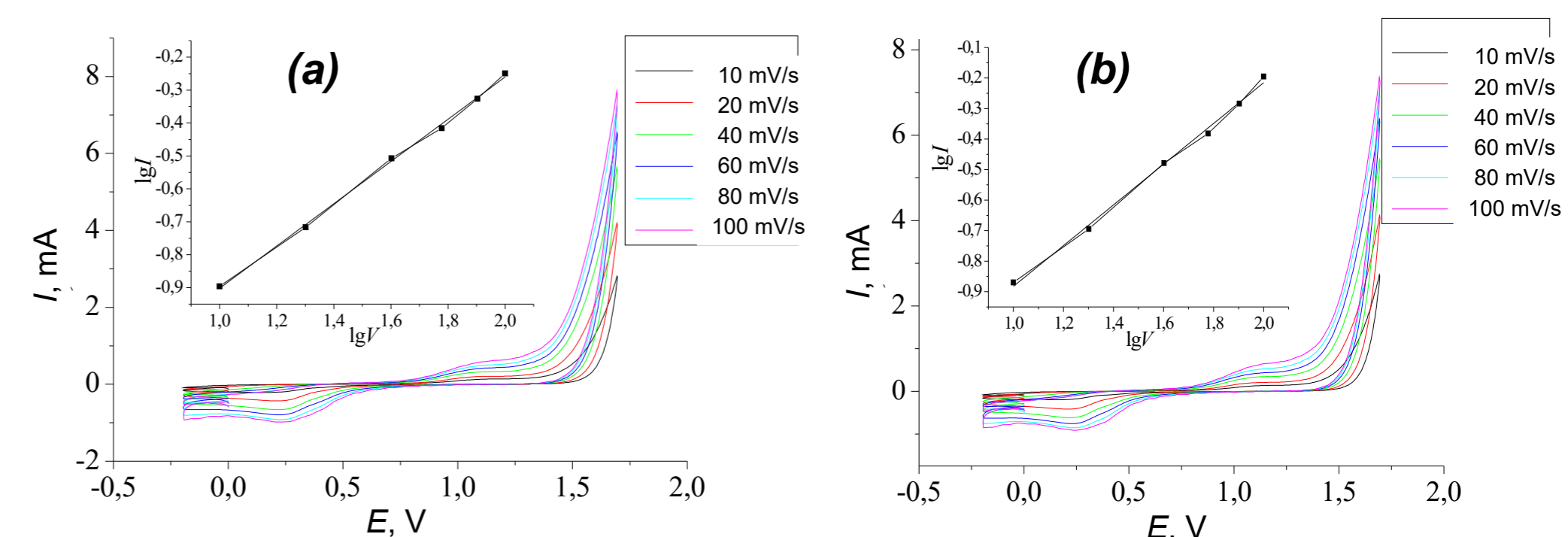


CVA obtained during electrochemical polymerization from an aqueous solution of 0.1 M AT on the SnO₂ (a) and Pt (b) electrodes, background electrolyte – 0.3 M (NH₄)₂C₂O₄, v = 20 mV/s



CVA obtained during electrochemical polymerization of 0.1 M AT in the presence of GO on Pt (a) and SnO₂ (b) electrodes, background electrolyte – universal buffer (pH=9.5) + 0.3 M LiClO₄, v = 20 mV/s

The addition of GO to the AT solution changes the voltage-current characteristics of AT electrooxidation. It may indicate the inclusion of GO in the PAT film during its formation. The presence of GO has a smaller effect on the electrooxidation of AT on the Pt than on SnO₂.



CVA of PAT (a) and PAT/GO (b) films on the Pt electrode at different scanning speeds, background electrolyte – 0.5 M H₂SO₄. Inset: dependence of the peak current on the sweep speed in logarithmic coordinates

Effective charge diffusion coefficients determined by the Randles-Sevcik equation:

$$D_{ef} = 1,36 \times 10^{-8} \text{ for PAT film,}$$

$$D_{ef} = 2,32 \times 10^{-8} \text{ for PAT/GO film}$$

References

1. Bıyıkođlu M., Çiftçi H. // Polym. Bull.-2020.-77.-P. 6161-6174.
2. Kashyap S. J., et al. // Med. Chem. Res.-2012.-21.-P. 2123-2132.
3. Qiu S., et al. // J. Alloys Compd.-2018.-747.-P. 60-70.