

# X-ray diffraction investigation of structure of gold nanorods and metal oxide nanoparticles for theranostic applications

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Magnetic and plasmonic nanoparticles can be used in medicine, for example as theranostic agents, combining diagnostic and therapeutic processes. Plasmonic nanoparticles exhibit qualities that make them perfectly suited for sensing, including biosensing. For determination of their properties, it is important to know their composition and structure, as it can affect their efficiency in their respective tasks. X-ray diffraction (XRD) can help to determine the crystallographic structures and phase content of the nanoparticles as well as to estimate the size of the nanocrystallites.

We have obtained diffractograms for iron oxide nanoparticles synthesized by coprecipitation of iron (II) and iron (III) chlorides in the presence of hyaluronic acid sodium salt (Na-HA), as described by Kasprzyk et al. 2025 [1] and for gold nanorods with plasmonic properties, synthesized using a modified seedless growth technique described by Ali et al. 2012 [2]. Then, we have determined mean diameter of the nanoparticles using the Williamson-Hall method and imaged the nanoparticles using Scanning Transmission Electron Microscopy (STEM), which allowed for a comparison between a direct and indirect size estimation. For the gold nanorods a conclusion on the anisotropic growth was drawn.

For plasmonic nanoparticles, their dimensions and material influence their absorption spectra, and, consequently the efficiency of photothermal conversion caused by localised surface plasmon resonance (LSPR). Size and composition are also crucial for superparamagnetic iron oxide nanoparticles (SPIONs), as they decide on their superparamagnetic properties. Thermographic measurements of a suspension of gold nanorods illuminated with 450 mW, 808 nm laser light will be demonstrated and compared to analogous measurements of a suspension of spherical gold nanoparticles. For SPIONs, magnetic measurements such as Vibrating Sample Magnetometry (VSM) results will be shown. The relationship between properties that can be derived from diffractogram analysis and their consequences for application purposes will be discussed.

[1] Kasprzyk, M., Opila, G., Hinz, A., Stankiewicz, S., Bzowska, M., Wolski, K., Dulińska-Litewka, J., Przewoźnik, J. Kapusta, Cz., Karewicz, A. (2025). ACS Appl. 17, 9059-9073.

[2] Ali, M. R. K., Snyder, B., El-Sayed, M. A. (2012). Langmuir 28, 9807-9815.

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