

Dislocation Dynamics Simulation

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Introduction

People have been approaching crystal plasticity as a continuum problem. And although this approach can describe the problem well enough it breaks down for small length scales. By now it has been very well established that defects in crystals govern plasticity, namely line defects, called dislocations. They move when under stress and allow the crystal to deform when they move, thus being the perfect candidate to be the fundamental carrier of plasticity. However it is their long-range anisotropic interaction that gives submicron-size plastic phenomena their rich variety. With Dislocation Dynamics Simulations we are trying to investigate the different aspects of plasticity especially down to small scales where modern technological applications care more about.

Description

We are investigating the motion of parallel straight edge dislocations under the long-range elastic stress interaction they produce in their host medium. In a square box of sides L , we place N straight parallel edge dislocations. They are allowed to glide along the x -axis only while they can interact in x and y directions. In that way we are simulating a single-slip system. Nothing happens in the z direction and while this is not very common in real dislocation systems it is not going to mask any of the characteristics we are probing.

A dislocation, under this long-range stress interaction with the rest and the external shear stress, moves in an overdamped manner, as indicated by experiments, where its velocity is proportional to the force it is experiencing. The differential equations of motion are solved by the adaptive-step 5th order Runge-Kutta.

To simulate the effect of bulk materials we employ periodic boundary conditions. To treat the long-range character of the dislocation interaction we found particularly straight forward and useful the Lekner summation method. According to that we introduced image cells around the basic simulation cell where each one of them contains N image dislocations at the same relative positions and following exactly what the basic N dislocations do.

The dislocation number is constant since for the time being we didn't consider creation nor annihilation. There is equal number of dislocations with positive, and negative Burgers vectors. We are also not allowing dislocation climb which is not very common in single-slip systems.

Objective

The existing sequential CPU code is very slow to allow us to simulate large system sizes and long running times that would allow the system to reveal its fundamental behavior. We are hoping that with parallelizing the different tasks of the simulation with CUDA(R) and running on GPUs we will be able to greatly decrease runtime and be able to simulate much larger systems.

Background

Since it is a physics application, classifiable as a N-body simulation it would be very helpful for people to know University Physics level Mechanics (e.g. phys211) and Ordinary Differential Equations (e.g. math285) especially systems of ODEs and ways to solve them numerically .

Resources

[1] For general knowledge on dislocations see here:

<http://en.wikipedia.org/wiki/Dislocation>

[2] Latest research with Dislocation Dynamics Simulations see here:

<http://cmn.fisica.unimo.it/zapperi/dislo.html>

[3] For general info on solving ODEs see here:

http://en.wikipedia.org/wiki/Numerical_ordinary_differential_equations

[4] For adaptive step 5th order Runge-Kutta see here: www.tat.physik.uni-tuebingen.de/~speith/Projekt1/numrec/c16-2.pdf

[5] Numerical Recipes in C++: the art of scientific computing. William H. Press et al. Cambridge University Press ISBN:0-521-75033-4

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