Microstrain was obtained by analyzing the configuration obtained from RMC fitting, following:

 (1)

where  is the total number of unit cells within certain analysis region (here, specifically, different shells within the nanoparticle).  and  refers to the individual and average lattice parameter of unit cells within the analysis region. Specifically, for the shell analysis, only complete unit cells are considered, i.e. no atoms are missing in the unit cell and all the six neighbors (namely, front, back, top, bottom, left and right) are also complete. The nanoparticle model is then divided into shells in such a way that each shell contains roughly the same number of complete unit cells – to guarantee the same level of statistics for all shells.