

# ATOMIC-CONTINUUM EQUIVALENCE AT NANOSCALE

Ryszard Pyrz

Department of Mechanical Engineering, Aalborg University  
Pontoppidanstræde 101, 9220 Aalborg East, Denmark

## Abstract

In order to predict macroscopic properties, a microscopic model should contain an expression, which relates the macroscopic fields quantities to the variables by which the microstructure is described. So, depending upon the level of description of microstructure there will be various expressions for the field quantities of a given system. We will use the term for the microscopic field quantities such as stress and strain to denote fields, which vary on the scale of atomic dimensions. An important issue is the development of definitions for continuum quantities that are calculable within a molecular structure. The most frequently used form for the stress at atomic level is based upon the Clausius virial theorem, which determines the stress field applied to the surface of a fixed volume containing interacting particles (atoms). The virial stress includes the mass and velocity of atoms, which describes the fact that mass transfer causes mechanical stress to be applied on the surfaces external to an atomic system, as well as it includes pair-wise interatomic forces and atomic positions. It has been shown that the virial stress cannot be directly related to the classical Cauchy stress and several modifications have been proposed. It is essential to recognize that the stress at the location of an atom depends on the details of the interatomic interactions and the positions of interacting neighbours. Hence, the atomic stress is a non-local function of the state of the matter at all points in some vicinity of the reference atom, in contrast to the local stress field used in classical continuum theories.

It seems that the relationship between local displacements of atoms and the strain tensor is not as ambiguous as the concept of atomic stress. Position of atoms is readily available from almost all molecular simulation algorithms and the atom displacement can be easily assessed. Strain measure is a relative quantity and one need two configurations, the reference and the present, in order to define the local atomic strain. The atomic strain should provide detailed local information about kinematics of the atom in relation to its neighbours and the true test of the atomic strain concept is how well it approximates total strain of the simulation cell by summing local atomic strains over all atoms present in the system. In the best case this sum should be equal or very close to the total strain calculated from boundary conditions of the simulation cell.

The atomic strain tensor is applied to investigate deformation of regular and disordered molecular systems. As classical continuum mechanics is inherently size-independent, inclusion of atomic strain gradients is used to analyse and predict the mechanical behaviour of nanomaterials in presence of size effects. It is shown that disordered systems exhibit significant nonaffine deformations. The characteristic length scale over which the nonaffine field is correlated serves as a lower limit beyond which classical continuum elasticity cannot be applied. The high nonaffinity of disordered (amorphous) nanomaterials possibly stems from a group of strongly bonded atoms behaving as a unit and therefore high moment stresses may result. This effect can be captured by the atomic strain gradient tensor in a way similar to the strain gradient elasticity solution.