

# PRE-RELAXATION EFFECT IN COMPUTER MODELING OF NANOINDENTATION

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## 1. Aim of the paper

The object of the paper is to examine the influence of the chosen method of preparation of computable a sample due to pre-relaxation of structure on the obtained result and numerical behavior of simulation of nanoindentation process. Two schemes based on pre-relaxation are investigated in this work: First, using a Molecular-Statics (MS) scheme with an empirical potential; and second, using Molecular-Dynamics (MD) with an empirical potential. It is found that in some cases the MS scheme, which does not take into account the self-vibration of the atoms, is a sufficient framework to use as a pre-relaxation tool for computational mechanics where non-equilibrium systems are to be simulated.

## 2. Introduction

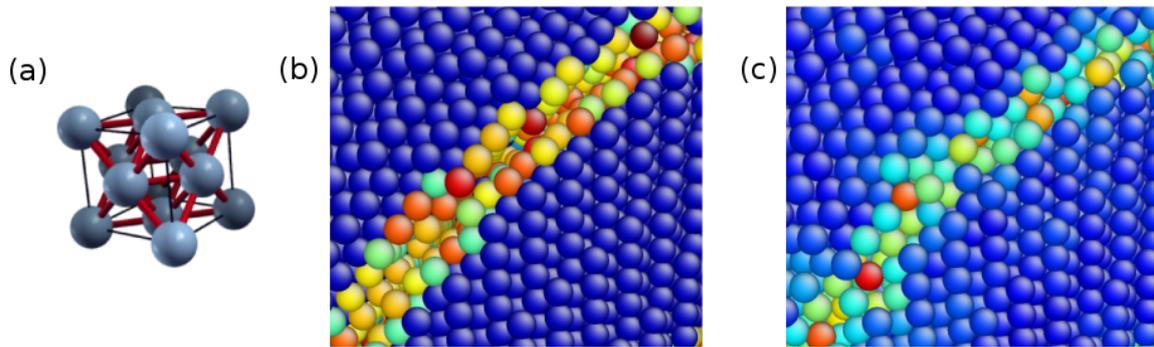
It is peculiar that MS [1, 4, 5] in comparison with MD is used much less frequently since MS is neither a marginal or not worthless method of calculation. In fact, due to the limitations of MD, *eg.* time scales, spatial scales, the lack of conservation of energy during the simulation, the problem of artificial reflected waves, its use is often questioned. MS does not have these drawbacks. Thus, MS is often used as a method of "Hard" verification checking whether the solution obtained in MD is "Correct", as a method simulation of molecular phenomena where MD can not be used because of its limitations.

Numerical simulation of the nanoindentation process [3] may explain the mechanisms responsible for nanodeformations, which does not are often available for direct observation and in particular the lack of continuity in the curve of loading-unloading. These phenomena are inextricably linked to the crystalline structure of the hidden material-usually in the form of the generation of structural dislocations. The nanoindentation process, due to its importance to studies in Mechanical Engineering and its use of very non-equilibrium molecular configurations, is a good ground on which to perform computational optimization tests. The development of such methods, however, is tricky task since we have take into consideration the differences between the microscopic and macroscopic approach.

## 3. Problem description

In molecular statics approach we model the elastic-plastic deformation utilizing the idea of the time-independent plasticity developed here at the molecular-statics level[1, 4, 5]. The time-dependency of the nanoindentation problem is reduced to a quasi-static adiabatic scheme. We analyze the indentation force-depth curve for loading-unloading of mono and polycrystalline structure and examine atomic bond-lengths and the arrangement of atoms in the bulk structure.

Very important element in these simulations is preparation of computable sample. Our computational algorithm for generation of the polycrystalline structure was based on a 'nucleation and growth mechanism'. It is a type of realization of Voronoi tessellation [7] – in which the orientation of the crystal lattices is determined by three Euler angles. In particular, a selected number of atoms is randomly spaced in an otherwise empty box, after which through a growth mechanism neighboring atoms were attached with randomly fixed orientations based on ideal f.c.c. lattice structure (see also



**Figure 1.** In panel (a) a schematic representation of the f.c.c phase of ideal crystalline copper. In panel (b, c) an illustration of the pre-relaxation process of a single grain boundary before (b) and after (c) relaxation.

Figure 1a). The growth mechanism stops when the surfaces of the growing crystal meet and thereby creating grain boundaries; see Figure 1b-c. Grain boundaries created in this geometrical way almost always have a structure that is less dense than those observed in real materials. In order to improve it and to move atoms at grain boundaries to their optimum, correct positions, the whole structure can be relaxed by MD or be initial step in MS. Then the resultant atomic positions were transferred to the MS-elastic model prior to simulation of the nanoindentation process.

This investigation determines whether MD relaxation is necessary for preparation of a computable atomistic-scale sample, and gives some background and worked examples for cases where a straightforward MS simulation of pre-relaxation suitably describes the numerical behavior of the simulation.

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