Research Seminar

And Journal Club Report Summer Semester 2020

Dislocation avalanches in plasticity

Technische Universität Bergakademie Freiberg

Die Ressourcenuniversität. Seit 1765.

Viswambhar Reddy Yasa

Computational Material Science

65074

Guided by
Dr.Hengxu song

Supervised by
Dr.Arun Prakash

July 20, 2020

1 Introduction

In plasticity model, plastic deformation depends on the internal state variables which are measurable variables like strain rate, temperature, stress and material variables. The relation between all the internal state variables is expressed using flow rule.

In general, flow rule is the resistance to the plasticity and expressed as the ratio of the plastic driving force to the flow resistance. During plastic deformation, the driving forces direct the internal slip mechanisms which causes shearing. A general power law flow rule representation equ.(1.1)[1]

$$\dot{\gamma}^{(\alpha)} = \dot{\gamma}_0 \left| \frac{\tau^\alpha}{g^\alpha} \right|^n \operatorname{sgn}(\tau^\alpha) \tag{1.1}$$

In equ.(1.1) $\dot{\gamma}^{(\alpha)}$ is slip rate of the slip system α, τ^α is the shear stress, g^α is the internal state variable which depends on temperature.

Plasticity is mediated through dislocation. The basic types of dislocations are edge, screw and mixed dislocation. During plastic deformation, dislocation motion will occur in multiple slip system simultaneously. This lead to the interaction of dislocation with dislocations of other slip systems. This collective dislocation dynamics plays an important role in understanding the material response like fatigue, creep, yield.[7]

The entanglement of different dislocation generate a complex stress field. These complex stress field creates a low energy barriers which act as obstacles for dislocation movement having long range interactions. This complex system of interaction leads to the formation of dislocation avalanches. Dislocation avalanches are the basic mechanism of plastic flow in solids at the nano-scale. Dislocation avalanches are also associated with strain bursts which is a sudden increase in strain rate. They follow power law distribution. [9]

A comprehensive overview on dislocation avalanche physics and the phenomena leading to strain bursts in crystal plasticity is discussed further.

2 Dislocation avalanches

Dislocation avalanches can be defined as collective movement of dislocations happening at irregular intervals. Dislocations at the nano-scale do not move smoothly,but instead they transition through bursts of activities which are due to dislocation avalanches. [9]

Forest dislocations are dislocation in active slip plane which interact with other dislocations having different Burgers vector. These forest dislocations act as pinning point for the movement of the dislocations. When the external force reaches a critical stress, the dislocations lend to overcome the energy barrier by breaking or by jumping over the forest dislocations.[2].

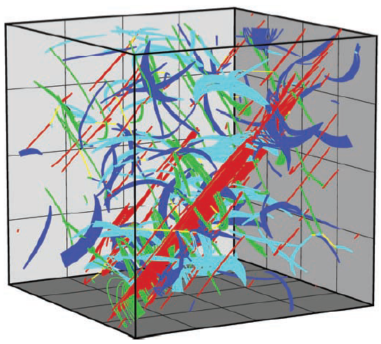

Figure 1: Progress of a large dislocation avalanche in [010] symmetrical multiple slip for a specimen.[2]

To understand dislocation avalanches. We should understand how dislocation accumulation occurs

- Pinning and de-pinning
- Jamming or clogging

In pinning and de-pinning, the obstacle are precipitates which impend the dislocation motion. Based on Orowan mechanism which depends on critical radius of the precipitates, the dislocation would cut or loop over the precipitate. The dislocation tend to accumulate at this pinning points. As the external force increases, dislocation jump over the obstacles and get pinned again at other location. The dislocations tend to move collectively in intermittent fashion. These pinning of dislocation lead to the formation of frank-read mechanism at precipitates which lead to the multiplication of dislocations.

When the external force reaches a critical stress, the dislocation line would bypass the precipitate by Orowan cutting mechanism. Thus The dislocation line tends to move continuously responds to steady plastic flow.

Jamming or clogging occurs in caged dynamics. Where the dislocation density is very high. This leads to the dislocation having self-induced constraints to there motion. Jamming or clogging is similar to traffic jams. When the external force is high enough, the dislocation tend to move in a collective manner causing plastic flow.

Grain Boundaries would also acts as barrier to the dislocation motion and impend dislocation until increasing external force causes a collective dislocation glide leading to sudden increase in strain-rate in plasticity.This process is repeated until the crack propagation is initiated.[8]

A quantitative analysis of multi-slip system can be expressed as the number of dislocation per unit length.The rate at which dislocation density increases is proportional to the number of precipitates. The yield strength can be expressed as the square root of the dislocation density.

$$\sigma_y \propto \sqrt{\rho} \tag{2.1}$$

The equ.(2.1) shows that as the dislocation density increases, the strength of the material increases.

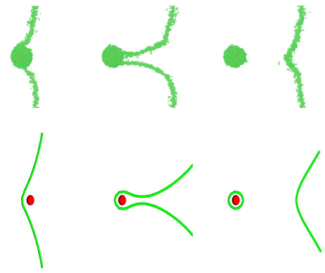

Figure 2: Orowan mechanism pinning of dislocation line

The atomistic simulation of dislocation avalanches will depend on the pinning point and dislocation density. The figure (1) is a simulation of large dislocation avalanche in a symmetrical cube. The lines in red, blue, pink are dislocation avalanche which occurred at different time steps.The yellow lines are the immobile dislocation which act as forest dislocations.

3 Atomistic modelling and simulation of dislocation avalanches

The magnitude of time scale in molecular dynamics (MD) simulation can hardly go beyond nanoseconds, which is magnitudes away from real time experiments. To over come this disadvantage we use an alternative approach of exploring the structure of the energy landscape and identifying the transition pathway and barrier. This information is incorporated in TST calculations. Many atomistic algorithms are developed like activation-relaxation technique (ART) and autonomous basin climbing (ABC) method to incorporate the energy barriers and pinning points .[4]

Slip avalanches also known as discrete stress relaxations and are strain-rate sensitive.The modelling of constant strain-rate simulation is done using transition state expression is given equ. (3.1) [4]

$$\dot{\varepsilon} = \dot{\gamma}_0 \exp\left(-E_b/k_{\mathrm{B}}T\right) \tag{3.1}$$

For atomistic modelling, The following step are to be performed:

- Energy minimization i.e the local energy of the system is minimum. For each iteration the energy minimization is performed to the system to equilibrium.

- Atomistic algorithms like ABC or ART must be applied to the system to generate local energy barriers and pinning points which are essential for dislocation avalanches.
- External load is applied and for small strain rate, the energy state is configured and saved
- The stored atomic configuration are used to calculate the single-atom displacement and strains.
- For each iteration, energy minimization with respect to the external load need to be achieved for the iteration to terminate. This process is continued till a maximum strain is achieved.

After reaching maximum strain, the subsequent plastic flow is essentially dominated by this shear localized region, involving sliding and thickening.

The figure (4) show the response of strains for different strain-rates.For all the strain-rates, the material shows elasticity till yield point represented by point 1.Then at point 2 there is sudden drop in stress due to impending of dislocation.A significant sharpening of stress is observed in plasticity.This variation of stress with strain-rate is called over-shooting. This signifies that the dislocation avalanches result in strain bursts.[4]

The dislocation statistics and there implications on stress-strains are discussed in the next section.

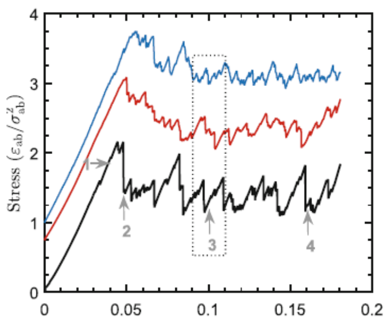

Figure 3: stress-strain graph.[4]

4 Dislocation avalanche statistics and machine learning

The result from MD and atomistic simulation like stress-strain and displacement-time graphs are used to generate the statistics of dislocation avalanches like size and velocity.

Dislocation avalanche size distribution can calculated from the stress-strain information. The magnitude of the dislocation slip is obtained by using Complementary Cumulative Distribution Function (CCDF) C(S,σ) equ.(4.1)[5] which on using scaling factor would give the dislocation avalanche distribution based on slip size.[5].where S is slip size and σ is stress

$$C(S,\sigma) \sim \int_{S}^{\infty} D\left(S',\sigma\right) dS' \sim S^{-(\kappa-1)} g\left(S\left(\sigma_c-\sigma\right)^{\frac{1}{\beta}}\right) \tag{4.1}$$

The fact that the dislocation avalanches depends on the size distribution implies that two response regimes exist. After yield point, small avalanches can be regarded as precursor events or an incubation stage leading up to the occasional major relaxation event. When the external force reaches a critical value all dislocation would glide continuously causing large dislocation avalanches having steady plastic flow.

From displacement-time information, velocities of the dislocation avalanches are calculated. The probability of a certain displacement magnitude to occur follows a power-law distribution over at least two orders of magnitude.[6]

Many supervised Machine Learning algorithms like neural network are capable of learning non-linear mapping of features to a desired output. Therefore, this method is used for predicting deformation.Due to dislocation avalanches there are irregularities in stress-strain relation as a result of strain bursts. These strain bursts follow power-law distribution until the system reaches criticality. The predictive model to simulate stress-strain curve can be achieved by using sample-specific information about the pinning landscape as well as the initial dislocation configuration as input. From these predicted stress-strain curves, the dislocation avalanche statistics can also be predicted.In figure (4) using CNN we predicted strain bursts.

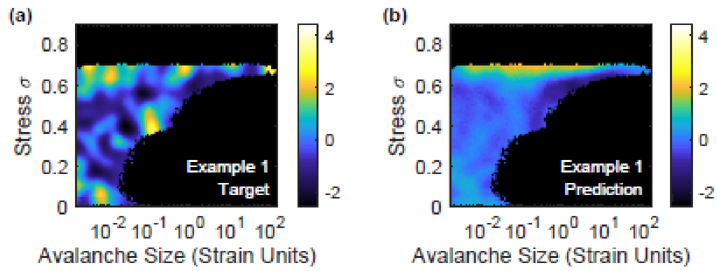

Figure 4: stress-strain graph.[4]

Conculsion:

References

[1] H. Chowdhury, H. Altenbach, and K. Naumenko. On the choice of the power law flow rule and its consequences in crystal plasticity. *Journal of Applied Physics*, 725:359–365, 2 2017.

[2] F. F. Csikor, C. Motz, D. Weygand, M. Zaiser, and S. Zapperi. Dislocation avalanches, strain bursts, and the problem of plastic forming at the micrometer scale. *Science*, 318(5848):251–254, 2007.

[3] K. M. Davoudi and J. J. Vlassak. Dislocation evolution during plastic deformation: Equations vs. discrete dislocation dynamics study. *Journal of Applied Physics*, 123(8):085302, 2018.

[4] Y. Fan and P. Cao. *Long Time-Scale Atomistic Modeling and Simulation of Deformation and Flow in Solids*, pages 237–263. Springer International Publishing, Cham, 2020.

[5] Y. Hu, L. Shu, Q. Yang, W. Guo, P. K. Liaw, K. A. Dahmen, and J.-M. Zuo. Dislocation avalanche mechanism in slowly compressed high entropy alloy nanopillars. *Communications Physics*, 1(1):61, Oct 2018.

[6] R. Maaß, P. M. Derlet, and J. R. Greer. Small-scale plasticity: Insights into dislocation avalanche velocities. *Scripta Materialia*, 69(8):586 – 589, 2013.

[7] U. Messerschmidt. *Dislocation Motion*, pages 73–154. Springer Berlin Heidelberg, Berlin, Heidelberg, 2010.

[8] T. Niiyama and T. Shimokawa. Barrier effect of grain boundaries on the avalanche propagation of polycrystalline plasticity. *Phys. Rev. B*, 94:140102, Oct 2016.

[9] S. Papanikolaou, Y. Cui, and N. Ghoniem. Avalanches and plastic flow in crystal plasticity: an overview. *Modelling and Simulation in Materials Science and Engineering*, 26(1):013001, dec 2017.