Stress propagation in crystals: molecular dynamics simulations with examples.

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→ Why molecular dynamics (MD) and what is that at all?

→ *classical (newtonian) dynamics of atoms with interatomic potential*
→ *iteration steps used to integrate time-trajectories of atoms*

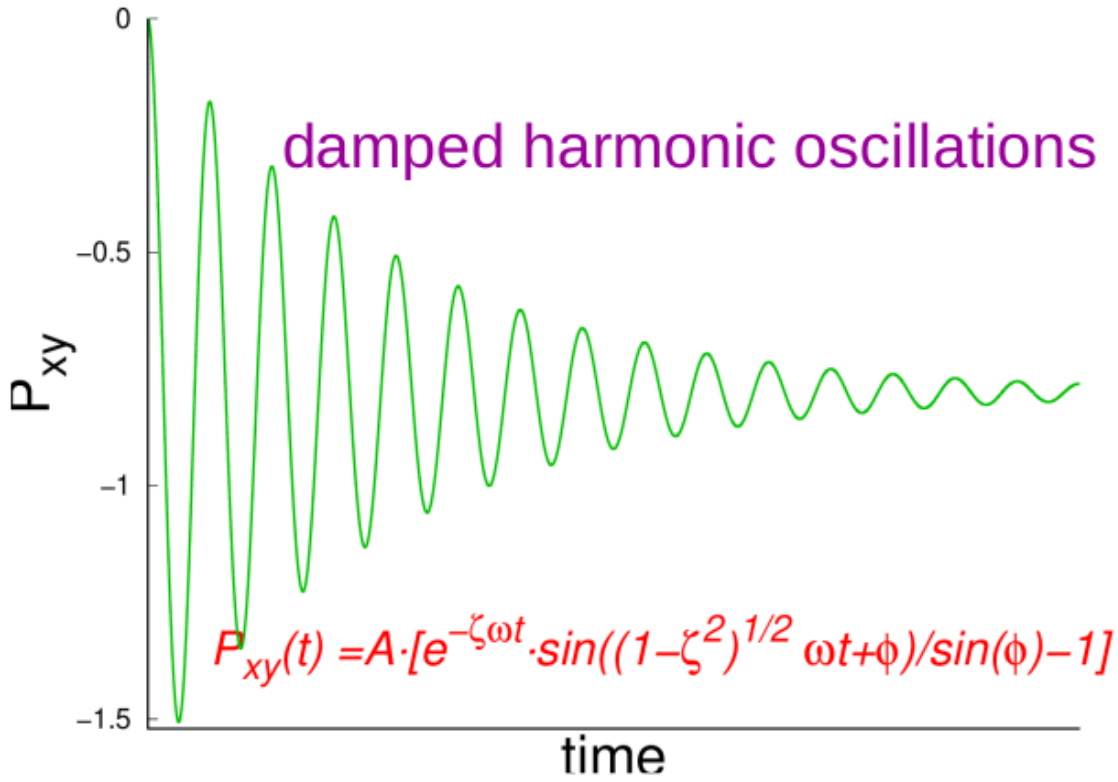
→ MD is the only simulation tool available for sub pico-second times

→ useful, for investigation of irradiation damage (defects, vacancies, collision cascades, etc)

→ **in this example** MD is used for investigation of dynamics of dislocations in steel 310S

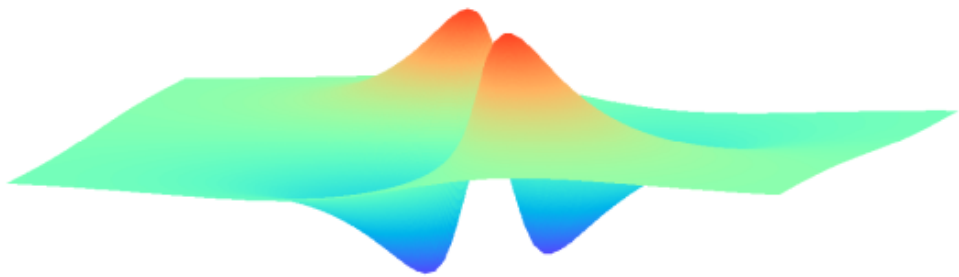
Graphical Abstract

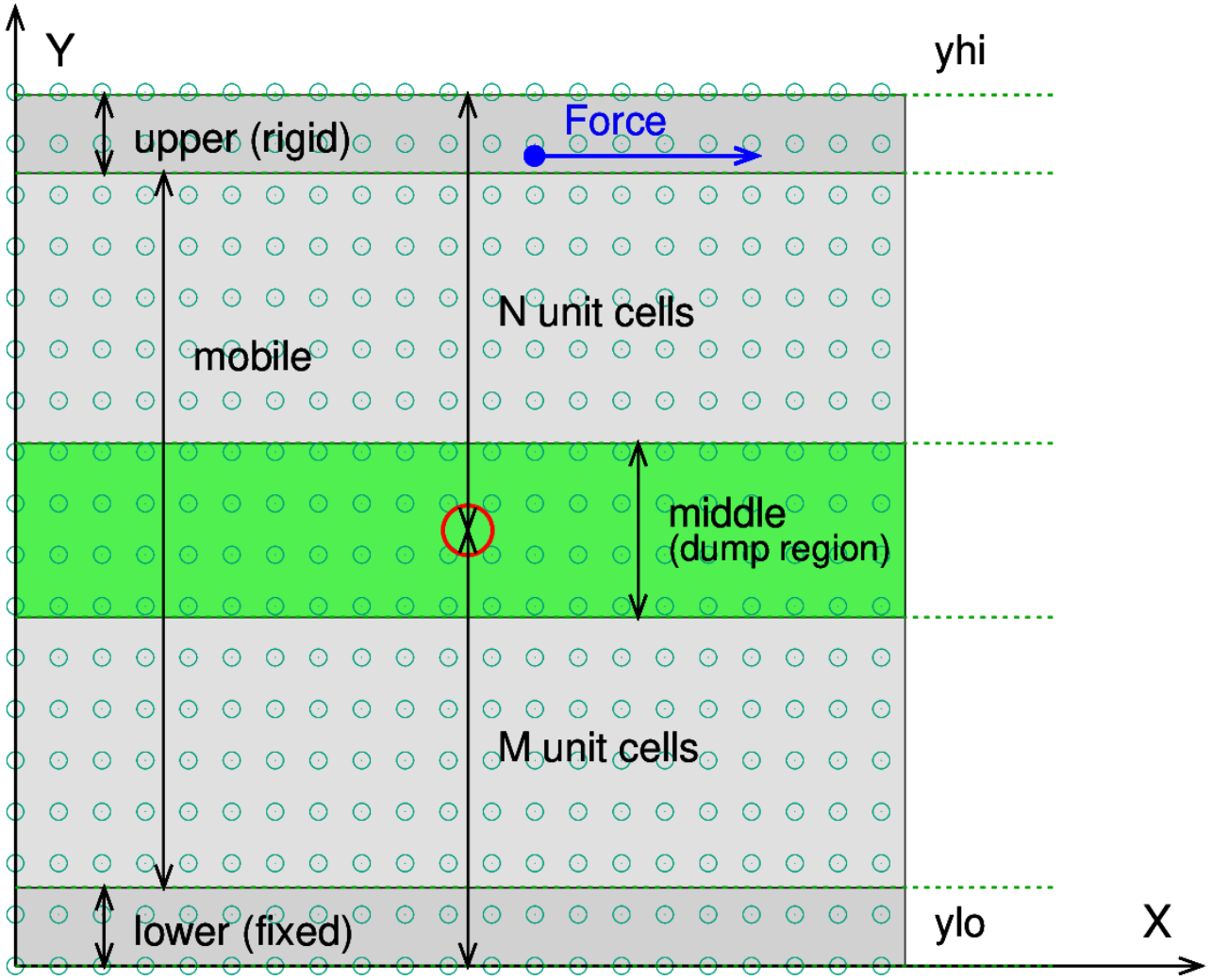
pressure penetrates sample interior as a sound wave
and interacts with strain field of dislocations



→ time effects

→ size effects

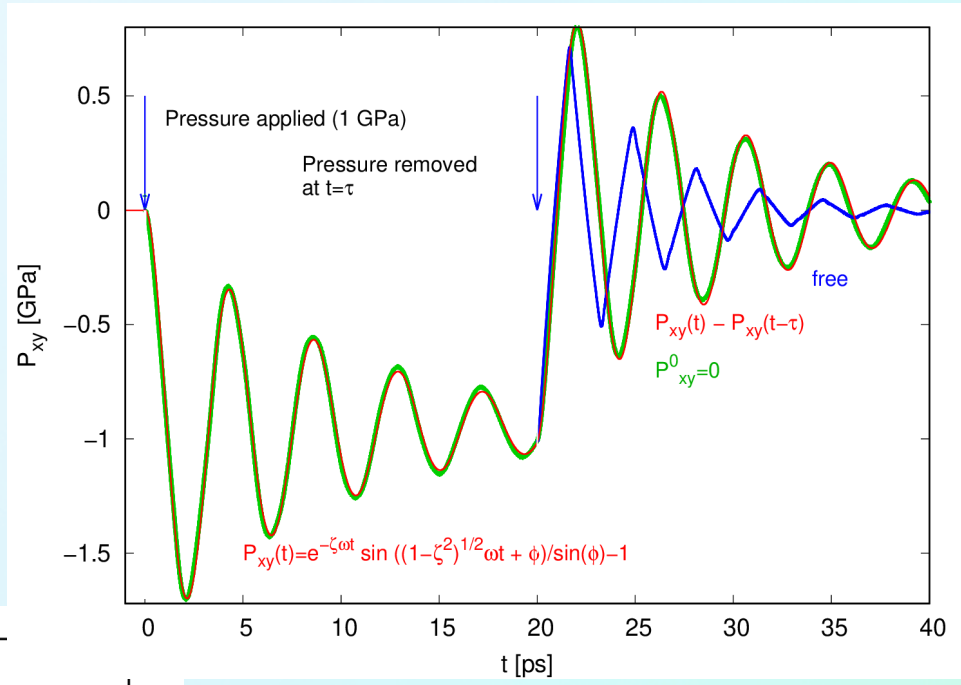


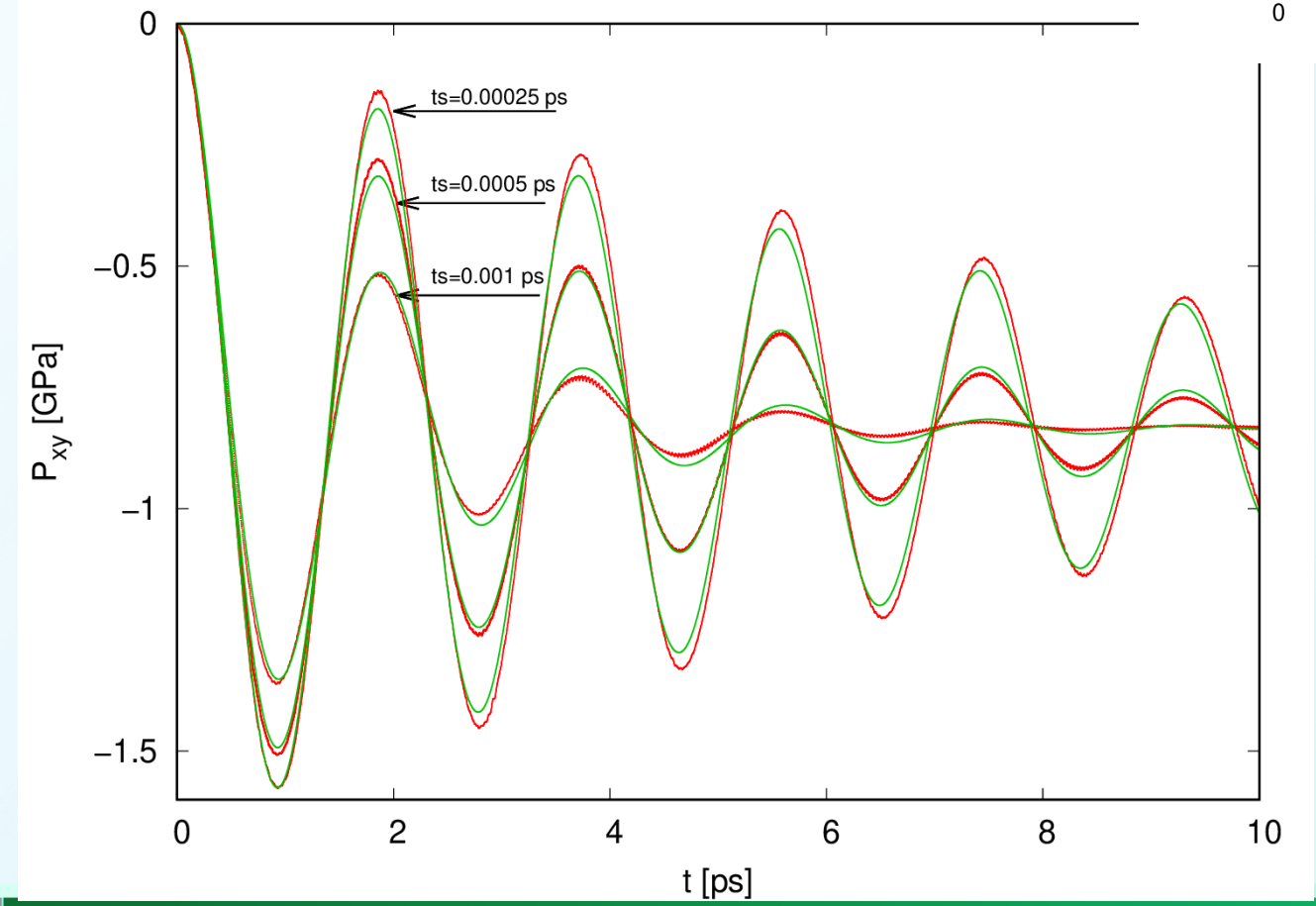


Sample cross-section.

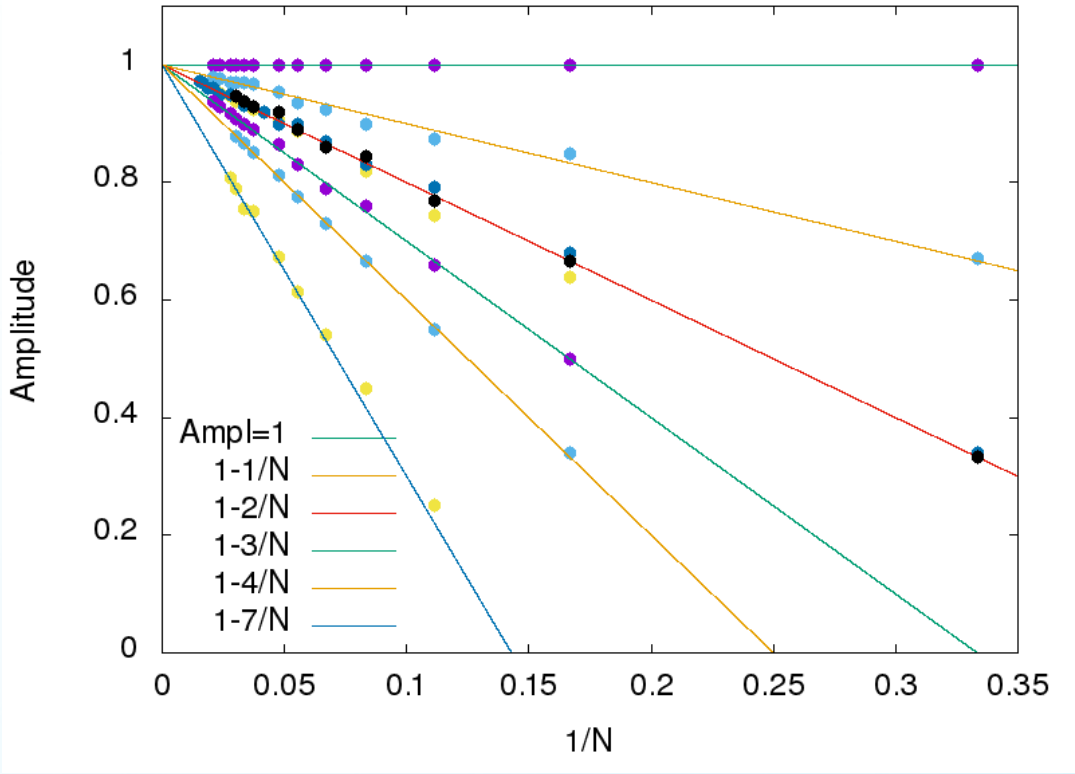
→ **Movie 1.** Typical movement of dislocations.

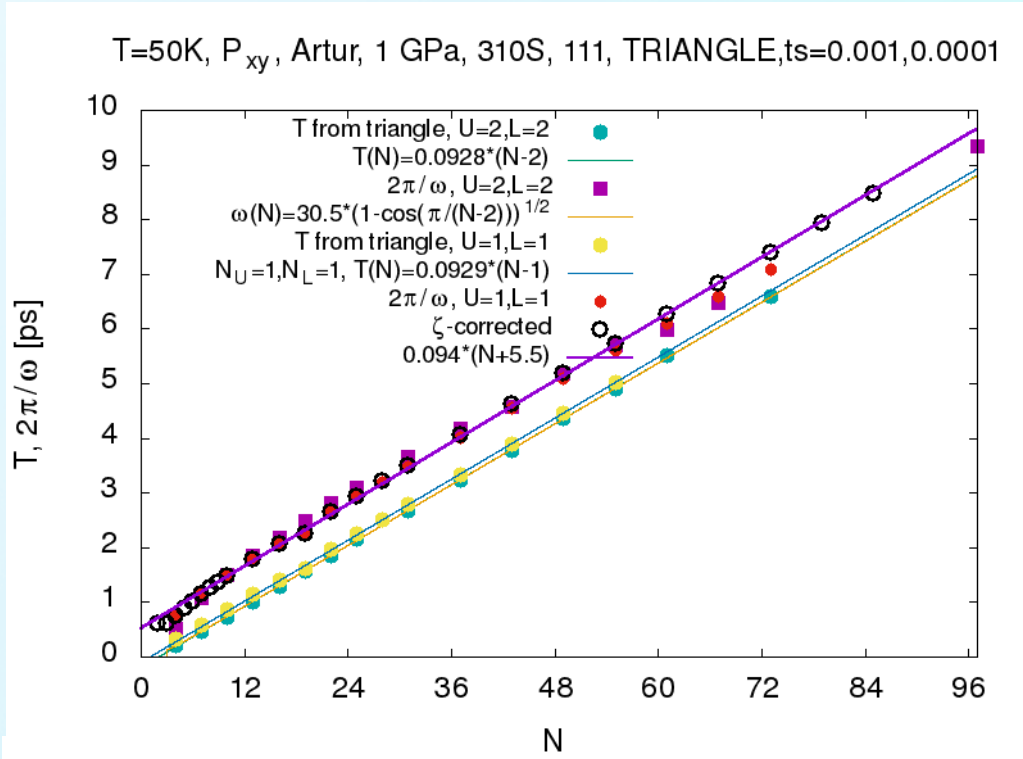
Importance of boundary conditions

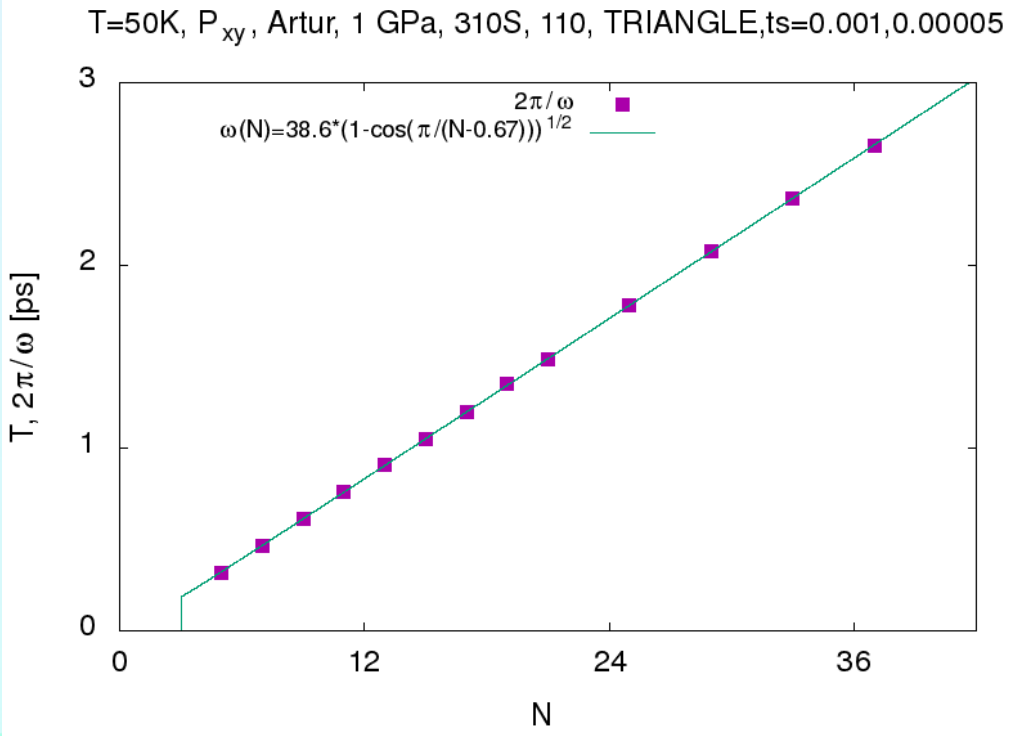




Why amplitude depends on time-step?







Properties of oscillations:

→ A=1-(U+L-2)/N

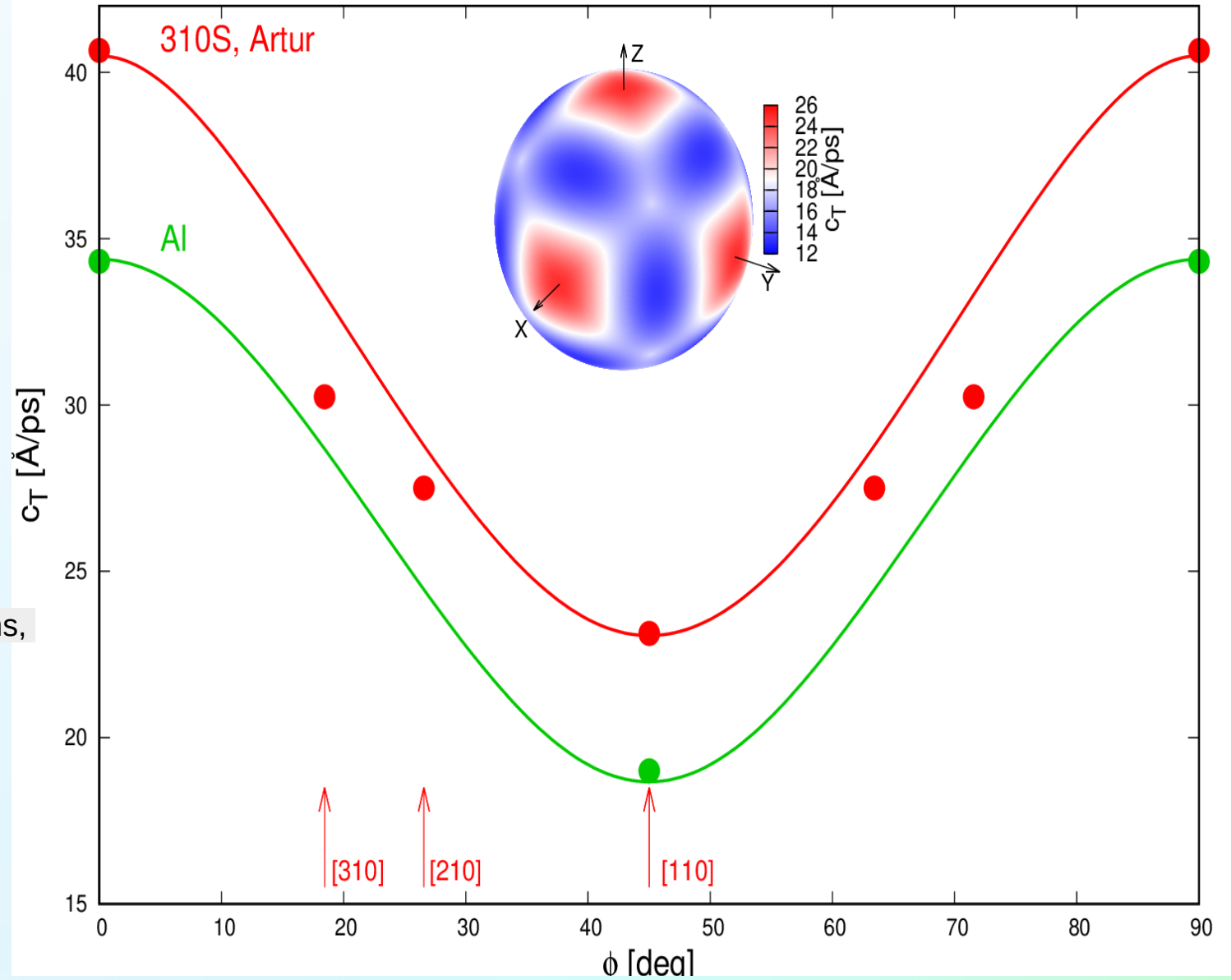
→ T proportional to N

→ dependence on direction

Hypothesis:

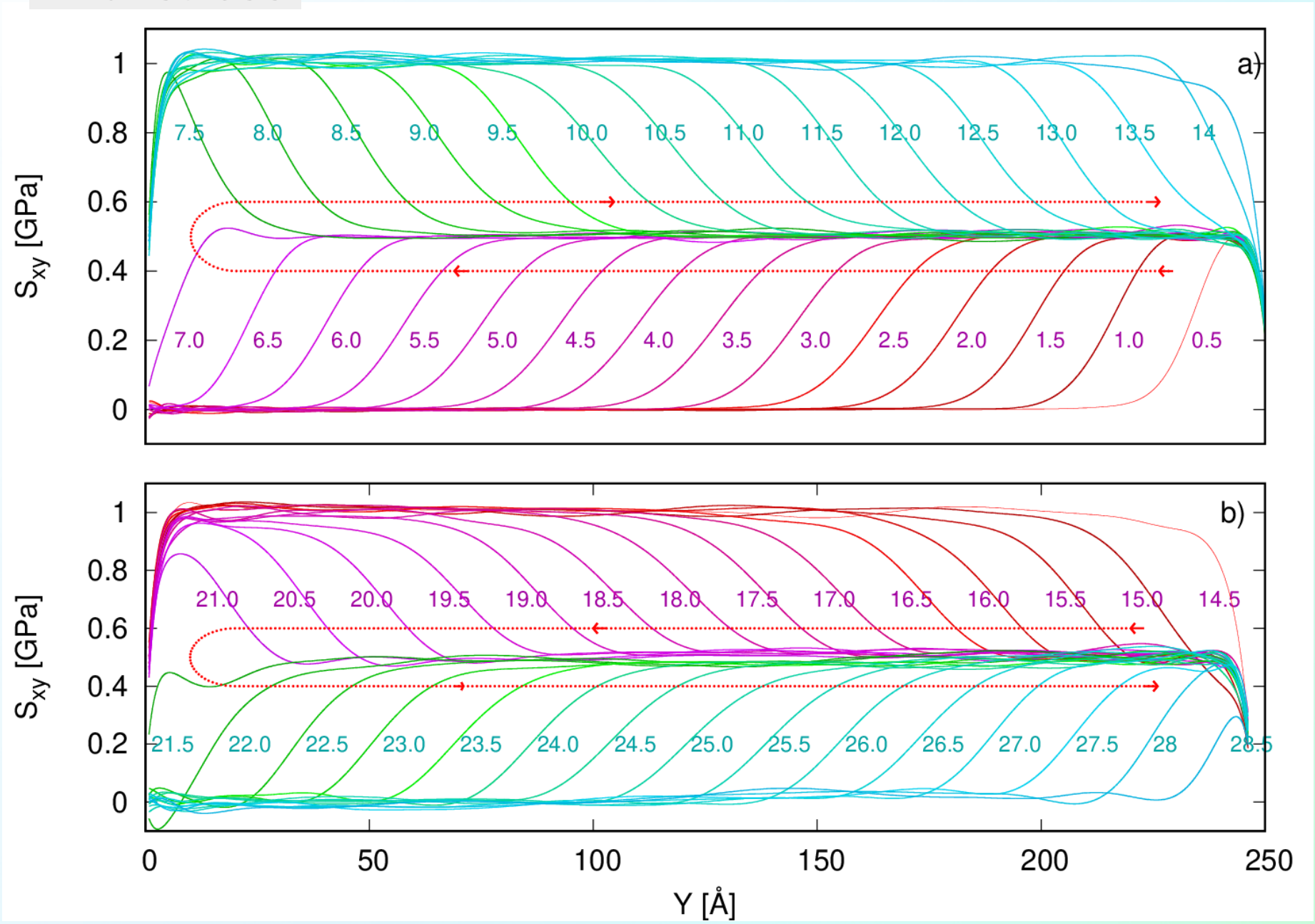
Period of oscillations T
is related to sample length
(N) and speed of sound.

Jan Jaeken,
Computer Physics Communications,
10.1016/j.cpc.2016.06.014



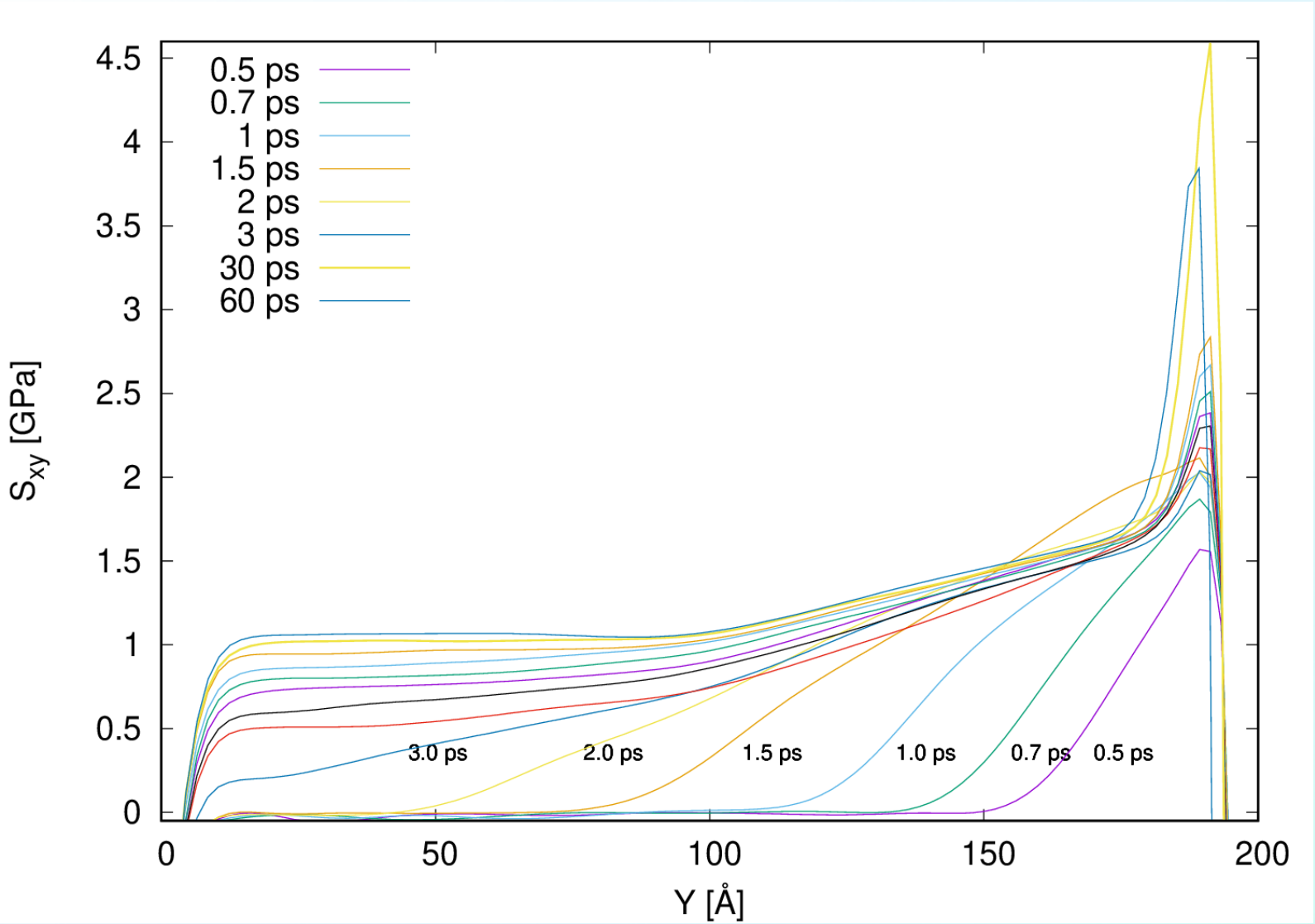
Lines and 3D plot of sound velocity by using Christoffel equation.
Red and green dots are our results for steel 310S and Al.

Virial stress.

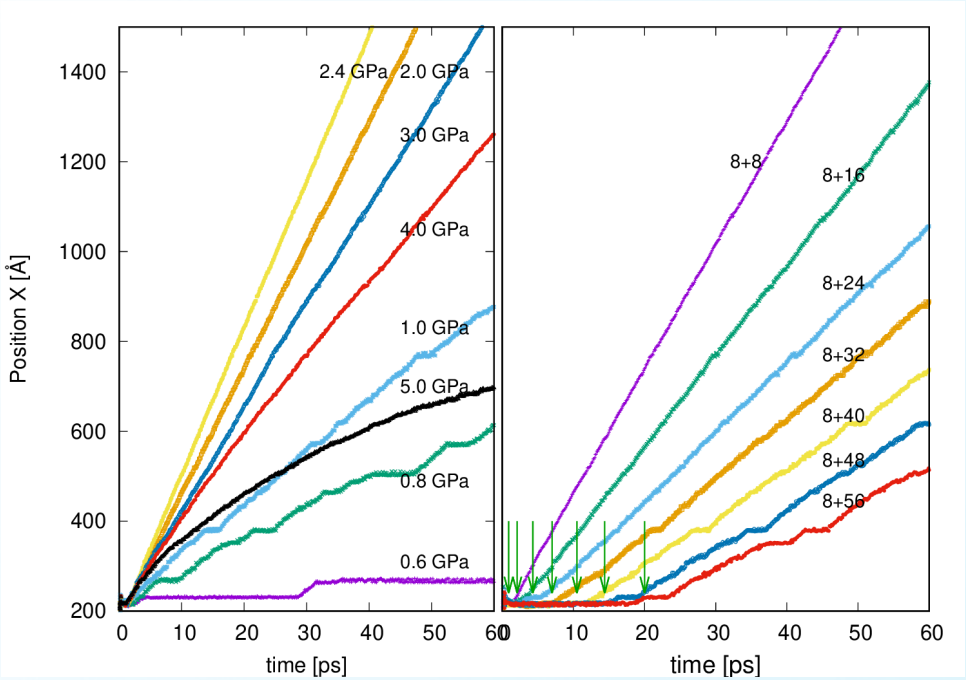


Evolution of virial stress profiles within the first period of oscillations.

→ **Movie 2.** Surface pressure and volume virial presure profiles. No dislocations inside.



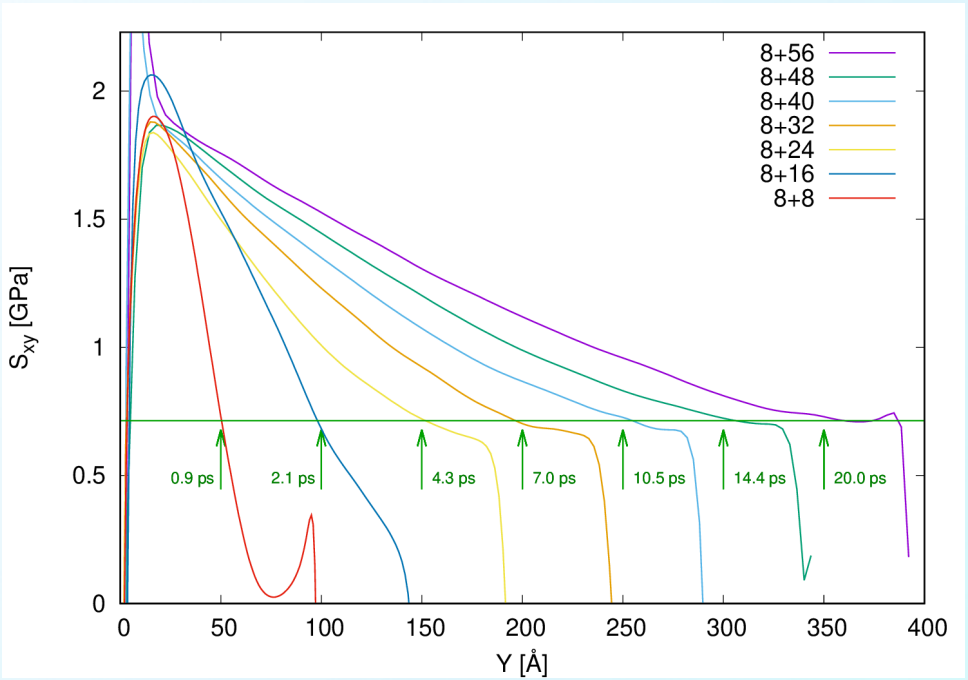
Volume virial presure profiles with dislocation in the center.



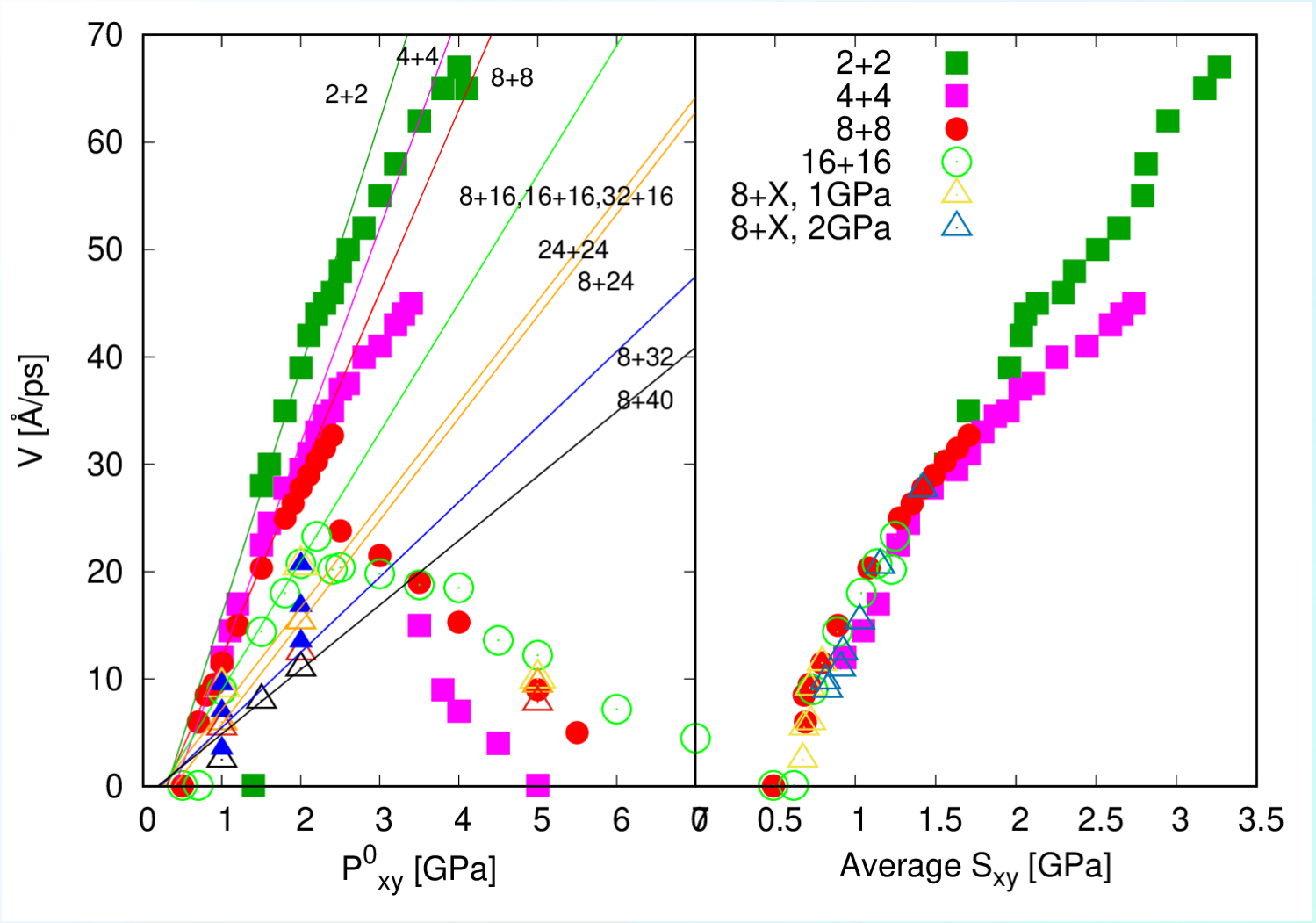
Dislocation displacement as a funcion of time.

On left: for several values of pressure.

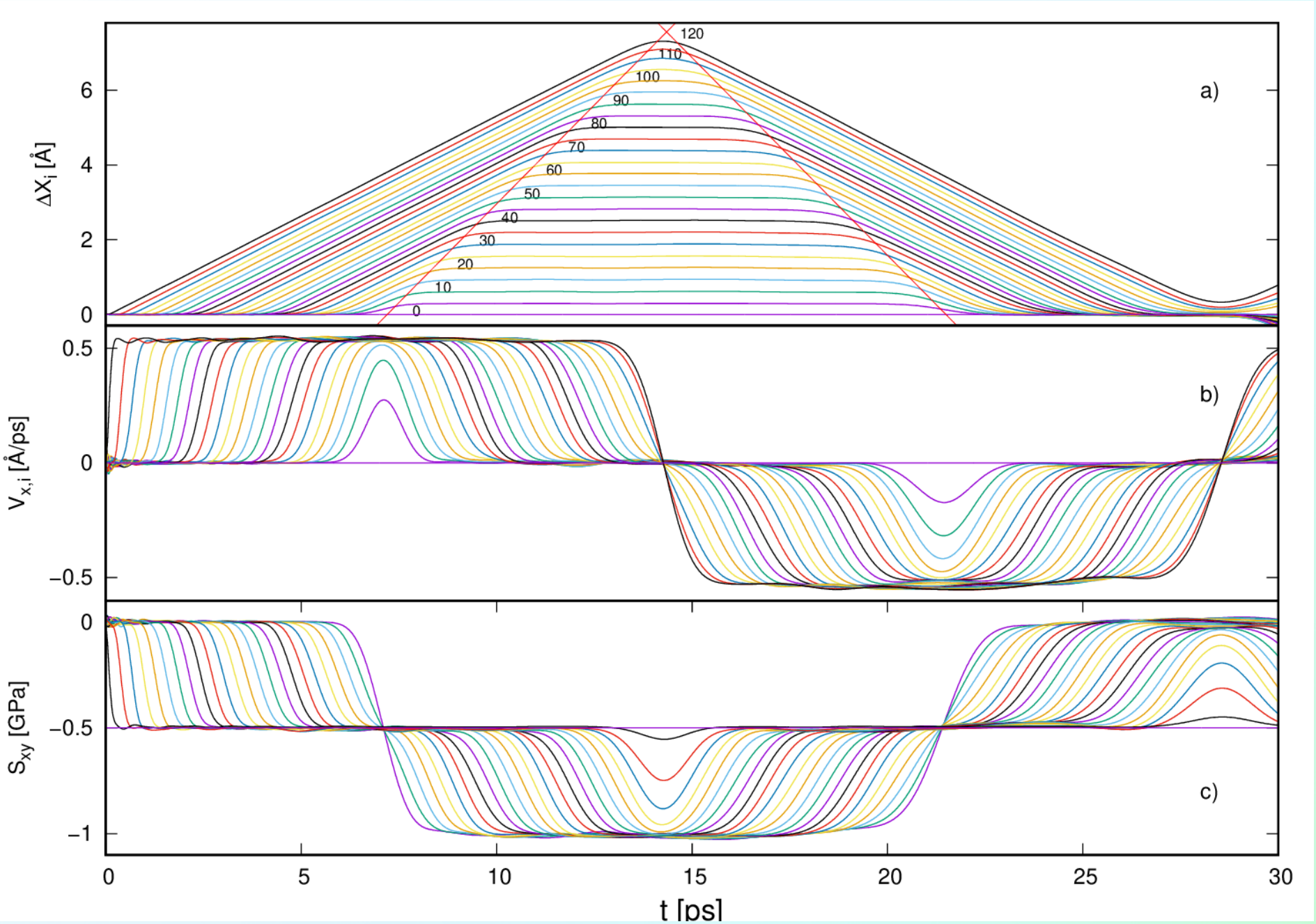
On right: for pressure 2 GPa for several sample sizes.



Virial stress profiles for several samples at time moments when dislocation starts moving.



Velocity of dislocations.
On the left scaling with applied pressure.
On the right scaling with average volume of virial pressure.

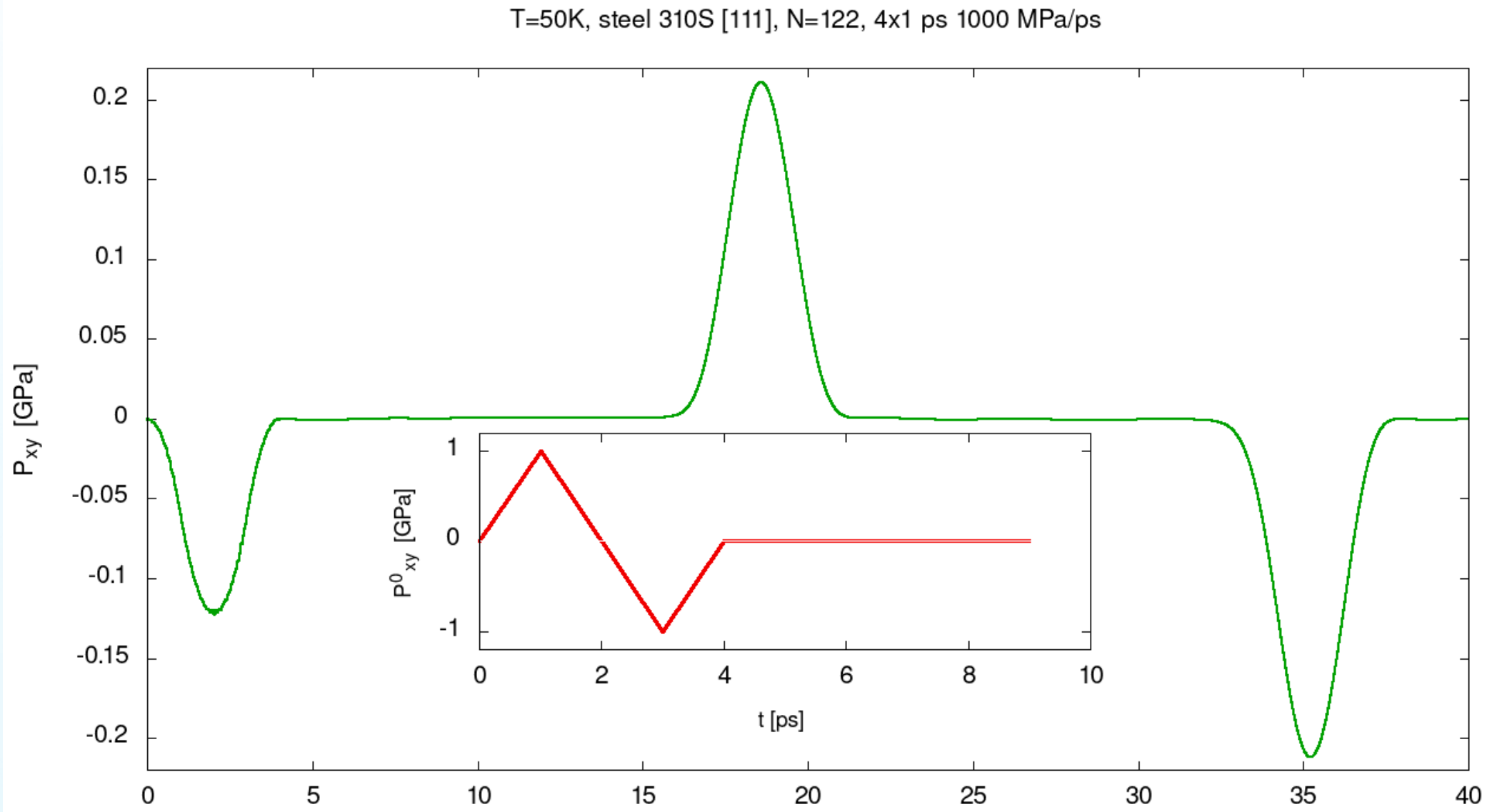


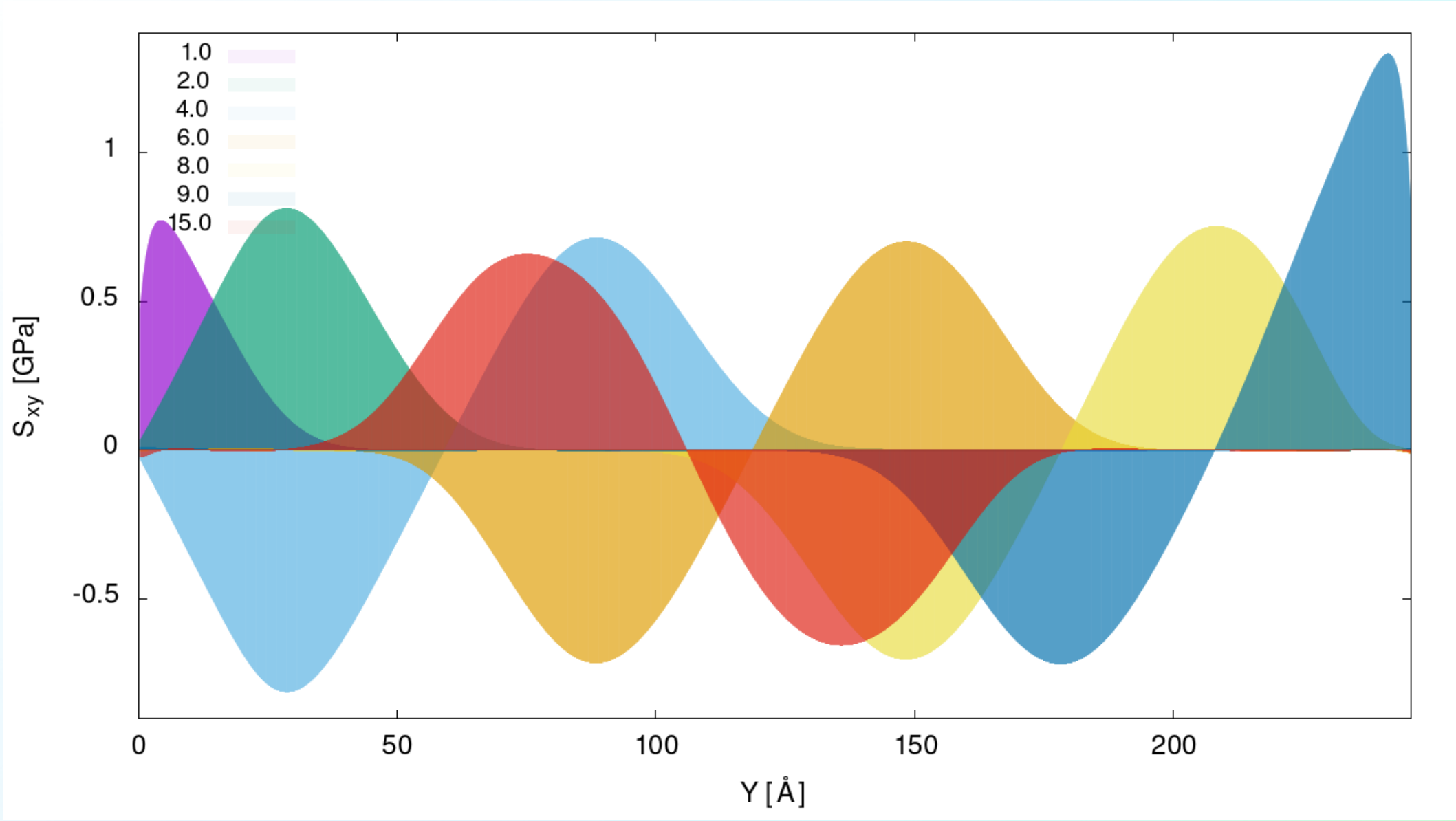
Average plane displacement, velocity, and virial stress as a function of time for crystallographic planes from bottom (0) to top (120) of Y.

Results shown so far are for an abrupt (Heavyside type) time dependence of external pressure.

Another often used method of modeling uses linear in time (ramp) pressure.

An interesting opportunities are in using solitary stress packets:




1.0
2.0
4.0
6.0
8.0
9.0
15.0
1
0.5
0
-0.5
S_{xy} [GPa]
0
50
100
150
200
Y [Å]

→ **Movie 3.** Dynamics of solitary stress packet.

More on this example:

Zbigniew Kozioł, *Size effects in stress propagation and dynamics of dislocations: Fe-Ni-Cr steel*, Modelling Simul. Mater. Sci. Eng., 2022, 10.1088/1361-651X/ac83de

+ another paper coming soon.

Advantages of LAMMPS:

→ well developed, continuously improved open source code (10 mln lines).
→ modular structure.
→ **compilation** and adding/changing features is within the range of abilities of users.
→ community support (mailing list, discussion fora).
→ interatomic potentials for hundreeds+ of compounts.
→ excellent documentation, broad range of examples, thousands of research papers.

Disadvanteges / problems:

→ more than minimum familiarity with Unix (Linux) is a must
→ well developed skills in working with and storing large amount of data (Terabytes), developed habits in documenting own procedures and results
→ while it is perfect for working on clusters, most of the time in case of any project is spent on testing, where cluster environment is usually not convenient for use; Therefore a modern desktop computer with efficient multi-core CPU is very desirable.
→ it is “only” for classical dynamics (though some methods allow to mimic quantum effects as well).
→ still a lot of interatomic potentials are missing or are too simplified.
→ steep learning curve, in particular initially. Gaining a broad and deep understanding of features would require years of intensive, practical using it.

Methodology

→ KISS rule.
→ Develop scripts and tools for simulations and data analysis and processing on principles of their independence of each other, “horizontally”, not “vertically”. This is the philosophy behind Unix.

Content of my toolbox

0. Working on Linux is a must. Open Source environment.
1. LAMMPS for MD simulations.
2. Atomsk for creating samples, voids, defects, dislocations.
3. LAMMPS and scripts in Perl/Python can be used for 2) as well.
4. Ovito for visualization of atomistic structures and data analysis.
5. Ovitos (Python) for data analysis.
6. Perl scripts for data analysis (Python is often used as well).
7. Gnuplot, Image Magick for graphing results.
8. Ovito, Image Magick, ffmpeg, gnuplot for creating movies.
9. Bash, grep, and all available Linux terminal environment for data manipulation.
10. ssh, tmate with scripts for remote connectivity; additional data server for data exchange desirable.

I am always interested in sharing my code and advise.

Thank you for your attention.