Dynamics of stress propagation in crystals: comparing molecular dynamics simulations and analytical models

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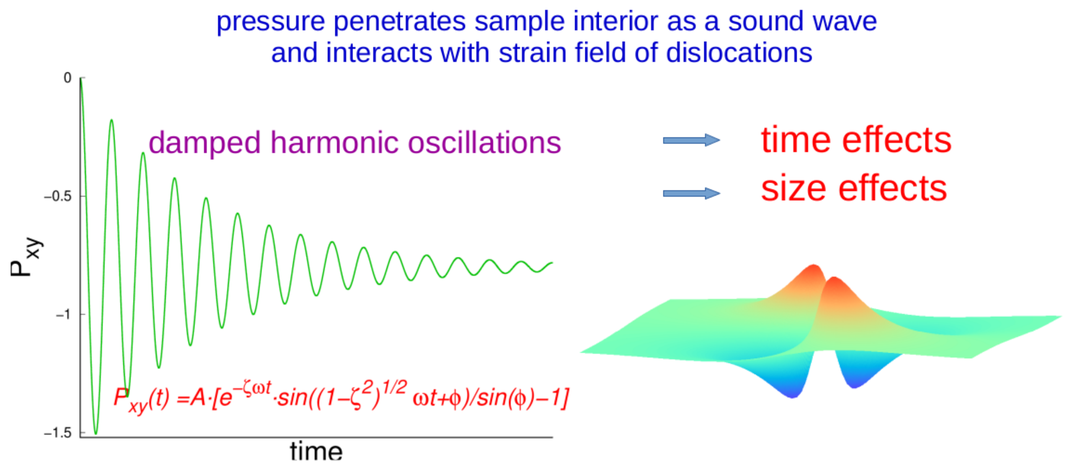
An overview



Simulations in molecular dynamics (MD) often are carried out in an applied pressure, as for instance in case of modeling the dynamics of dislocations in materials. In analysis of results a crucial role is played by the proper understanding of underlying process of pressure penetration itself, since this is a dynamic process occurring at the same time scales as the studied properties of material.

We use a combined approach to describe in details the phenomenon of pressure penetration: results of MD simulations performed on Steel 310S are guiding our analytical analysis based on a simple mechanical model of crystallographic lattice planes as a chain of masses undergoing oscillations described by equations of damped harmonic waves.

When external pressure is exerted on material surface, it penetrates it's interior with the speed of sound, and, depending on used boundary conditions, that wave may be reflected from the opposite side and interfere with the incoming wave. In case of ideal materials where energy losses can be neglected, the process is easy for description in mathematical therms. In real situations, adding energy damping leads to less straightforward picture that although qualitatively understood has not been so far discussed in details.

We show how the frequency of oscillating waves and damping process depend on intrinsic material properties, on crystallographic direction of sound propagation, and how the amplitude of waves depends on details of MD simulation procedure itself (size and geometry of sample, time step used, etc).

The worked out description is helpful in case of analysis of any MD simulations under pressure, as well it offers a convenient alternative way to already existing methods deriving elastic properties of materials from MD simulations.

Molecular dynamics results.

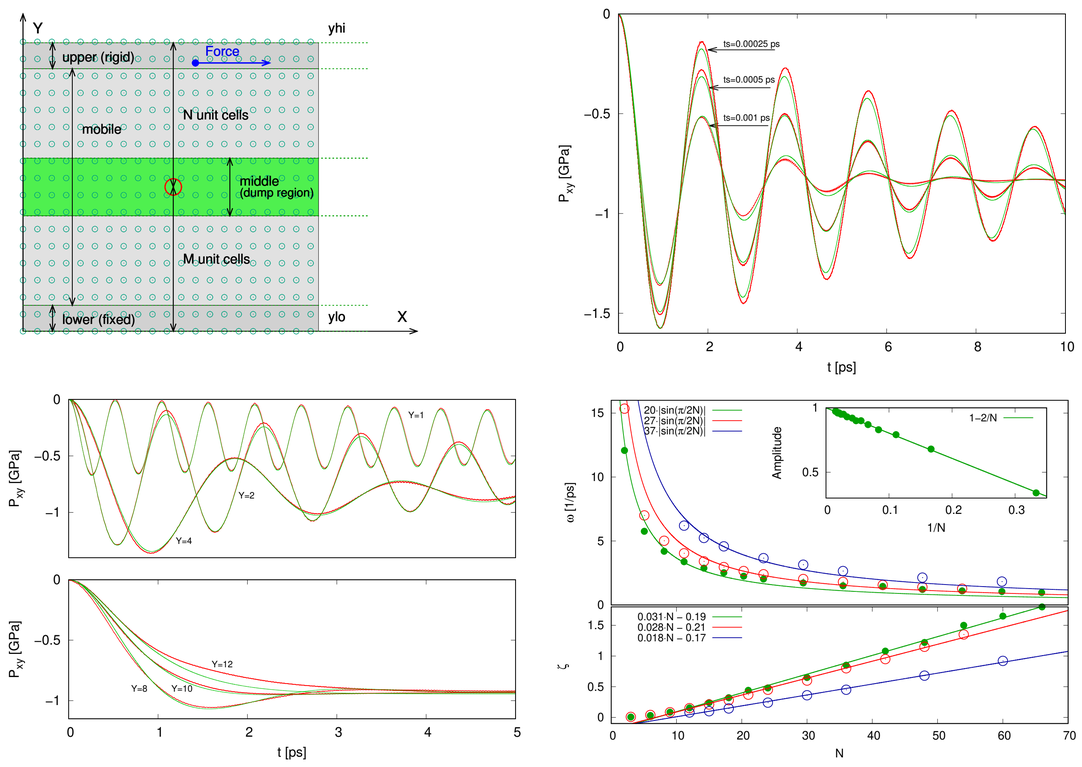


Figure 1. Sample crossection in X-Y directions for modeling dynamics of dislocations (not to scale).Open circles symbolize atoms arranged in X-Z layers: there are two layers in this case in **upper** and two in **lower** regions.

Figure 2. Shear pressure P_{xy} as a function of time reported by LAMMPS at the upper surface of sample of size Y=4 (4 unit cells). Three pairs of curves are shown for 3 values of time-step used in LAMMPS, as shown in the figure. Red data points are results of MD simulation while green curves are computed with Eq. 1. The applied pressure at the surface, $P^0_{\rm xy}$, is 1 GPa.

Figure 3. $P_{\rm xy}(t)$ dependencies, similar to these in figure 2, for samples of sizes from Y=1 to Y=12, when the same time-step is used in MD simulations, $ts = 0.001$ ps. Red data points are results of MD simulation while green curves are computed with Eqs 1 or 2. The applied pressure at the surface, $P^0_{\rm xy}$, is 1 GPa. In case of curves at the figure (b) the damping parameter ζ approaches (Y=8) and exceeds the critical damping ratio ($\zeta = 1$). The curve for Y=12 is in overdamped regime. In this case we see that green lines, as computed by Eq. 2 start to depart from MD simulation results. That difference increases when ζ grows more above 1.

Figure 4. Dependencies of ω, ζ and amplitude of oscillations A used in equations Eq. 1 and 2 on number of atomic layers in Y-direction, N, as deduced from analysis of MD simulations. The data points in green (full circles and curves) are obtained for simulations using Artur potential, while these in red and blue for Bonny potential. Data points and curves in blue are for direction $[11\bar{2}]$ while all other for Y in direction $[111]$.

$$P_{\rm xy}(t) = A \cdot \left[{\rm e}^{-\zeta\omega {\rm t}} \sin\left(\sqrt{1-\zeta^2}\omega {\rm t} + \varphi \right) / \sin(\varphi) - 1 \right], \quad \zeta < 1 \tag{1}$$

$$P_{xy}(t) = A \cdot \left[{\rm e}^{-\zeta\omega {\rm t}} \sinh\left(\sqrt{\zeta^2-1}\omega {\rm t} + \varphi \right) / \sinh(\varphi) - 1 \right], \quad \zeta > 1 \tag{2}$$

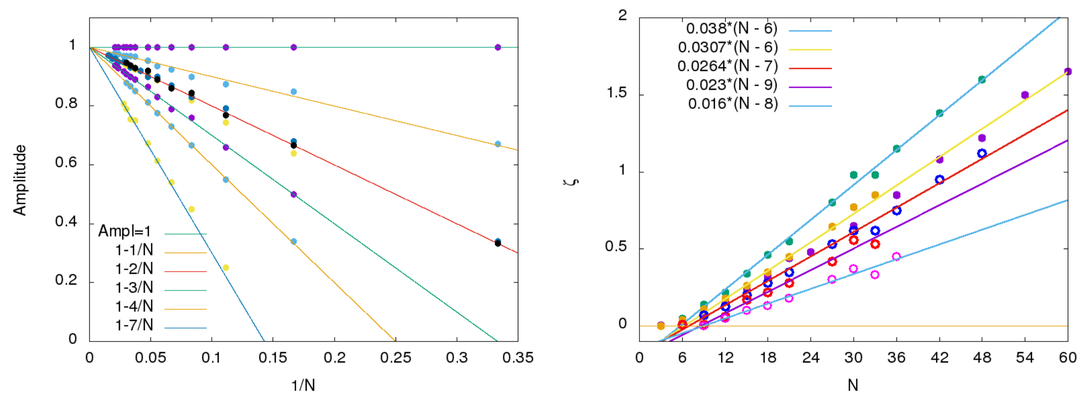


Figure 5. Amplitude of oscillations depends as $1 - Q/N$, where $Q = N_U + N_L - 2$, N_U and N_L are number of layers in regions upper and lower, respectively.

Figure 6. Damping factor ζ has a linear dependence on N and it depends also on N_U and N_L, the number of layers in regions upper and lower.

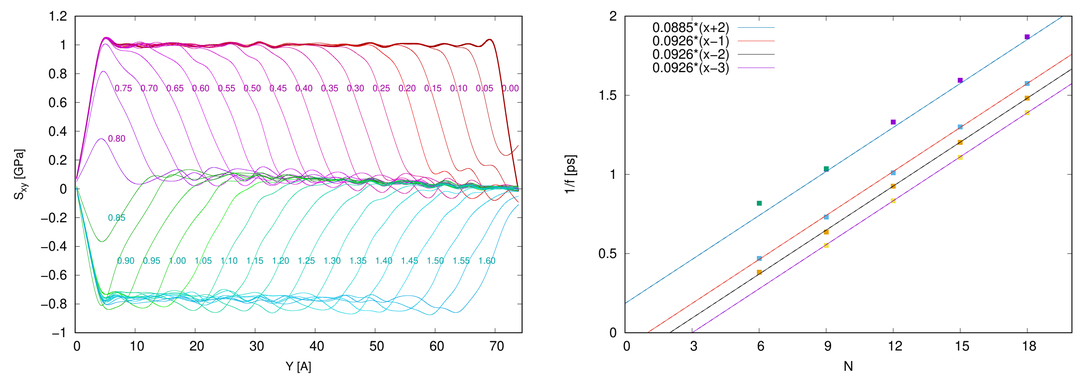


Figure 7. After pressure has been applied for a long time, it is removed at t=0. That results in traveling pressure wave, oscillating and decaying with time, as shown by the sequence of profiles of virial pressure component S_{xy}.

Figure 8. Period of oscillation of pressure P_{xy} at the surface, in cases like that in Fig. 7, depends linearly on sample size and it depends also on number of layers in **lower** and **upper** regions (Fig. 1).

Mathematical model: a chain of masses and springs.

Damped oscillator motion equation.

$$\ddot{x} + 2\zeta_0\Omega\dot{x} + \Omega^2 x = 0, \quad \Omega = \sqrt{\frac{\lambda}{m}}, \quad \zeta_0 = \frac{\kappa}{2\sqrt{m\lambda}}. \tag{3}$$

A chain of masses and springs

$$\ddot{x}_n + 2\zeta_0\Omega\dot{x}_n + 2\Omega^2 x_n - \Omega^2 x_{n+1} - \Omega^2 x_{n-1} = 0, \tag{4}$$

Traveling wave solution.

$$x_n = A \cdot exp(ikna - i\omega t) \quad \rightarrow \quad \omega^2 + 2i\zeta_0\Omega\omega - 4\Omega^2 \sin^2\left(\frac{ka}{2}\right) = 0. \tag{5}$$

$$\text{where :} \quad \omega_0 = 2\sin({\rm k_1 a}/2) \cdot \Omega, \quad \zeta = \zeta_0/(2\sin({\rm k_1 a}/2)), \quad {\rm k_1} = \pi/{\rm Na}. \tag{6}$$

$$x_n(t) = \exp(-\zeta\omega_0 t) \cdot \left(\sin(kna - \sqrt{1-\zeta^2}\omega_0 t + \varphi)/sin(\varphi) - 1 \right). \tag{7}$$

Summary and Conclusion

1. The mathematical model of chain of masses and springs explains relation of $\omega(N)$ and $\zeta(N)$.
2. For explanation of $A(N)$, a tri-diagonal matrix approach is needed.
3. The model describes very well the penetration in time of stress field in sample volume, in an agreement with MD results **(please request movie presentations)**.

References

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