MPI molecular dynamics on torus

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Abstract. The molecular dynamics method in multiprocessor mode based on a new type of ensemble with constant tension is developed. The new method uses the representation of classical mechanics in \( T^6 = S^6 \) manifold. Six true topological dimensions of the torus surface are represented by six scalars: three relative strains and three shear angles. The separation of spaces, which address the deformation and the coordinates of the particles greatly simplifies the equations of motion. Instead of the stress, the new equations contain the generalized tension forces acting on each atom. The notions of surface and surface forces are absent in new concept based on a new type of ensemble with a constant tension force \( NfE \). A much simpler principle of virtual work provides a number of advantages over the widespread isostress ensemble \( NtE \) in molecular dynamics based on Parrinello Rahman method. The method is demonstrated by the example of torsion deformation in aluminium polycrystalline. It is shown that at stresses near the creep threshold, the main mechanism of deformation is the flow of nanocrystals in the grain boundary region.

1. Introduction

The modern molecular dynamics suggests a compilation of continual and many particle mechanics. One of the example is the most widely used program LAMMPS, which allows using different types of statistical ensembles, including the most realistic isothermal-isobaric ensembles. That program implements the method of Parrinello and Raman (PR)\(^1\) in terms of isostress \( NtT^6 \) ensemble. The inclusion of deformations there is made by applying dynamic bonds, which are a consequence of scaling the coordinates of atoms, adapted to the type of deformation of the MD cell under the action of external stress. This algorithm is based on conventional continuum mechanics according which the components of stresses, being a continuous field, act over an area. It doesn’t look quite natural from the point of molecular dynamics whose equations of motion inherently exploit molecular variables. You have to use some constraint to scale coordinates of particles to a flexible MD cell.

The new approach developed in Refs.\(^2-3\) is quite natural for a molecular dynamics implementation, since only pointwise forces caused by the stress act to atoms making a body deform. It is based on a description of classical mechanics on the surface of the torus \( T^6 = S^6 \). In contrast to usual treatment in \( \mathbb{R}^3 \), the equations of motion of particles in the this multifold treat deformation and stress in terms of vector variables. Besides, the principal difference between the approaches is in an implementation of the principle of the virtual work under external forces/stresses. Standard theory uses the second Piola-Kirchhoff stress instead of true (Cauchy) stress as external load. It is not convenient due to a changing of instantaneous orientation and size of surface elements while the body deforms. In new ensemble with constant tension force \( NfT^6 \), this principle is realized by the use of a conventional homogeneous external field being a linear function of stretches so this problem is absent.
This paper is devoted to the development of molecular dynamics program TORUS in terms of a new ensemble with constant tension, supporting multiprocessor and associated with the visualization program. As a representative example of the use of the program, section 4 will present the results of modeling of the deformation in polycrystalline aluminum in inelastic region characterized by a high strain rate.

2. Equations of motion

All six deformations in three dimensional space $\mathbb{R}^3$ can be described on the surface of $T^6 = S^6$ torus by the six scalar parameters $\lambda_a$ and $\varphi_a$, $\alpha = x, y, z$. The kinematic relation for coordinates is the same

$$x_a = \frac{R_a}{R_0} \theta_a = \lambda_a \theta_a$$

while the transformation of the central angles $\theta_a$ is given by a matrix $A_{\alpha \beta}$:

$$\theta_a = A_{\alpha \beta} (\varphi) \theta_\beta$$

which follows from the kinematic relation for imaginary “rotation”

$$\frac{\partial \theta_a}{\partial \varphi_\beta} = \theta_\gamma, \quad \alpha \neq \beta \neq \gamma$$

In the initial configuration, $\lambda_a = 1$, $\varphi_a = 0$ and $u^0_a = x^0_a$ (hereinafter upper index 0 refers to the reference configuration). What we have achieved? Now the deformation is determined by six scalars related rather to surface parameters then to vectors belonging to this surface.

Variation of this kinematic equation allows introducing other kinds of deformation combined with a rotation. For example, the rigid rotation is provided by the relation $\partial u_a / \partial \varphi_\beta = e_{a\beta\gamma} u_\gamma$ ($e_{ijk}$ is the permutation matrix). The simple shear in 2D which involves rigid rotation can be introduced by the relations $\partial u_x / \partial \varphi = u_x$ and $\partial u_y / \partial \varphi = 0$

$$\begin{align*}
\partial u_x / \partial \varphi &= u_x, \\
\partial u_y / \partial \varphi &= 0.
\end{align*}$$

Similar, other inextensibility and orientation constraints can be introduced in dynamics without additional force contributions normally required for enforcing the holonomic constraints for coordinates.

To determine the velocity of the particle on torus surface we must keep in mind that a rotation of principal curvatures doesn’t like a rigid rotation. The particle skates on the surface but not rotate together with cylinder surface. To exclude rigid rotation, we have to consider rotating coordinate system where the velocity of the particle becomes equal to

$$v_a = \dot{x}_a - \lambda_a A_{\alpha \beta} \dot{\theta}_\beta = \lambda_a A_{\alpha \beta} \dot{\theta}_\beta = \lambda_a v_a$$

In this system the rate of change of angular variables becomes equal to

$$\dot{\theta}_a = v_a + A_{\alpha \beta} \dot{\theta}_\beta = v_a + \Omega_{\alpha \beta} \dot{\theta}_\beta$$

where the symmetric matrix $\Omega_{\alpha \beta} = A_{\gamma \beta}^{-1}$ has zero diagonal elements and expressed through the rate of shear angles.
\[ \Omega_{\alpha\beta} = \dot{\phi}_\gamma, \quad \alpha \neq \beta \neq \gamma. \] (7)

It is clear that the kinematics is the main brand of the concept \([2,3]\). As soon as relationship between the position of the particle on the surface and deformation variables establishes, all else that are forces or equations of motion follow in accordance to standard procedure.

Our task now is to formulate the classical dynamics in \( T^6 \) manifold. Consider a system of interacting particles with a potential energy \( U(\{x_i\}) \). Three generalized tensions \( f^\lambda_{\alpha} \) affect the uniaxial stress along each direction while tree others, \( f^\phi_{\alpha} \) relate to shear stress. These six generalized forces and the interaction force \( f_{i\alpha} = -\partial U / \partial x_{i\alpha} \) are applied to \( i \)-th atom of mass \( m \) independently, causing the system to oscillate and deform.

Taking into account kinematic relations we can write down the Lagrangian of joint deformation and vibrational dynamics of an ensemble of particles on the torus under a constant external field \( f^\lambda_{\alpha} \) in form

\[ \mathcal{L} = \frac{m}{2} \sum_{\alpha=1}^{N} \left[ \dot{C}_{\alpha}^i \dot{\lambda}_\alpha^2 + C_{\alpha}^\phi \dot{\phi}_\alpha^2 + \nu_{i\alpha}^2 \right] - U - N \sum_{\alpha=1}^{3} \left( f^\lambda_{i\alpha} \dot{\lambda}_\alpha + f^\phi_{i\alpha} \dot{\phi}_\alpha \right) \] (8)

where \( C_{\alpha}^i = R_{\alpha}^{02} \) and \( C_{\alpha}^\phi = R_{\alpha}^{02} \).

In this expression, one can see a fundamental difference with a standard tensor-based approach. The external potential used here is the usual potential of a uniform field, the same as, for example, in electrodynamics. This contrasts with the potential under the standard theory, which is a product of the finite strain tensor on the second Piola-Kirchhoff stress. The Cauchy (true) stress is "sewn" here in the directions of planes changing with strain. It does not add simplicity to the equations of molecular dynamics.

Standard procedure gives Euler equations of motion for \( 3N + 6 \) dynamical variables \( \dot{\lambda}_\alpha, \dot{\phi}_\alpha \) and \( \ddot{\theta}_{i\alpha} \).

For the particles one obtains

\[ m \frac{d}{dt} \chi_{i\alpha} \dot{\lambda}_\alpha^2 \chi_{i\alpha} = -\frac{\partial U}{\partial \theta_{i\alpha}} \] (9)

Coming back to Cartesian coordinates yields

\[ \dot{\theta}_{i\alpha} = \frac{f_{i\alpha}}{m \chi_{i\alpha}} - B_{\alpha\beta} \chi_{i\alpha} \] (10)

where the matrix

\[ B_{\alpha\beta} = \begin{pmatrix} 2 \dot{\lambda}_\alpha / \dot{\lambda}_\alpha, \\ \Omega_{\alpha\beta} \left( \dot{\lambda}_\alpha / \dot{\lambda}_\alpha \right)^2 \end{pmatrix}, \quad \alpha \neq \beta \] (11)

The equations of motion for deformation variables are

\[ C_{\alpha}^\lambda \dot{\lambda}_\alpha = \dot{f}_{\alpha}^\lambda - \ddot{f}_{\alpha}^\lambda, \]
\[ C_{\alpha}^\phi \dot{\phi}_\alpha = \dot{f}_{\alpha}^\phi - \ddot{f}_{\alpha}^\phi. \] (12)
Here $C_{a}^{\gamma}m$ and $C_{a}^{\alpha}m$ are barostat masses (their dimension is a mass times a squared length). Generalized tensions are equal to

$$
\begin{align*}
 f_{a}^{\lambda} &= \frac{1}{\lambda_{a}}\sigma_{aa}, \\
 f_{a}^{\gamma} &= \frac{\lambda_{\beta}}{\lambda_{\gamma}}\sigma_{\beta\gamma}, \quad \alpha \neq \beta \neq \gamma.
\end{align*}
$$

(13)

where the values

$$
\sigma_{\beta\gamma} = \frac{1}{N} \left( m \sum_{i=1}^{N} v_{\beta i} v_{\gamma i} + \sum_{j=1}^{N} f_{\beta j} x_{\gamma j} \right)
$$

(14)

Recall, that these values are presented in the expressions for the components of internal pressure $P_{\beta\gamma} = \sigma_{\beta\gamma} / v$. Hence, the external tensions are associated with the external uniaxial $P_{\alpha\alpha}^{ext}$ and shear $P_{\beta\gamma}^{ext}$ stresses by means of relations $f_{a}^{\alpha} = V_{\alpha}P_{\alpha\alpha}^{ext}$ and $f_{a}^{\gamma} = 2V_{\gamma}P_{\beta\gamma}^{ext}$, $\alpha \neq \beta \neq \gamma$ (hereinafter index 0 refers to the reference configuration). The dynamics of the $N\Phi$ ensemble of particles preserves the instantaneous enthalpy $\Phi$ following from the Lagrangian in due course.

3. Calculations

Algorithm described above was realized in program TORUS developed for CSDPMF NRC “Kurchatov Institute” using MPI technology. Spatial decomposition of the calculation area is divided into subdomains, each of which is accompanied by a separate computational kernel. The input data sets the spatial grid parameters for the decomposition. The uniform grid is determined by a prescribed step over spatial coordinates.

Inside the spatial subdomain, a spatial grid is defined with the parameters related to the effective radius of interaction between the particles. Thus, a particle in the element of the volume formed by such a grid can interact only with particles located in neighboring volumes. The number of adjacent volumes for the considered volume in this model can be no more than 26. Neighboring volumes are used to build images on the boundaries of spatial subdomains through which information is exchanged. The migration of particles between subdomains is calculated using images that are repeated MD crystallite to fulfill periodic boundary conditions. The grid allows to reduce the time of calculation of interactions during the run. In options with changes of the volume of the system, a linear transformation into an orthogonal coordinate system was used to build images followed by an inverse transformation to the original coordinate system while calculating the force field. The parallel algorithm used is well scaled as long as the time of solving the equation of motion for the particles in the subdomain is greater or comparable to the time of data exchange between the subdomains. TORUS was used on 1000 cores for an ensemble of several million particles. The input and output data in the calculation are consistent with the format of the LAMMPS.
As an example of using the ensemble, the stress-strain curve for mono and polycrystalline aluminum was calculated. An interest to plastic deformation of nanocrystals is related to the opportunity of observing exceptionally high strain rates of \( t \sim 10^9 \text{ sec} \) (obviously faster than in experiments), which makes them available for numerical MD modelling on the nanosecond time scale. The attractiveness of this kind of calculation is in the possibility to trace detail the realistic mechanisms of plasticity in the conditions of achieving equilibrium (when the external stress is compared with the applied load). The key step for modeling of polycrystalline material is to be accurate enough to represent the microstructure of the real material. During the last decades, several models for microstructure simulation have been developed. In this paper, we will use the Voronoi section for separation of MD cell with grains of different orientation and size and the subsequent procedure of optimization. The procedure begins by simulations of the grain center vectors \( \mathbf{R}_k, k = 1 + n_g \), so that the average distance between them is \( \bar{I}_{av} = \left( \frac{N V}{n_g} \right)^{1/3} \). The planes with these directions intersect the middle of all of vectors connecting the centers of the grains, including 26 located in the MD images of a crystallite. Further, the obtained grains are filled with atoms of a randomly oriented lattice. Some atoms near the grain boundaries creating a density significantly higher than mean atomic one, are removed. The condition for minimum rapprochements of atoms was varied in runs, to ensure the minimum of the potential. The nanocrystal thus obtained was heated to a temperature close to the melting point, then cooled to zero. The result of this procedure for MD cell with \( N = 500025 \) is shown in Fig.1. Only atoms with a shift of the center of symmetry are shown (i.e. whose positions differ significantly from the host of the grain structure).

The resulting structure was used to obtained the equation of state. A system consisting of \( N = 2048000 \) of Al atoms in a nanocrystal with \( n_g = 6 \) grains was considered. The calculations used a chain of two thermostats with mass \( Q = 0.1 \) and barostat mass \( C^e = C^\alpha = 0.1 \) in the temperature range \( T = 100 \sim 600K \). The equations of motion using the EAM potential Al99.eam.alloy were solved by program TORUS in MPI mode with 512 cores.

In this paper, we investigated the shear stresses that occur during torsion of samples. Torsional deformation for constant sample length represents the simple shear. In generally accepted MD programs (such as LAMMPS), direct modelling of simple shear is not feasible, since it contains a rigid rotation (in the optimization PR procedure only a pure shear is available). Here we use the kinematic relation of Eq. (4) for simulation of simple shear.
The applied shear stress varied within $f_{xy} = 0 \pm 3.0 \text{eV}$ which corresponds to $P \sim \text{GPa}$. The procedure of optimization for polycrystalline began with zero pressure, since the equilibrium lattice parameter $d = 0.40557 \text{nm}$ did not meet the minimum potential. The calculation yields the stretch ratio $\lambda = 6.293 \times 10^{-3}$. Equilibrium tension is established at the time $\sim 1 \text{nsec}$. After that, a shear stress was applied to the MD cell. Conservation of the longitudinal length of the cell causes additional stress along the axis $Z$ (Poynting effect). Note in this connection that the analogous calculation with zero axial pressure and the corresponding uniaxial deformation did not lead to a noticeable difference in the results. Fig. 2 shows the dependence of the shear strain on the applied stress up to the plasticity threshold. For $P_{xy}^{\text{ext}} = 0 \pm 100 \text{MPa}$ it coincides with the linearly elastic part of the curve calculated for the ideal FCC crystal of Al. Plastic flow has actually begun at room temperature with a pressure of $P_{xy}^{\text{ext}} \sim 500 \text{ MPa}$.

Fig 3 shows the time evolution of deformation at $P_{xy}^{\text{ext}} = 500 \text{MPa}$. After a short linearly elastic phase, creep $\sim 10^3 \text{sec}^{-1}$ begins. The experimental creep value in pure aluminium for $P_{xy}^{\text{ext}} \sim 100 \text{MPa}$ does not exceed the values of $10^0 \div 10^1 \text{ sec}^{-1}$ [4]. Unlike the case of uniaxial stress, no hardening phase was observed here. In the extreme case of high temperatures $T = 500K$ and pressures $P_{xy}^{\text{ext}} = 500 \text{ MPa}$, the strain rate reached the values of $\sim 10^5 \text{ sec}^{-1}$ (Fig.3).

As for the creep mechanism, in contrast to the case of uniaxial stress, the analysis of animation revealed the origin of complete $1/2 [110]$ dislocations from the grain boundary, despite its small size ($\geq 10 \text{ nm}$), cf. [5]. Although in the initial stage, the movement of grains was due to their relative movement along the amorphous boundaries.

4. Conclusions
A detailed scheme of calculation of the equations of motion by the method of molecular dynamics based on the isothermal $NRT$ ensemble with constant tension is presented. As an example, the process of aluminium polycrystalline torsion was considered, where the advantages of proposed method were demonstrated quite clearly. Namely, the ability to reproduce the results of various isothermal isothermal ensembles (including $NtT$) due to the simpler potential of the external stress field. In addition, it was demonstrated the ability taking into account of combinations of pure strain with rigid rotation, often present in real experiments for determination of stress– strain curves.
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References
1. Ryabov V A 2017 Cont. Mech. Thermodyn. 29 715.
2. Ryabov V A 2018 Comp. Meth. Appl. Mech. and Engrng. 342 240.
3. Ryabov V A 2018 Principles of Statistical Physics and Numerical Modeling (Bristol: IOP Publishing)
4. Ishikawa K, Okuda H, Kobayashi 1997 Y Mat. Sc. Engrng. A234-236 154
5. Yamakov V, Wolf D, Philpot S R, Mukherjee A K and Gleiter H 2004 Nat. Mat. 3 43