Abstract of “Grain Boundary Field Projection Method and Atomic Lattice Interferometer for Nanometrology” by Chien-Kai Wang, Ph.D., Brown University, May 2014.

The aim of this thesis is to investigate how grain boundary (GB) strength and separation mechanisms affect strength and ductility of nanocrystalline materials. Such nanoscale materials are highly nonlinear and thus have different energy profiles in different atomic configurations. Therefore, failure of GBs under straining is highly cooperative and process-dependent in nano-granular materials. To ascertain the strength and toughness of GBs, accurate and quantitative assessments of GB field descriptions with atomic features are required. Two new means of establishing connections between global loadings to nanoscale GB traction distributions are developed: the interior and exterior field projection methods of GBs for computation and experiment respectively.

Three mechanisms of Cu symmetric tilt GB deformation are introduced through the GB field projection methods. First, symmetric atomic rearrangement reduces concentrated compression of the GB tractions due to the ease of intergranular incompatibility. Second, asymmetric atomic rearrangement or dislocation emission decreases the concentrated tension leading GB opening and triggers the shear traction fluctuations as a new strain energy reservoir. Thus the GB separation toughness is enhanced. Third, Pb impurities at the GBs maintain the tension peaks of normal traction fluctuations and then retard the traction transformation. Hence, the GB becomes brittle.

In addition to the GB field projection methods, we introduce an invention of an experimental instrument – atomic lattice interferometer, which can give us sub-angstrom scale resolution of deformation measurement. The corresponding calibration experiments

were implemented on highly ordered pyrolytic graphite (HOPG), and the atomic-scale strain fields of a crinkle structure in HOPG were successfully measured. The measurement results show that the crinkle ridge line has a highly concentrated surface curvature involving localized atomic-scale deformations. With the help of simulation-assisted data analyses, the experimental data reveal that the typical width, the kink angle and the minimum radius of the ridge as 1.76 nm, 6.2° and 8.51 nm, respectively.

In summary, this thesis develops novel scientific computational projection methods and experimental metrology instrument for investigating unexplored global physical phenomena of materials associated with minute and localized atomic deformation at nanometer scales.