

A SURFACE EVOLUTION SCHEME TO OPTIMIZE NANOSCALE GEOMETRY FROM AFM EXPERIMENTAL DATA

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Abstract

The geometrical properties of metallic nanoparticles like the size and morphology have significant effects on the structure and stability of the adsorbed biological entities as well as the nano-scale structural performances. To identify the nanoscale geometry, there are two major types of measuring devices to obtain the nanoscale properties. One is a type that uses an electron beam which interacts with the atoms that make up the signals about the sample, such as scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The other type is the atomic force microscopy (AFM) that uses the deflection of cantilever according to the force between the specimen and the probe at the end of cantilever is one of the foremost tools for imaging, measuring, and manipulating in nanoscale. It is a type of scanning probe microscopy that has a very high-resolution, with a demonstrated resolution on the order of a nanometer which is more than 1,000 times better than the optical diffraction limit. The AFM gathers the information by scanning the surface with a mechanical probe and could provide the high resolution images of height and phase in nanoscale.

To analyze the nano-scale intrinsic geometry from the height images in AFM, we developed a curvature-dependent evolution scheme that can eliminate the noise and smoothen the surfaces. The principal curvatures are computed directly from the first and second derivatives of the discrete AFM height data. The principal curvatures and directions correspond to the eigenvalues and eigenvectors of shape operator matrix, respectively. The evolution equation using the principal curvature flows is smoothing out the images in the corresponding principal directions. For an idealized model, k_2 flow successfully identifies the major valley lines to represent the boundary of nanoparticles without referring to the phase information, whereas the mean curvature flow eliminates all the minor ones and optimally leaves only the major feature of the boundary. The developed numerical scheme is also applied to real AFM data to demonstrate the capabilities of noise removal, smoothing surfaces, the identification of ridge and valley lines, and the extraction of intrinsic geometry. It is demonstrated that the application of developed scheme to experimental AFM data includes the capabilities such as the removal of experimental noise, smoothing surfaces, the ridge and valley line identification for the nanoparticles, polymers, and substrate, and the extraction of intrinsic geometry to mathematically enhance the resolution of the experimental data.

KEY WORDS: Evolution equation, Curvature flow, Eigenvalue problem, Ridge line, Valley line, AFM image, Metallic Nanoparticle

Note: Poster presentation