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Atomistic modeling of the dislocation dynamics and evaluation of static yield stress

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Abstract. Static strength characteristics of structural materials are of great importance for the analysis of the materials behaviour under mechanical loadings. Mechanical characteristics of structural materials such as elastic limit, strength limit, ultimate tensile strength, plasticity are, unlike elastic moduli, very sensitive to the presence of impurities and defects of crystal structure. Direct atomistic modeling of the static mechanical strength characteristics of real materials is an extremely difficult task since the typical time scales available for the direct modeling in the frames of classical molecular dynamics do not exceed a hundred of nanoseconds. This means that the direct atomistic modeling of the material deformation can be done for the regimes with rather high strain rates at which the yield stress and other mechanical strength characteristics are controlled by microscopic mechanisms different from those at low (quasi-static) strain rates. In essence, the plastic properties of structural materials are determined by the dynamics of the extended defects of crystal structure (edge and screw dislocations) and by interactions between them and with the other defects in the crystal. In the present work we propose a method that is capable to model the dynamics of edge dislocations in the fcc and hcp materials at dynamic deformations and to estimate the material static yield stress in the states of interest in the frames of the atomistic approach. The method is based on the numerical characterization of the stress relaxation processes in specially generated samples containing solitary edge dislocations.

1. Introduction

Plastic deformations of crystals are controlled by the presence of extended defects of crystal structure, primarily, dislocations. Dynamics of the dislocations due to external stresses determines the kinetics of plastic deformations and thus plays an important role in the controlling of the mechanical characteristics of structural materials. It is well known that the yield stress depends substantially on the deformation rate. This becomes more evident at the deformation rates exceeding $\sim 10^3 - 10^4\,\mathrm{s}^{-1}$. At low plastic deformation rates (that is, at low dislocation sliding velocities) the dislocations overcome potential barriers impedimental their sliding as a result of combined action of the applied external stress and thermal fluctuations. While for the high rate plastic deformations one needs to apply much higher stress. At the high plastic deformation rates (exceeding $10^4\,\mathrm{s}^{-1}$ for the most of elemental hcp and fcc metals) acting stresses are sufficient to provide for dynamic potential barriers overcoming without additional help of the thermal fluctuations. In the high plastic deformation rate regimes the dominant mechanism of the dislocation drag is the dislocation energy transfer to the lattice vibrations (phonon excitations). Here we present a method that allows not only to study the dynamics of the edge dislocations in the hcp and fcc materials under dynamic loading, but also estimate static yield stress of the materials in the frames of atomistic modeling. The method is based on the numerical characterization of the stress relaxation processes in specially constructed samples containing solitary edge dislocations.

2. Traditional methods of edge dislocation dynamics simulations

The dynamics of edge dislocations in close-packed materials under dynamic loading has been studied earlier in the frames of classical molecular dynamics (CMD) by other researchers [1–7] as following. Typical scheme of the simulation model is presented in Fig. 1. The lab-frame axes are oriented in congruence to the dominant sliding system of edge dislocations in the fcc crystals. The full edge dislocation Burrgers vector is aligned along the x-axis ($[1\bar{1}0]$-direction). The dislocation sliding occurs in the xz – (111) plane. In order to generate the sample containing solitary edge dislocation the following procedure is widely used. In ideal non-defective crystal structure one removes two mono-atomic half-planes (110). Then the sample is slightly compressed, and atomic layers nearest to the cutaway draw together and cohere. Then the thermalization of the sample at the conditions of interest takes place. During the thermalization a constitutive process occurs, namely, a splitting of the ideal edge dislocations to a pair of partial dislocations $\frac{a}{2}[110] \rightarrow \frac{a}{6}[121] + \frac{a}{6}[21\bar{1}]$ with the formation of stacking fault area between them. In order to reproduce in the frames of CMD the processes related to the plastic deformations of fcc crystals one needs to be sure that the model of the interatomic interactions used is capable to describe basic properties of the edge dislocations. One of the constitutive

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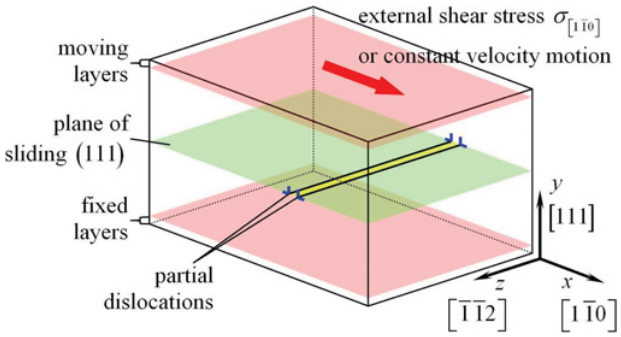

Figure 1. Typical schematic of the model for the edge dislocation dynamics in fcc crystal simulations. Along the x and z directions periodic boundary conditions are used. The sample part in-between two red planes consists of freely moving atoms. Atoms laying bellow the lower red plane are fixed, while the atoms laying above the upper red plane are allowed to move along the x-axis only either with a constant velocity v_x or due to a constant external force F_x. The applied external force or the constant velocity motion of the upper part of the sample cause plastic deformation of the sample (the edge dislocation sliding along x-axis). In the first case the shear stress acting on the sample is controlled, while in the second – the plastic deformation rate.

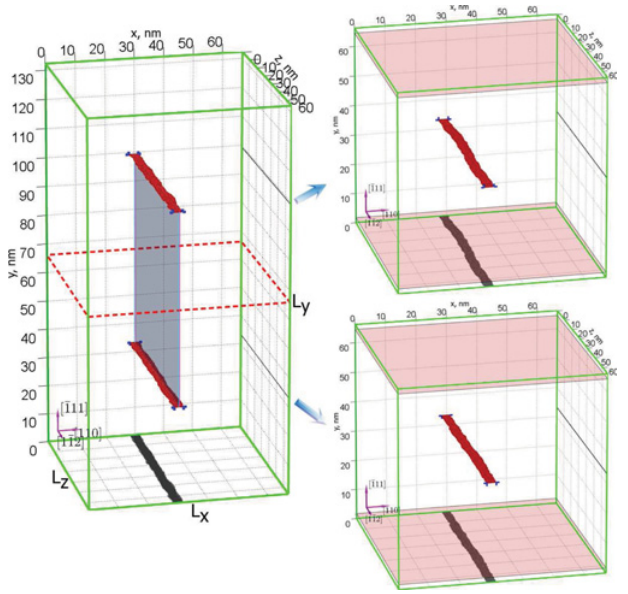

Figure 2. Initial samples generation for the shear stress relaxation method by example simulations of copper with the EAM interatomic potential [8]. From the ideal non-defective samples with the sizes $L_x \times L_y \times L_z$ and the orientation shown on the left in periodic boundary conditions in all directions we removed two mono-atomic layers of (110) type with $\frac{1}{4}L_y < y < \frac{3}{4}L_y$. As a result two edge dislocation of opposite signs are formed in the sample. Then the sample was thermalized at the conditions of interest for at least 2 ns. During the thermalization the dislocations obtain their equilibrium width and all the undesirable elastic waves caused by the artificial removing of the atomic layers decay. After that we divide the sample as it is shown, and change the boundary conditions in the new smaller samples: in the x and z directions periodic boundary conditions are used, while in the upper and bottom parts of the samples we fix all the atoms separated by the red planes. So we get two samples containing solitary relaxed equilibrated edge dislocations at the conditions of interest.

characteristics of the edge dislocations in the close-packed materials is its energetics in other words the energy stored in the defect itself and energy of elastic deformation of the crystal around it. The energy balance between the dislocation core and elastic shear deformation energy caused by the presence of the dislocation determines the dislocation core structure.

The described above approach to the CMD modeling of the edge dislocation dynamics in close-packed lattices was demonstrated to be quite an effective method. However, despite of its effectiveness the method has significant drawbacks. All the simulations had been performed so far with the rather small samples, that corresponds to the gigantic deformation rates and rather high dislocation densities considerably exceeding dislocation densities in real materials. Moreover the CMD simulations with the fixed deformation rate (dislocation velocity) or fixed shear stress provides for only one point of $v(\sigma)$ dependence in a stationary regime. In the stationary simulations it is impossible to obtain an estimate for the static yield stress (Peierls-Nabarro stress). Here we propose instead of the fixed deformation rate or fixed shear stress calculations to perform CMD simulations of the dislocation motion during the relaxation of shear stress. In such approach one can obtain in a single simulation an entire dependence of the dislocation velocity on the actual shear stress and get Peierls-Nabarro stress as the limit when the dislocation stops.

3. Stress relaxation approach

Detailed description of the initial sample generation procedure for the proposed method is given in the caption of Fig. 2 by example simulations of copper with the Embedded Atom Model (EAM) interatomic potential [8]. All the CMD simulations presented here were carried out using CMD code MOLOCH [9]. The samples containing solitary relaxed equilibrated edge dislocations at the conditions of interest are subjects for the instantaneous shear deformation ϵ_{xy} of various values. As the result of the instantaneous shear deformation ϵ_{xy} there are elastic shear stresses σ_{xy} in the samples, that cause the edge dislocation sliding along the x-direction. As a result of the dislocation motion (plastic deformation) the relaxation of the elastic shear stresses σ_{xy} takes place in the samples.

In Fig. 3(a) a typical time dependence of the shear stress σ_{xy} in the sample at the ambient conditions is presented. Initial shear deformation in the simulation was set $\epsilon_{xy} = 0.004$. At the moment $t = 0$ the shear stress has its maximum. Then the dislocation starts to move, and the shear stress decreases because of the plastic deformation. It is important that the shears stress decrease does not reach zero value, but stops somewhere around 5 MPa. This value corresponds to the shear stress when the dislocation motion stops (Peierls-Nabarro stress), while the Peierls-Nabarro stress corresponds to the minimal estimate of the engineering yield stress. In Fig. 3(b) the corresponding time dependence of the dislocation position in the same simulation is presented. The position of

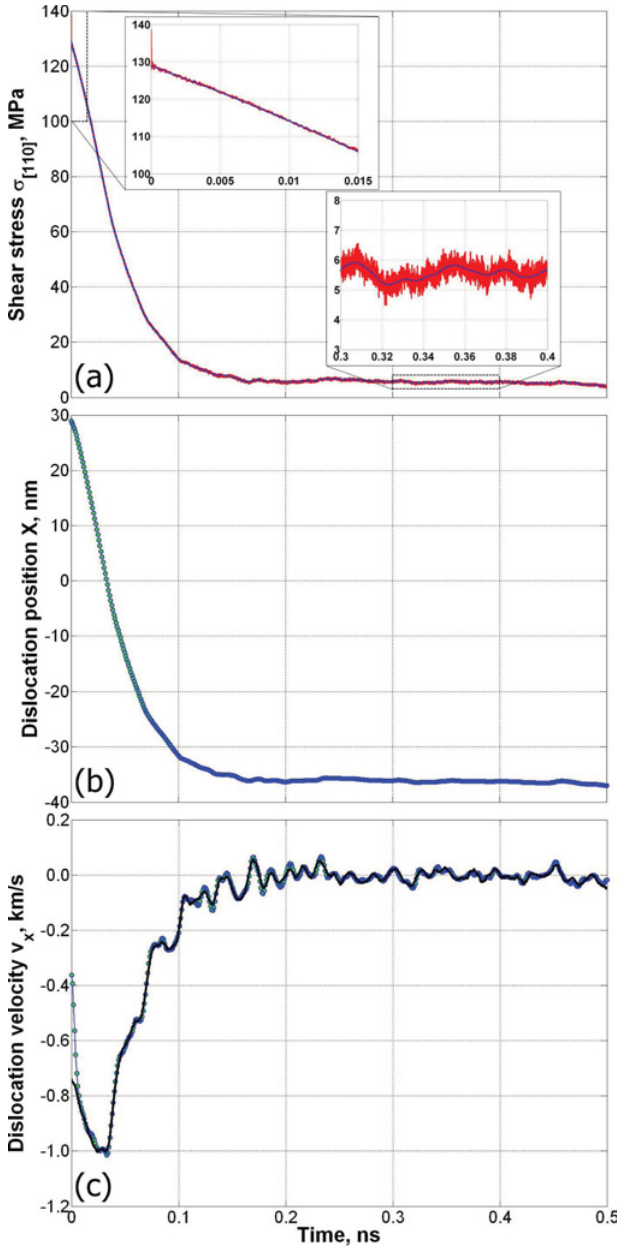

Figure 3. Time series of the shear stress $\sigma_{[110]}$ – (a), dislocation position x – (b), and dislocation sliding velocity v_x – (c) in the shear stress relaxation simulation of copper with the deformation $\epsilon_{xy} = 0.004$ at the ambient conditions.

the dislocation was determined using Adaptive Template Analysis (ATA) [10] which allows to analyze precisely crystal structure of virtual samples at finite temperatures even approaching melting. In particular, the ATA method determines with high confidence all the stacking fault atoms forming the edge dislocation. The dislocation position x is determined as average of x coordinates of all atoms in the stacking fault positions. If one takes time derivative of the dependence presented in Fig. 3(b) one gets the velocity of the edge dislocation sliding as a function of time shown in Fig. 3(c) by dots. Combining the time series from Fig. 3(a) and (c) we get the dependence of the dislocation velocity v_x on the applied external shear stress σ_{xy} presented in Fig. 4. In Fig. 4 one can see non-stationary

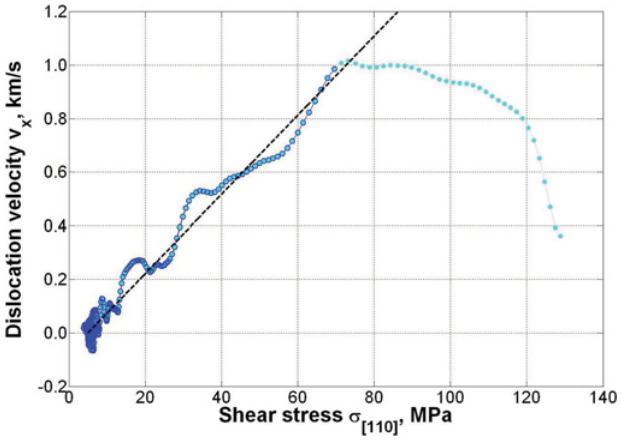

Figure 4. Dependence of the dislocation sliding velocity on the shear stress in the copper sample after the shear deformation $\epsilon_{xy} = 0.004$ at the ambient conditions.

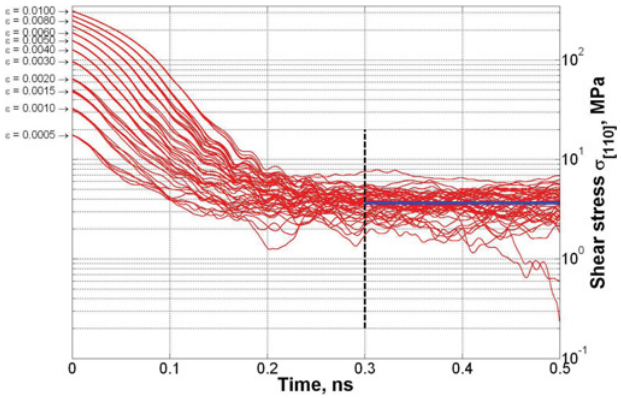

Figure 5. Time dependence of the shear stress in the copper samples containing solitary edge dislocations after various shear deformations ϵ at the ambient conditions. Blue solid line represents overall time average for all the curves calculated for the last 0.2 ns. The Peierls-Nabarro stress estimate is $\sigma_0 = 3.65$ MPa with the standard deviation $\Delta\sigma_0 = 1.08$ MPa.

initial stage when the dislocation velocity increases while the shear stress decreases. One can see also oscillations of the dependence due to circulations of elastic waves caused by the motion of the dislocation. Notice one more time that the dislocation stops not at zero shear stress but at some other one corresponding to the Peierls-Nabarro stress.

Besides the direct observation of the dislocation motion we can determine its velocity indirectly using the rate of the shear stress relaxation. At low deformations the total deformation of the sample ϵ can be expressed as the sum of plastic ϵ_{pl} and elastic deformation ϵ_{el} components. Taking time derivative of the total deformation ϵ and retaining that the total deformation of the samples does not change during the shear stress relaxation simulations we get $\dot{\epsilon}_{pl} = -\dot{\epsilon}_{el}$. In the case of low deformation the elastic shear stress is determined by the Hooke's law. Thus the rate of the plastic deformation in our simulations can be calculated as

$$\dot{\epsilon}_{pl} = \frac{\dot{\sigma}_{xy}}{G_{xy}}, \tag{1}$$

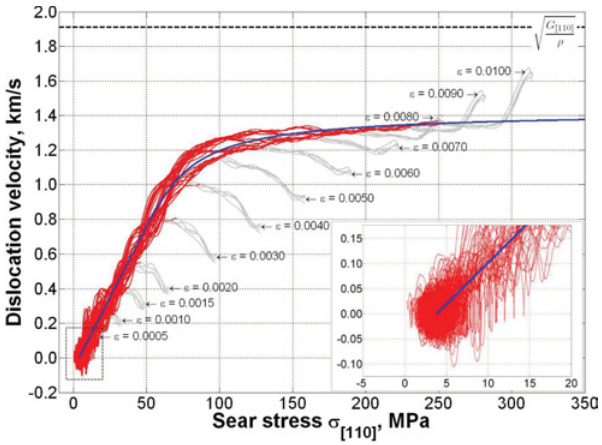

Figure 6. Dislocation sliding velocity v_x *vs.* shear stress σ_{xy} in the copper samples containing solitary edge dislocations after various shear deformations ϵ at the ambient conditions. Black dashed line represents shear sound velocity, blue solid line is approximation of the red brunches of the v_x on σ_{xy} curves. The light gray sections of the v_x on σ_{xy} curves were not used for the approximation construction.

where G_{xy} is corresponding to the deformation elastic shear modulus. In the case of the pure shear deformation of the sample with the solitary edge dislocation the plastic deformation rate $\dot{\epsilon}_{pl}$ directly proportional to the linear velocity the dislocation sliding. Thus, knowing the sample size and the shear modulus G_{xy} we can reconstruct the time dependence of the dislocation sliding velocity from the shear stress relaxation curve. In Fig. 3(c) one can see a comparison of the time dependence of the dislocation velocity obtained as the time derivative of the dislocation positions from ATA-analysis (line with dots) and one calculated from the shear stress relaxation curve (black solid line).

In Fig. 5 the time series of the shear stress in the copper samples obtained for various initial shear deformations are presented. All the curves consist of the branch where the shear stress decreases with time and stationary brunch with nearly constant non-zero value of the shear stress. That value corresponds to the stop of the dislocation sliding, *i.e.* the estimate of the Peierls-Nabarro stress σ_0. Blue solid line in Fig. 5 represents overall time average for all the curves calculated for the last 0.2 ns. The Peierls-Nabarro stress estimate is $\sigma_0 = 3.65$ MPa with the standard deviation $\Delta\sigma_0 = 1.08$ MPa. The yield stress is scaled as $\sigma_y = 2\sigma_0$. Thus, according to the EAM model with the parameterization [8] the estimate of the static yield stress of copper at the ambient conditions is $\sigma_y = (7.3 \pm 2.2)$ MPa. It should be noted that the choice of copper as a material for current investigation was made to check the sensitivity of the proposed relaxation method, because copper possesses extremely low yield stress. Indeed, the experimentally measured yield stress in high purity well annealed single crystal copper at the ambient conditions is in the range from 1.0 MPa to 4.4 MPa [11–15]. Thus, the obtained here value is only slightly higher than the experimental ones.

From the time series of the shear stress presented in Fig. 5 one can reconstruct the dependence of the dislocation sliding velocity v_x on the shear stress σ_{xy} presented in Fig. 6. Black dashed line represents shear sound velocity, blue solid line is the approximation of the red brunches of the v_x on σ_{xy} curves. The light gray sections of the $v_x(\sigma_{xy})$ curves were not used for the approximation construction. Notice that the approximation crosses zero velocity line not at zero shear stress point, and the shear stress corresponding to the zero dislocation velocity is the Peierls-Nabarro stress.

4. Conclusion

In the present work we introduce a novel approach to the simulations of the dislocation dynamics in close-packed materials. The method is based on the numerical characterization of the shear stress relaxation processes in specially generated samples containing solitary edge dislocations of particular orientations. The method allows obtaining in a single numerical experiment the entire dependence of the dislocation sliding velocity on the applied shear stress. Besides, the method provides for the capability to estimate the shear stress when the dislocation sliding stops, *i.e.* to estimate the Peierls-Nabarro stress at the condition of interest.

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