

ATOMIC-CONTINUUM EQUIVALENCE: ATOMIC STRAIN TENSOR

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1. Introduction

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 [1, 2]. 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 needs 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 was calculated in [3] to better understand changes in local structure. However, it has not been determined whether or not the sum of local atomic strains corresponds to the total deformation of the simulation cell when loaded by external forces.

In this work we describe an atomic strain measure related to the transformation matrix between two deformation states. This measure is further modified in order to take into account nonaffine deformations taking place in molecular disordered systems. Localized areas of nonaffine deformations indicate non-elastic response which evolves during loading [4].

2. Atomic strain measure and analysis

The atomic strain will be defined in terms of Voronoi tessellation. The atoms are assumed to be in their equilibrium positions, and thermal vibrations are averaged. The Voronoi polyhedron around central atom is composed of a set of sub-polyhedrons (interaction cells) whose number is determined by a number of neighbours to the central atom. During motion, the Voronoi polyhedron associated with the atom changes its shape. The interaction cell is defined for each pair consisted of a central atom and its neighbors. It is a part of Voronoi polyhedron that contains points situated closer to this pair of points than to any other. It is build of two sub-polyhedrons (parts of polyhedron surrounding a central point and a neighboring point) having common face. This is a unique region for which it can be assumed that it is influenced only by these points.

The atomic strain is defined through the deformation gradient that is calculated by minimizing the sum of squared separation distances between neighbouring atoms and subsequently weighted by corresponding polyhedra [5].

As an example, molecular modeling and strain calculations has been performed on CNT-polypropylene nanocomposite. At first, the system is constructed and subject to energy minimization using Polak-Ribiere conjugate gradient method. Molecular dynamics simulation is performed next using NTP ensemble in order to obtain an equilibrium state, which simultaneously serves as a reference state. The nanocomposite has been subject to uniaxial tension along the nanotube axis and the analysis has been performed for nine deformation steps with equilibration runs after each step. The total atomic strain of the system resembles very closely the strain of the simulation cell calculated from boundary conditions. For instance, the strain from boundary conditions is 0.0185 at third loading step whereas atomic strain gives 0.0179.

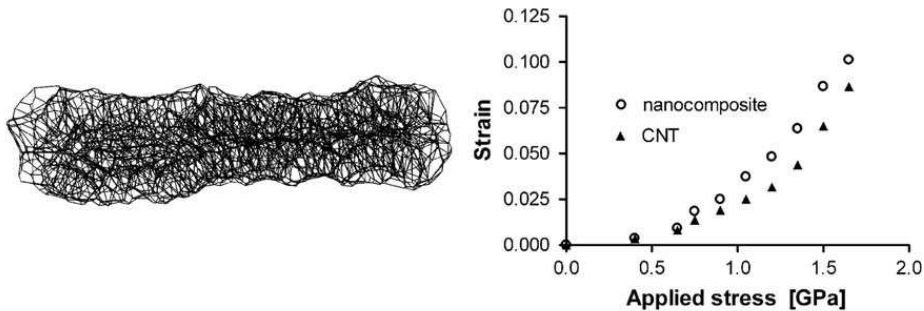


Figure 1. Voronoi tessellation of CNT at third step of deformation and evolution of the total CNT strain as compared to the total nanocomposite strain.

Figure 1 shows Voronoi tessellation only for atoms belonging to carbon nanotube at third loading step and the evolution of CNT total strain during loading history. The nanotube strain follows the strain of nanocomposite to a certain loading level and then lags after it as loading of the nanocomposite increases. This is clear evidence that we need to deal with an interfacial sliding. A detailed analysis atom by atom would be necessary to disclose and characterize an atomic nature of interfacial debonding.

3. Conclusion

The most important conclusion to emerge from present investigation is that atomic strain concept based on the construction of Voronoi cells provides means to bridge molecular and continuum length scales. This concept will be illustrated further with other examples comprising slippage of functional nanowires at interfaces in polymer based nanocomposites and cohesive fracture phenomena at interfaces.

References

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