A comparative microstructural characterization for gold nanoparticles and thin-films using integral breadth methods

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The study of the microstructure, such as the size of the domains or type and quantity of lattice defects is one of the most frequent applications of X-ray powder diffraction. In this study, we focused on the microstructure of Au nanoparticles (AuNPs) and Au thin-films (AuTFs) prepared from two different methods. A series of integral breadth methods were used to analyze parameters such as crystallite size, microstrain, strain anisotropy, and dislocations. The peak broadening was analyzed using the full-width-at-half-maximum parameter directly obtained from the Marquardt-Levenberg and trust-region-reflective algorithms. In contrast, the Scherrer plot, Uniform Deformation Model, Williamson-Hall, Williamson-Hall-Kröner, Balzar, and Halder-Wagner methods were analyzed to assess the crystallite size and the upper limit of the strain. Our quantitative estimation was evaluated from the modified Williamson-Hall method. The average crystallite size is 14.15 nm for AuNPs and 18.64 nm for AuTFs, while the average distance between dislocations is 40.82 and 163.27 nm for AuNPs and AuTFs, respectively, the dislocation density is 6.0×10^{14} m^{-2} for AuNPs and 3.75×10^{13} m^{-2} for AuTFs. From contrast factor calculations, it was observed that both screw and edge dislocations conduct deformations in the lattice. For both samples, such deformations are observed as peak broadening mainly in the planes (200) and (400). It is determined that AuNPs present more anisotropy of strain and deformation than AuTFs, which can be attributed to the synthesis and sample preparation method. The obtained results enable us to study the elastic deformation in polycrystalline solids of Au comparing the anisotropy on the as-prepared specimens, and thus to discuss their specific microstructure properties for further applications. Microstructural analysis plays a significant role in materials science to develop and define the applications of novel materials, such as nanoparticles and thin-films.