



Atomistic modeling of different loading paths in single crystal copper and aluminum

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ABSTRACT. Utilizing molecular dynamics (MD) integration model we have investigated some of the relevant physical processes caused by different loading paths at the atomic level in Cu and Al monocrystal specimen. Interactions among the atoms in the bulk are modeled with the standard realistic Embedded Atom Method (EAM) potentials. MD simulation gives us the detailed information about non-equilibrium dynamics including crystal structure defects, vacancies and dislocations. In particular, we have obtained result that indicate increase in the total energy of the crystal during loading (especially cyclic) that provides us direct quantitative evidence of the metal weakening. For the basic response, we have deformed copper and aluminum single crystal according to the simple loading path and a series of multiaxial loading-paths including cyclic repetition. We compute equivalent stress-strain diagrams as well as dislocation total length vs time graphs to describe signatures of the anisotropic response of the crystal.

KEYWORDS. Molecular dynamics; Fatigue, Multiaxial; Copper; Aluminum; LAMMPS.



Citation: Pezer., R., Trapić, I., Atomistic modeling of different loading paths in single crystal copper and aluminum, *Frattura ed Integrità Strutturale*, 38 (2016) 191-197.

Received: 15.05.2016

Accepted: 20.06.2016

Published: 01.10.2016

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INTRODUCTION

One of the landmark observation found in a macroscopic piece of polycrystalline engineering metal materials is existence of well-defined mechanic properties like yield stress or ultimate tensile strength. Tension test is most common experimental approach to examine structural materials. However, as great physicist and originator of our modern understanding of plasticity E. Orowan beautifully stated [1]: "The tensile test [is] very easily and quickly performed but it is not possible to do much with its results, because one does not know what they really mean. They are the outcome of a number of very complicated physical processes.". Even today our ability to quantitatively predict plasticity and fatigue properties like dislocation nucleation and multiaxial stress state properties are rather limited. The



problem is not only due to the immense complexity of the dislocation dynamics coming from atomic degrees of freedom but also because it is governed by phenomena at multiple length and time scales. In last two decades we witness substantial improvement of computing power and accompanied development of the sophisticated physical models [2,3] providing us with possibility to complement information from simple tensile test with numerical simulation. This fact calls for computational experiments that give us direct control over the whole range of scales involved so that we can avoid difficulties like short length ultraviolet divergences in standard crack dynamics laws. Crystals are among the most prominent examples of the decisive role of the sub micrometer scales governing the dislocation dynamics. Another prominent example is crack propagation accompanied with crystals surface production energy ("Fracture Energy") that is orientation dependent so that crystal response can be highly anisotropic even in a piece of material that is completely isotropic on the macroscale. At the atomic level in metal systems, interactions that capture complexity that accounts for fatigue and fracture must include terms beyond pairwise interactions. Such realistic potentials exist [4, 5] and are constantly improved to provide us with detailed information about non-equilibrium dynamics including crystal structure defects like vacancies and dislocations.

The task to develop successful dislocation theory to model plastic phenomena in metal materials proved to be very difficult one. Indeed, a great deal of theoretical work has been expended in the past 5 decades in attempts to explain the phenomena of metal plasticity by means of dislocation theory yet no comprehensive theory has been achieved. There has been substantial progress in modeling nucleation and growth of fatigue cracks under multiaxial stresses like Fatemi-Socie [6] parameter applied to steel specimens. However, at the fundamental atomic scale it turns out that the full resolved stresses play also very important role [7, 8].

Here we utilize MD simulations to help elucidate how the principal and resolved stress components on the primary slip plane(s) impact dislocation nucleation in FCC Cu and Al perfect crystals at room temperature. In contrast to prior studies of those systems here we perform both multiaxial and fatigue tests where we quantitatively examine sensitive dislocations effects that govern materials response under the plastic deformation. We are focused mostly on the yielding deformation zone where dislocation nucleation starts at the very high rate. In this sense, Cu and Al (apart from applicative interest in itself) are interesting FCC candidates. Those metals share crystal structure but behave very differently: soft Cu contains almost no discernible straight part while Al experience very graduate transition from straight to the curved zone of the stress-strain diagram. In short the goal of this work is to examine correlation of the loading axis orientation, stress components resolved onto the $\{1\ 1\ 1\}$ primary slip plane and dislocation density dynamics. Here we have found that dynamic properties in FCC single crystals critically depend on the magnitude and loading axis orientation. For the basic response, we have deformed Cu and Al single crystal according to simple loading path including cyclic fatigue harmonic tensile deformation. In order to further study complex patterns of fracture effects in crystal sample we prepare whole range of different loading-paths. This way we are able to specifically probe anisotropic response in the sample subject to different loading directions and look for the signatures of the multiaxial stress states at the atomic scale.

In order to show distinct features of stress-strain relationship for several loading paths first we have simulated evolution by deforming entire model system at the usual ps time scale isothermally at 300 K. The strain rate is several orders higher than we usually see in LAB or industry setting but is due to the intrinsic limit of the MD time propagation of the atomistic system dynamics. However, since we are following trajectories at individual atoms level the time scales separation is part of the complex process of information transport to meso and macroscale. What is the real information at the atomic level that survives and govern tensile test in the experiment is one of the important questions in solving mechanical properties puzzle.

SIMULATION MODELS AND METHODS

Embedded Atom Method

The semi-empirical embedded-atom method (EAM) potentials are energy functions and govern the interaction among the neighboring atoms. It is commonly used approach for metals because it captures main features of the metallic bonding. The potential proposed by M. S. Daw and M. I. Baskes [9, 10], was based on the quantum mechanical density functional theory. They combined theoretical considerations with a fitting of parameters to the main properties of the bulk crystal. Their approach leads to the following expression for the total potential energy of a crystal:

$$E_{\text{tot}} = \frac{1}{2} \sum_{i \neq j} V(r_{ij}) + \sum_i F_i(\rho_{b,i}) \quad (1)$$



First term is central repulsive short range pairwise interaction while the second one is a multi-body term (attractive interaction) that models “embedding” a positively charged pseudo-atom core into the “sea” of free electrons created by the surrounding atoms. It is described by the semi-empirical energy function F_i with argument describing host electron distribution at atom i . Due to the weak bonding directionality Cu is an ideal FCC material for accurate characterization by the non-directional generic feature of the EAM. Essentially all of the physics is contained in Eq. (1) and the calculated properties are complex manifestation of the huge number of atoms mutually interacting with one another. During the time evolution atoms are simultaneously exposed to environment forces that give raise to deformation response and defects nucleation that is subject of this work. Interatomic potential for aluminum is also very well established and thoroughly checked against many basic equilibrium properties like the elastic constants, the vacancy formation and migration energies, the stacking fault energies and the surface energies. For both, Cu and Al potentials, it is expected to be applicable to different local environments encountered in present simulations of dislocation and plastic properties within the MD simulation framework.

Simulation Modeling

As already mentioned in the introduction section, the time step size is difficult to decide because of the intrinsic simulation limits of the method. Trial and error process is usual choice but whatever the strategy we take most important is to make sure the total energy conservation is not violated to cause system instabilities. It is desirable to propagate the system as far as possible but characteristic time scale relevant for atoms makes 100 ps as appropriate option.

Property\Metal	Copper	Aluminum
box size (in lattice constants)	25	25
box size before relaxation (nm)	9.025	10.125
box size after relaxation (nm)	9.080	10.160
temperature (K)	300	300
number of atoms	62500	62500
equilibration time (ps)	20	20
simulation time (ps)	75	75
strain amplitude ϵ_A , period t_p (ps)	0.18, 25	0.18, 25

Table 1: Parameters used for MD simulations.

After the perfect crystal is prepared (initial lattice constants 0.361 and 0.405 nm for Cu and Al, respectively) in the desired crystallographic orientation, the system of atoms is equilibrated for 20 ps. Usual MD thermostating procedure has been employed in the isobaric-isothermal (NPT) ensemble at a zero pressure and temperature of 300 K. Periodic boundary conditions were used along all three axis. Summary of all parameters is given in Tab. 1. Equilibration and simulation time are chosen in order to cause appreciable dislocation nucleation and fatigue phenomena.

At the beginning of the simulation, atoms just vibrate around their perfect crystal positions. As the load increase after initial elastic response dislocation nucleation starts and we see characteristic signature of the process qualitatively similar to usual tensile test. MD simulation generate huge and abundant information about atomic system and here we use several sophisticated algorithms to extract relevant physical information. However, it is important to keep in mind that physical observables we see in this numerical simulation do not represent measured macroscopic quantities in LAB conditions. Although correlated quantities, they are distinct. We stress that nevertheless we use even millions of atoms our crystal system is still far from anything to be considered macroscopic. This correlation proves to be difficult tasks to accomplish in theory development and is still part of the ongoing research.



RESULTS AND DISCUSSION

Fig. 1 and 2 shows the equivalent stress-strain diagrams and resolved shear stress onto the $\{1\ 1\ 1\}$ primary slip plane for Cu and Al monocrystal at room temperature, respectively. Equivalent tensile stress is defined in terms of principal values as usual:

$$\sigma_{eq} = \frac{1}{2} \sqrt{(\sigma_1 - \sigma_2)^2 + (\sigma_2 - \sigma_3)^2 + (\sigma_3 - \sigma_1)^2} \quad (2)$$

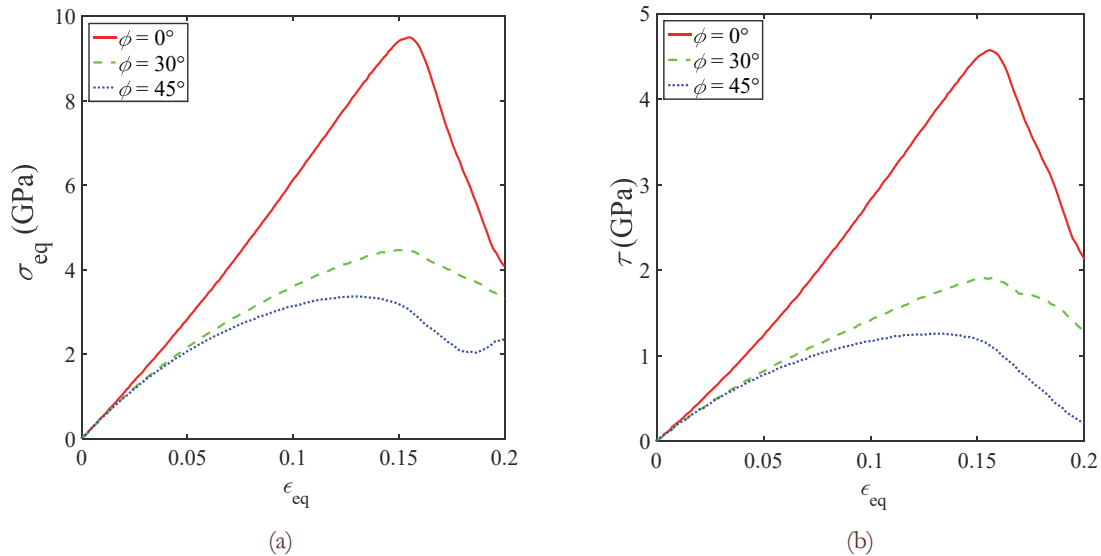


Figure 1: Different loading paths defined by deformation speeds along system axis. Loading speeds are expressed as $\Delta\varepsilon/\Delta t$ and total magnitude is 0.01 ps^{-1} . (a) Equivalent stress-strain diagram (see Eq. 2). (b) A resolved shear stress upon the $\{1\ 1\ 1\}$ slip plane in the slip direction.

The graphs clearly show strong dependency of the stress-strain correlation to multiaxial character of the loading to crystal system orientation. We note not only quantitative differences but also completely different curvature and smearing out of the peak stress value. Effects are much less pronounced in Al than in Cu system. Nevertheless both metals show strong orientation dependency, which alarms for careful analysis when we develop phenomenological or qualitative models of polycrystalline materials.

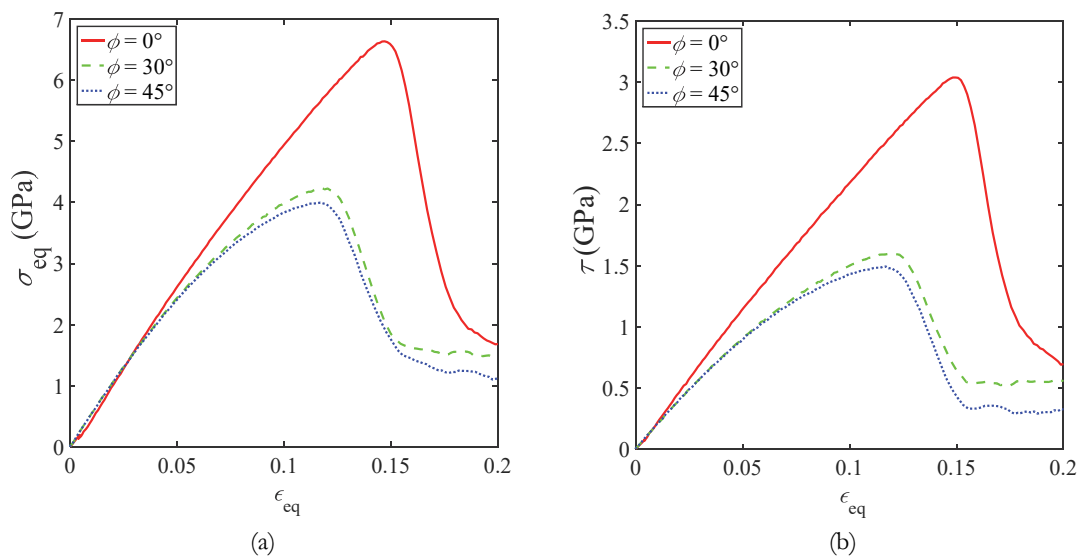


Figure 2: Same as Fig. 1 but this time for Al.



It is unlikely that we will develop a single model applicable for all materials and states of stress for the multiaxial fatigue even for the metallic systems. Therefore, an important ingredient for successful theory is to take into account whole range of important properties heavily influenced by atomic distribution symmetries in space coordinates. They are associated with the crystallography of the grains and the structure of grain boundaries [8].

Fig. 3 shows stress-time evolution during cyclic loading in three directions with respect to x axis in the xy perfect crystal plane where cyclic loading was harmonic and in phase given by following general formula for the strains along x and y axis (angle ϕ is given in legend of the figures):

$$\epsilon_x(t) = \frac{\epsilon_\Lambda \cdot \cos(\phi)}{2} \left(1 + \sin \left(2\pi \cdot \frac{t}{t_p} - \frac{\pi}{2} \right) \right) \tag{3a}$$

$$\epsilon_y(t) = \frac{\epsilon_\Lambda \cdot \sin(\phi)}{2} \left(1 + \sin \left(2\pi \cdot \frac{t}{t_p} - \frac{\pi}{2} \right) \right) \tag{3b}$$

The simulation parameters are given in Tab. 1. Cycling strain amplitude has been selected so that deformation reaches deep enough into the plastic zone in order to get substantial dislocation density as seen on Fig. 4 where it is clear that dislocation nucleation dynamics for Cu and Al crystal is quite different depending on the deformation direction.

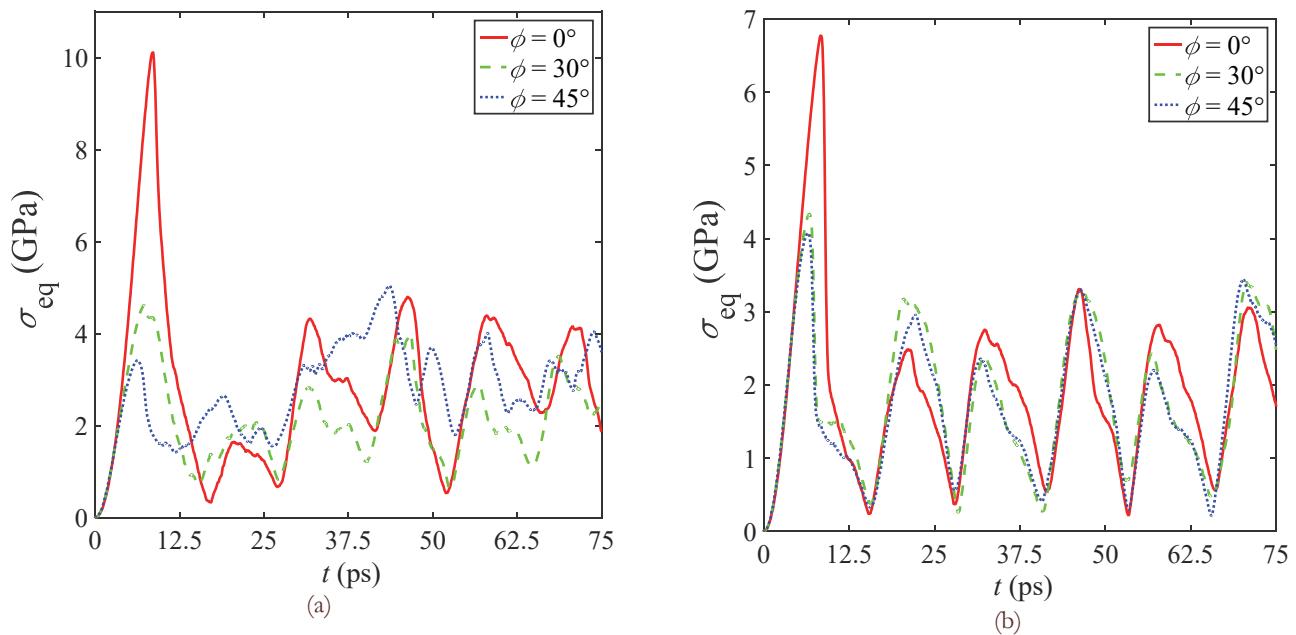


Figure 3: Stress during cyclic loading providing fatigue test for different loading paths defined by deformation angle of stress direction and x-axis in xy plane of the perfect crystal (see Eq. 3a, b). (a) Copper. (b) Aluminum

We clearly see completely different response of the Cu and Al crystal to cyclic in phase (uni)multiaxial loading. While Al single crystal shows no significant difference with regard to multiaxial stress state. In a way, Al crystal is able to recover after loading no matter what deformation direction we apply.

There is also significant difference regarding stress response phase among different deformation orientations. Cu system tends to go out of the phase for $\phi=45^\circ$ angle of simulation box deformation. One of the obvious physical properties to be reason for this discrepancy between two FCC metals is the stacking-fault energy (SFE). As is well known low SFE is usually accompanied by the lower mobility of a dislocation in a crystal. For Al it falls within 160-200 mJ/m² range, and for the Cu it is considerably smaller 70-80 mJ/m².

Critical resolved shear stress in Cu and Al is affected by the normal stress components acting to the slip plane as shown in [11] suggesting that factors beyond standard given by Schmid are necessary for dislocation nucleation description.



Motivated by this observation we have performed full atomistic simulation and dislocation identification using advanced DXA algorithm [3]. In Fig. 4 we show dislocation density (total length of dislocation line is divided by the system volume) during simulation. We note similar differences between Cu and Al behavior as we saw in Fig. 3 for equivalent stress dynamics. The dislocation morphology is rather consistent for both metals since they are mostly of Shockley partial dislocation type. This result is consistent with stacking faults presence mentioned in context of Fig. 3 regarding different cyclic loading response in Cu and Al single crystal.

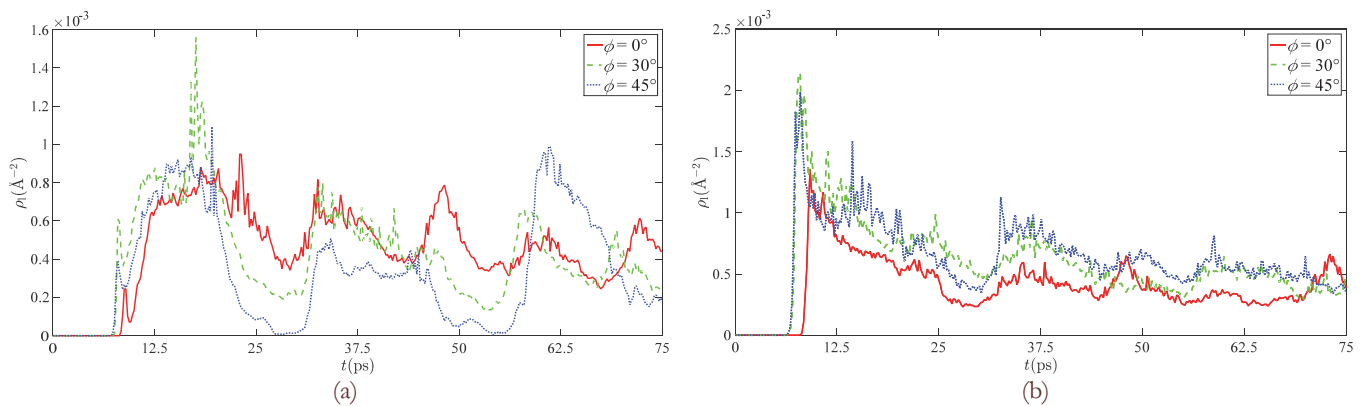


Figure 4: The dislocation density during cyclic loading for different loading paths defined by deformation angle of stress direction and x -axis in xy plane of the perfect crystal (see Eq. 3a, b). (a) Copper. (b) Aluminum.

CONCLUSIONS

In this paper atomistic simulations of multiaxial strain, including cyclic fatigue harmonic loading, in face centre cubic (FCC) single crystal have been performed for two common metals: Cu and Al. In addition, we have examined dislocation nucleation as identified during time evolution. The stress response behaviors on main slip plane $\{1\ 1\ 1\}$ have been investigated using resolved shear stress. It has been found that the response to the fatigue significantly differs for Cu and Al system. Time evolution of the dislocation density shows completely different pattern for two metals. Connection with significantly different SFE for two metals is discussed. We conjecture that development of a single universal model applicable for all metallic materials and states of stress and the multiaxial fatigue is practically ruled out by complexity of the physical properties at the atomic level.

ACKNOWLEDGMENTS

This work has been supported by Croatian Science Foundation under the project Multiscale Numerical Modeling of Material Deformation Responses from Macro- to Nanolevel (2516).

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