

Strain Determination in Nanoparticles

Shangmin Xiong and I.C. Noyan

¹Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY, 10027, USA

Understanding strain is of great importance in characterizing and designing nanomaterials. X-ray diffraction technique is widely applied in determining strain distribution in nanoscale. The strain properties of nanocrystals are significantly different from their bulk counterpart due to surface and size effect. Here we determine the strain distribution in nanoparticles by combining molecular dynamics simulations and virtual X-ray diffraction experiments. This analysis will lead to further understanding of the mechanical properties of nanoparticles.