The morphology of nanoparticles plays an important role in determining their physical and chemical properties and, consequently, their performance in different applications. For example, nanoparticle shape can influence drug delivery in pharmaceutical applications, while in fuel science, particle shape and surface structure can affect catalytic activity. Characterizing nanoparticle morphology from transmission electron microscopy (TEM) images has been very challenging because particle populations often exhibit substantial variability in shape, may evolve over time, and contain geometric features that are difficult to quantify from two dimensional images. Conventional approaches frequently rely on simplified shape descriptors that cannot adequately capture the heterogeneity, dynamic nature and geometric complexity of particle populations. To address these limitations, this dissertation makes three main research contributions in the area of statistical characterization of nanoparticle morphology.

The first contribution introduces a finite mixture modeling method for analyzing heterogeneous and multimodal nanoparticle shape populations. Particle boundaries are represented using the square-root velocity function (SRVF) within an elastic statistical shape analysis approach. This method allows shape variability to be studied while accounting for differences in translation, rotation, scale, and boundary parameterization. A probabilistic mixture model is formulated in a reduced-dimensional representation of the shape space, and an expectation–maximization (EM) algorithm is developed to estimate component mean shapes, covariance structures, and mixing proportions. Simulation studies and analysis of real experimental nanoparticle data demonstrate its ability to identify distinct morphological subpopulations and characterize within-population shape variability.

The second contribution extends the finite mixture modeling method to the case of dynamically changing nanoparticle populations. A time-series based approach is proposed that characterizes temporal evolution through changes in the proportions of the underlying shape populations. Mixture proportions estimated at successive observation times are transformed and modeled using autoregressive and related time-series methods, including autoregressive integrated moving average (ARIMA) models. This framework provides a means of describing temporal dependence in population composition and forecasting changes in the relative prevalence of different nanoparticle shapes. The proposed approach is applied to real time-resolved nanoparticle data, demonstrating how statistical shape modeling can be extended beyond static characterization to analyze and predict changes in morphological distributions over time.

The third contribution develops a regularized polygonal approximation approach for automated determination of facets from nanoparticle boundaries. Facets are important because their geometric characteristics can influence the surface properties of nanoparticles, particularly their catalytic activity and chemical reactivity. An approach is proposed that combines greedy backward vertex pruning with Akaike information criterion (AIC)-based model selection, an uncertainty-guided

model simplification, and an uncertainty-guided edge-merging procedure. This three-stage framework balances geometric fidelity and model complexity while reducing sensitivity to boundary irregularities and image noise. Simulation studies involving regular and rounded polygonal shapes evaluate the method under different particle sizes, degrees of corner rounding, and noise conditions. A real data study is presented in which the proposed approach is applied to TEM images of palladium nanoparticles supported on crystalline and amorphous substrates, where comparisons of vertex counts, edge lengths, internal angles, edge orientations, and Voronoi-based spatial characteristics provide insights into particle morphology and spatial organization across the two support environments.

Together, these contributions provide a statistical framework for studying nanoparticle morphology at complementary levels. The elastic shape mixture model characterizes heterogeneity and multimodality in shape populations, the dynamic extension describes and forecasts changes in their composition, and the polygonal approximation method quantifies local geometric features associated with faceting. By integrating statistical shape analysis, finite mixture modeling, time-series analysis, and uncertainty-aware geometric approximation, this dissertation advances quantitative and reproducible characterization of nanoparticle morphology from microscopy images.