A complete methodology for the simulation of large nanostructures and quantitative analysis using Z-contrast images

Pedro L. Galindo, Joaquín Pizarro, Elisa Guerrero, Andrés Yáñez, M. Paz Guerrero, Giovanni Scavello, Sergio I. Molina

Departamento de Lenguajes y Sistemas Informáticos, Universidad de Cádiz, Campus Río San Pedro, s/n, 11510 Puerto Real, Cádiz, Spain,
pedro.galindo@uca.es

During the last few years, a complete methodology has been developed at the University of Cadiz for the simulation of High Resolution Electron Microscopy images of large nanostructures. Z-contrast imaging in scanning transmission electron microscopy (STEM) constitutes a powerful approach to investigate strained heterostructures on the nanometer scale and it has been proved to be extremely reliable for characterizing nanomaterials[1]. The proposed methodology allows the modeling and simulation of Z-contrast Electron Microscopy images of large nanostructures in reasonable time and it can be used to study materials in the presence of defects, being therefore very useful for a better knowledge of their mechanical properties and therefore of a great technological interest.

Figure 1 depicts the steps for a complete analysis of experimental and simulated HAADF images and quantitative characterization of nanostructures, and it comprises three steps, 3D nanostructure description (geometry, composition, etc.), 3D nanostructure modeling (Finite Element Modeling and/or Molecular Dynamics) and Image simulation.

A) Geometry Description: a commercial package (COMSOL^{TM}) is used to describe the geometry of the nanostructure (subdomains, boundaries, constraints, symmetries, etc.) and to define the local parameters (composition, initial strains, elastic constants…). The geometry of the nanostructure is usually described based on a-priori knowledge but the compositional distribution is usually extracted from experimental images by electron energy loss spectroscopy and aberration-corrected high-resolution Z-contrast imaging.

B) Nanostructure modeling: once the geometry is fully described, an atomistic model must be generated. This goal can be accomplished by modeling the nanostructure using finite element analysis (FEA) and solving the equations of the anisotropic elastic theory to obtain the displacement field [2,3]. *SIC_Supercell* software developed at the University of Cadiz provides the corresponding 3D atomistic model from a supercell described as a sequence of (x, y, z) coordinates that have been obtained from FEA model at equilibrium, i.e. atom coordinates according to the local displacement field and occupancy or Debye-Waller factors according to the local composition. A second approach based in Molecular Dynamics is usually applied in our research group in order to obtain the 3D atomistic model [4] Molecular modeling involves theoretical and computational methods needed to model the behavior of a system at atomic scale. The collective behavior of atoms allows the understanding of how the material undergoes deformation, phase changes or other phenomena, providing links between the atomic scale to macro phenomena.

The resulting strain obtained by any of these two techniques may be compared with that obtained directly from experimental images applying a strain mapping technique. Using high-resolution electron microscopy images and under some limitations we may assume there exists a constant spatial relationship between the intensity maxima and the location of atomic columns in the studied material [5]. This relationship appears in the form of a spatial shift of the intensity maxima positions with respect to atomic columns. *Peak Pairs Analysis* is a strain mapping technique developed at the University of Cadiz[6] and implemented in a Digital Micrograph plug-in. It is distributed by HREM Research[7] and

improves both, the speed of computation, and memory requirements with respect to other strain mapping approaches.

C) Image simulation: STEM image simulation of a few unit cells can take hours and the simulation of medium-size nanostructures, where millions of atoms are involved, is unfeasible in the state of the art personal computers. To overcome this problem, a parallel HAADF-STEM simulation software has been developed [8].The software runs in the University of Cadiz cluster, having 320 nodes and 3.8 Tflops and it is capable to simulate images from nanostructures represented by about 1 million atoms in a couple of days. The software can generate one dimensional line scans, two dimensional images and focal series and its results has been successfully compared with WinHREM[4,8] software.

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Figures

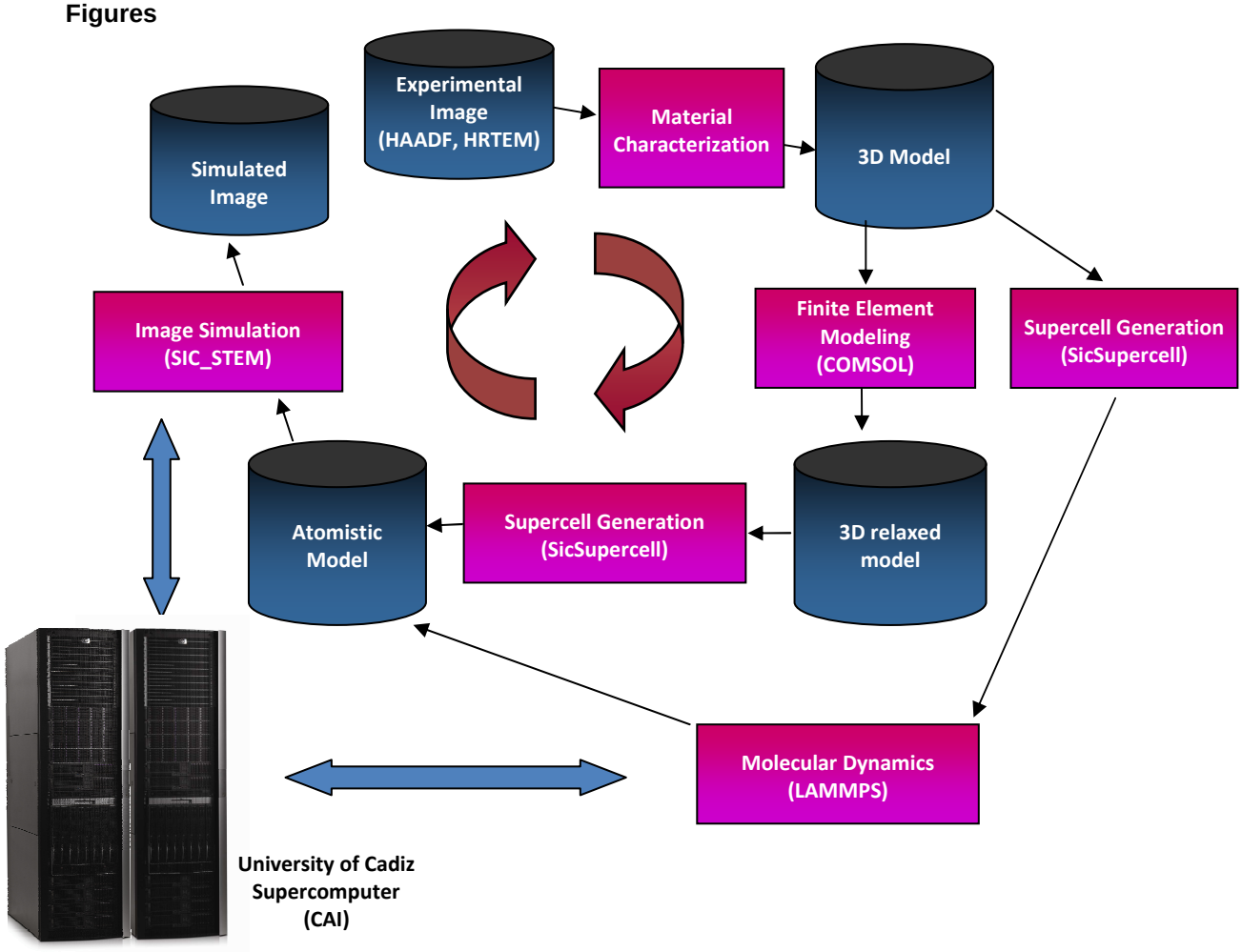

Figure1: Schematic diagram of the nanostructure modeling methodology developed at the University of Cadiz