STABILITY OF IDEAL INFINITE CRYSTAL UNDER FINITE UNIFORM DEFORMATION

Pavel V. Tkachev

Institute for Problems in Mechanical Engineering Russian Academy of Sciences, Molecular and Particle Dynamics Simulation Group , Bolshoy pr. V. O., 61, 199178 St. Petersburg, Russia

St. Petersburg State Polytechnical University, Dep. of Theoretical Mechanics, 195251 St. Petersburg, Russia

Summary. Strong deformation and fracture are very difficult to describe using macroscopic continuum methods. Lack of a material continuousness makes description of such processes to be a serious challenge. In the presented paper the onset of the material fracture is studied from both micro- and macroscopic points of view. First an ideal infinite crystal lattice is considered. Transfer from microstructure to continuum mechanics is made using long-wave approximation. This allows obtaining nonlinear continuum equations of the infinite crystal under finite uniform deformation. These equations are found without limitation to the space dimension. For the stability verification a small deformation is superposed to a finite deformation of the crystal lattice being described by the obtained nonlinear macroscopic equations. Criterions of the material stability and their relevance to the crystal structure are obtained.

INTRODUCTION

A lot of facts give evidence about crucial role of the internal structure in the processes which attend deformation. That is why an influence of the material structure to its mechanical behavior requires a serious attention. Most of classic continuum methods have serious problems describing strong deformation and fracture, because the material is not really continuous in this case.

Generally the microstructure can be considered by the following three ways. The first way is to analyze microstructure and obtain stability criterion for the crystal cell [1] using microscopic equations for the atoms motion. The second way is to compute deformation and fracture processes using molecular dynamics method [2, 3, 4, 5, 6]. The third way is to consider the microstructure in the classic continuum mechanics equations, in other words make transfer from the microstructure to continuum mechanics [7, 8, 9]. In the presented paper we will follow the third way and then use the continuum mechanics methods to analyze stability of the material under finite deformation.

METHODS AND ANALYSIS

The material is represented as an infinite crystal. The dynamics of the particles (atoms) forming the crystal is described by Newtonian equations of motion, where each particle is interacting with the other particles via prescribed potential interaction forces. Transfer from microstructure to continuum mechanics is made using long-wave approximation [7, 10]. This allows obtaining nonlinear continuum equations of the infinite crystal in the Piola [11] form

$$\rho \ddot{\underline{u}} - \overset{\circ}{\nabla} \cdot \underline{\underline{P}} = 0 \,, \tag{1}$$

where ρ is the material density in the reference configuration, $\underline{u}$ is the displacement vector, $\overset{\circ}{\nabla}$ is the vector differential operator in the reference configuration, $\underline{\underline{P}}$ is the Piola stress tensor, which can be expressed in the terms of the microscopic parameters as following [7]

$$\underline{\underline{P}} \equiv \frac{1}{2v_*} \sum_{\alpha} \Phi\left(A_\alpha^2\right) \underline{a}_\alpha \underline{A}_\alpha \;; \tag{2}$$

where v_* is the volume of the elementary crystal cell in the reference configuration; $\underline{a}_\alpha$ is the vector from the current particle to the particle number α in the reference configuration; $\underline{A}_\alpha$ is the vector $\underline{a}_\alpha$ in the actual configuration;

$$\Phi\left(A_\alpha^2\right) = -\frac{\Pi'\left(A_\alpha\right)}{A_\alpha} \,, \tag{3}$$

where $\Pi(r)$ is the pair potential of interaction between the particles, which is a function of the distance between the particles. These equations are valid for both 2D and 3D considerations.

For the stability verification a small deformation is superposed to a finite deformation of the crystal lattice being described by the obtained nonlinear macroscopic equations. As a result the system of equations in variations can be obtained. Criterions of the material stability and their relevance to the crystal structure are obtained and will be presented in the lecture. Instability is considered as non-oscillation motion of the crystal lattice.

CONCLUSIONS

Using long-wave approximation it is possible to consider interaction only within a limited vicinity of the current particle. However, using the presented method it is possible to take into account not only the nearest neighbors, but as many coordination shells as needed. Thereby this method can describe materials for which the interaction between the particles decreases relatively slowly with respect to the distance between them.
The material is represented as an infinite crystal. Consequently in the paper the influence of the boundary effects and material imperfections is neglected. But in spite of these rude assumptions the method allows describing the important feature of all materials — stability loss under strong deformations in correlation with the material microstructure, which is difficult to describe using purely continuum considerations.

ACKNOWLEDGEMENTS

This work was supported by Russian Foundation for Basic Research, grant No 02-01-00514. The author is grateful to A. M. Krivtsov for the statement of the problem and D. A. Indeitsev, P. A. Zhilin for the discussions.

References

[1] Tkachev P. V.: Stability of particle triangle under compression. Proceedings of the XXX Summer School "Advanced Problems in Mechanics", St.–Petersburg, 2002, p. 593-595.
[2] Allen M. P. and Tildesley A. K. Computer Simulation of Liquids. – Oxford: Clarendon Press. 1987.
[3] Gilabert F. A., Krivtsov A. M., Castellanos A. Computer simulation of mechanical properties for powder particles using Molecular Dynamics. Proc. of XXX Summer School "Advanced Problems in Mechanics", St. Petersburg, Russia, 230-239.
[4] Hockney R.W. and Eastwood J.W. Computer simulation using particles – IOP Publishing. 1988.
[5] Krivtsov A. M., Wiercigroch M. Molecular dynamic simulation of mechanical properties for polycrystal materials. Materials Physics and Mechanics, 2001, 3(1), 45-51.
[6] Tkachev P. V., Krivtsov A. M.: Computer simulation of 2d dynamic fracture. Book of abstracts of the XXXI Summer School "Advanced Problems in Mechanics", St. Petersburg, 2003, p. 91.
[7] Krivtsov A.M. Constitutive Equations of the Nonlinear Crystal Lattice. ZAMM Z. angew. Math. Mech. 1999. 79(S2). 419-420.
[8] Krivtsov A.M. Relation between Spall Strength and Mesoparticle Velocity Dispersion // International Journal of Impact Engineering. 1999, 23, 477-487.
[9] Krivtsov A. M. From nonlinear oscillations to equation of state in simple discrete systems. Chaos, Solitons & Fractals, 2002, 17(1), 79-87.
[10] Born, M. and Huang, K. Dynamical Theory of Crystal Lattices. Oxford, England: Clarendon Press, 1954.
[11] Lurie, A. I: Nonlinear theory of elasticity. North-Holland Series in Applied Mathematics and Mechanics. 1990.