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Simulation of current-activated pressure-assisted densification

UNIVERSITÄT
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Offen im Denken

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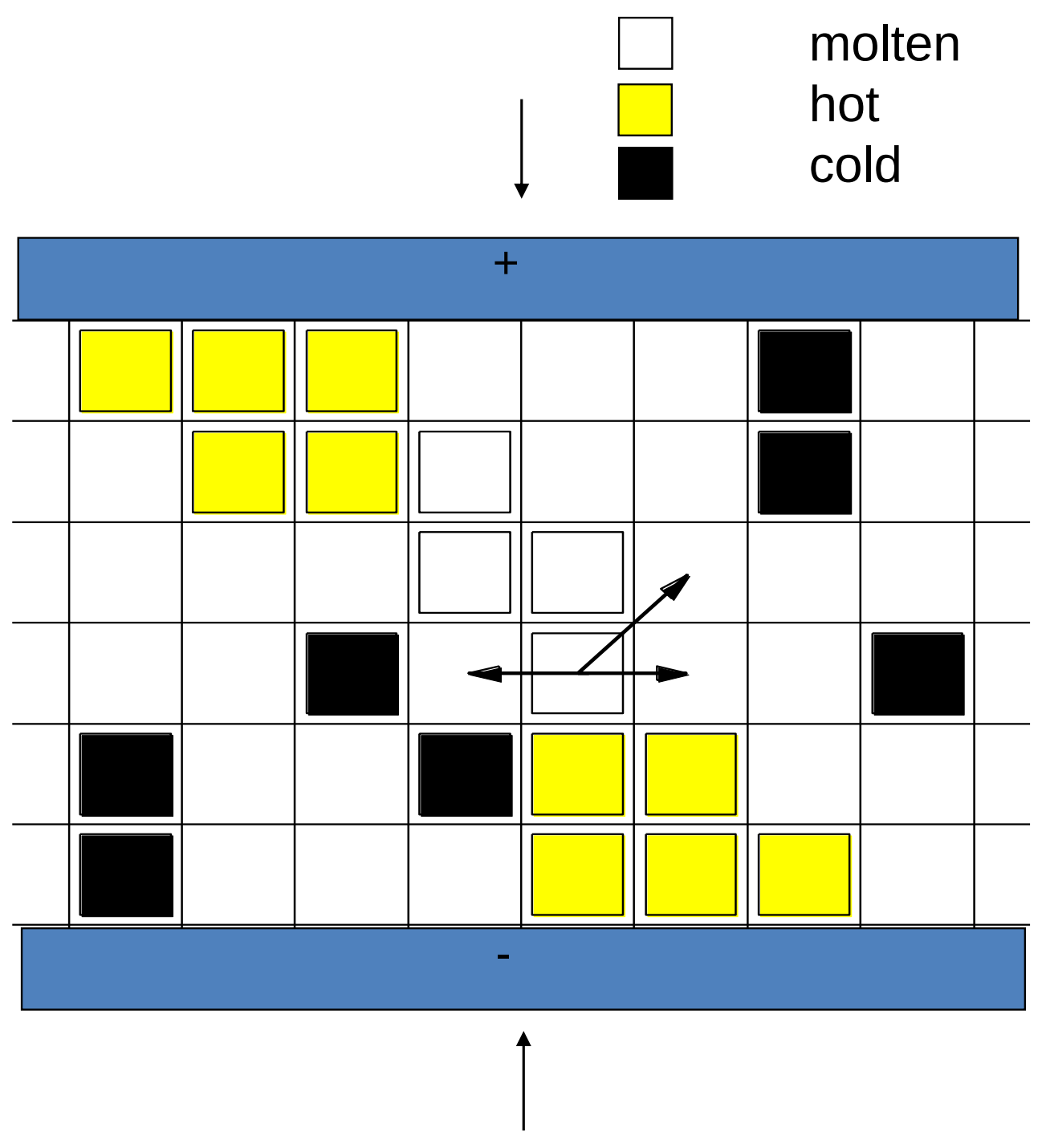
Introduction

Current-activated pressure-assisted densification (CAPAD) leads to a rapid consolidation, while maintaining the grain size. Particles or their surfaces melt due to locally deposited Joule heat which lowers the consolidation pressure.
Two models: A) kinetic lattice model, B) dynamic off-lattice model.

A) Resistor network model

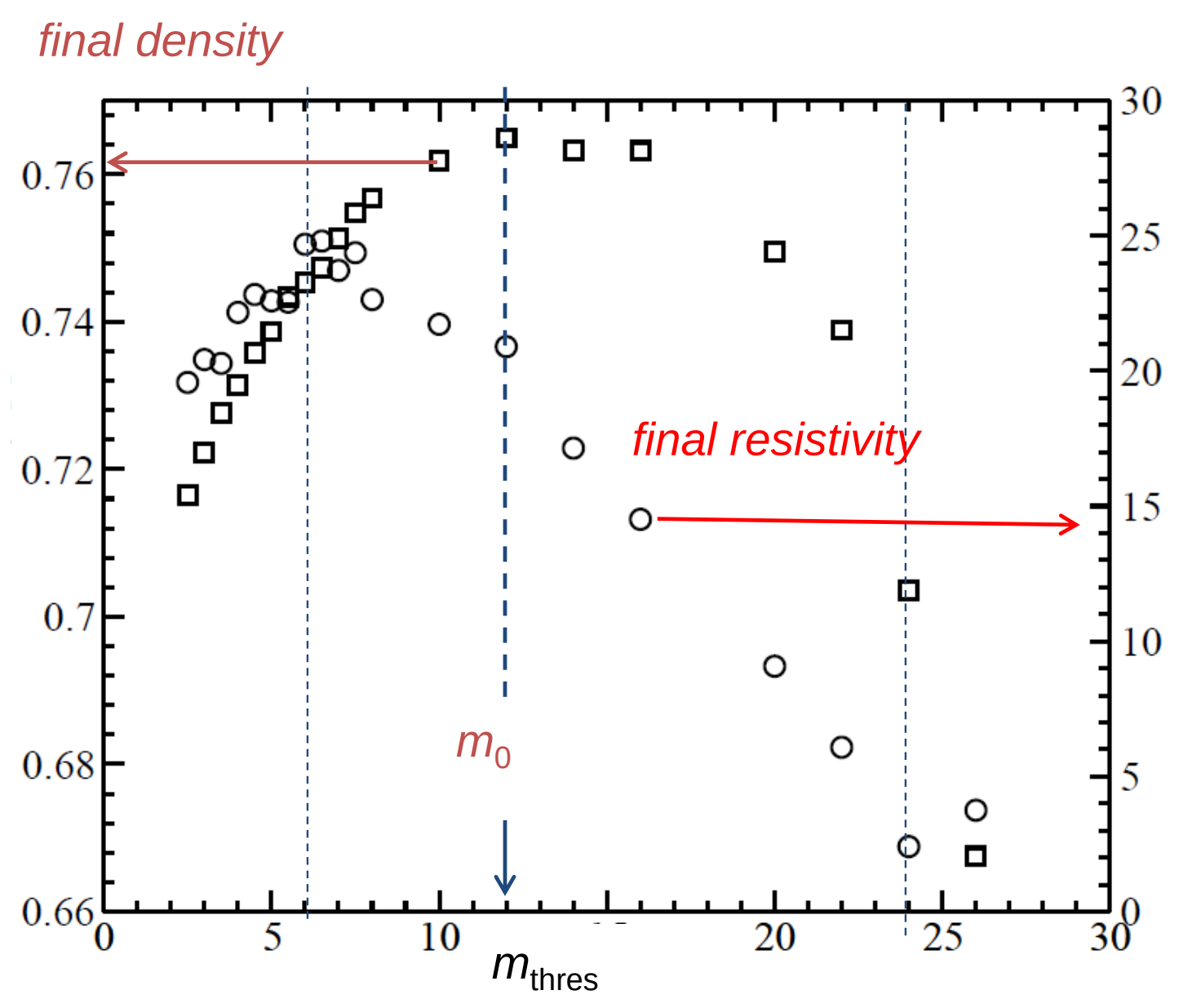


- Sites of a two-dimensional square lattice are occupied by randomly distributed particles, such that a percolatiting cluster between two electrodes forms. Neighboring particles are connected by an resistor. Giving the total current between the electrodes, the current between two particles can be calculated. and the Joule heat produced at a contact is delivered in equal parts to both sides: $\Delta Q_i = \frac{1}{2}\sum_j RI_{ij}^2$

- Particles melt if $\Delta Q_i > mQ_{avg}$ with average Joule heating Q_{avg} . Molten particels are moved randomly into neighboring voids. If the percolation is interrupted, the upper electrode and all particles connected to it are moved downwards until a percolating cluster is re-established.

Final states: Resistance and density

Unexpected correlations



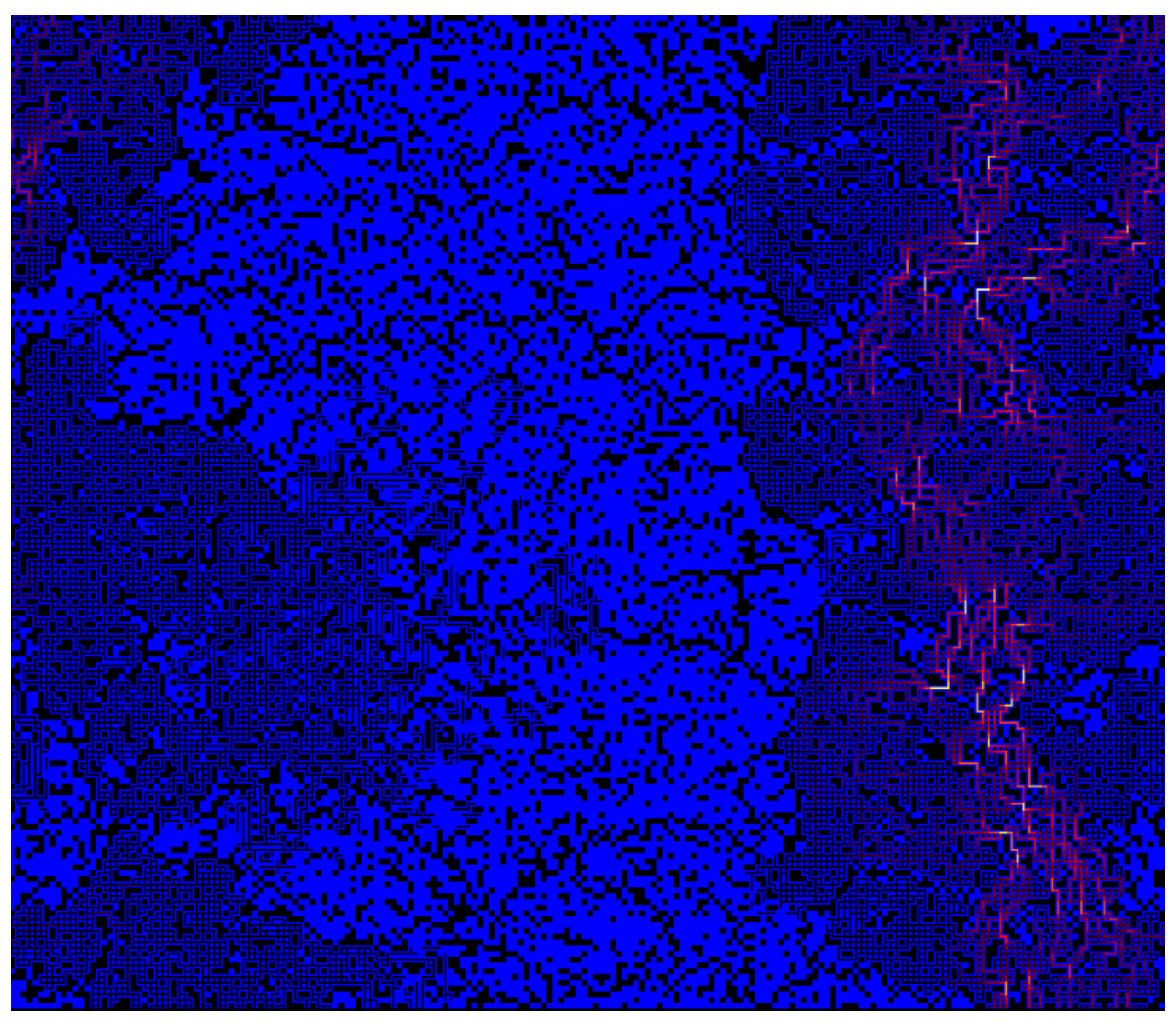
- The density increases and the resistance of the sample decreases with time until the melting threshold is not exceeded anymore.

- The final density and the final resistivity vary in a non-monotonic and correlated way with *m*.

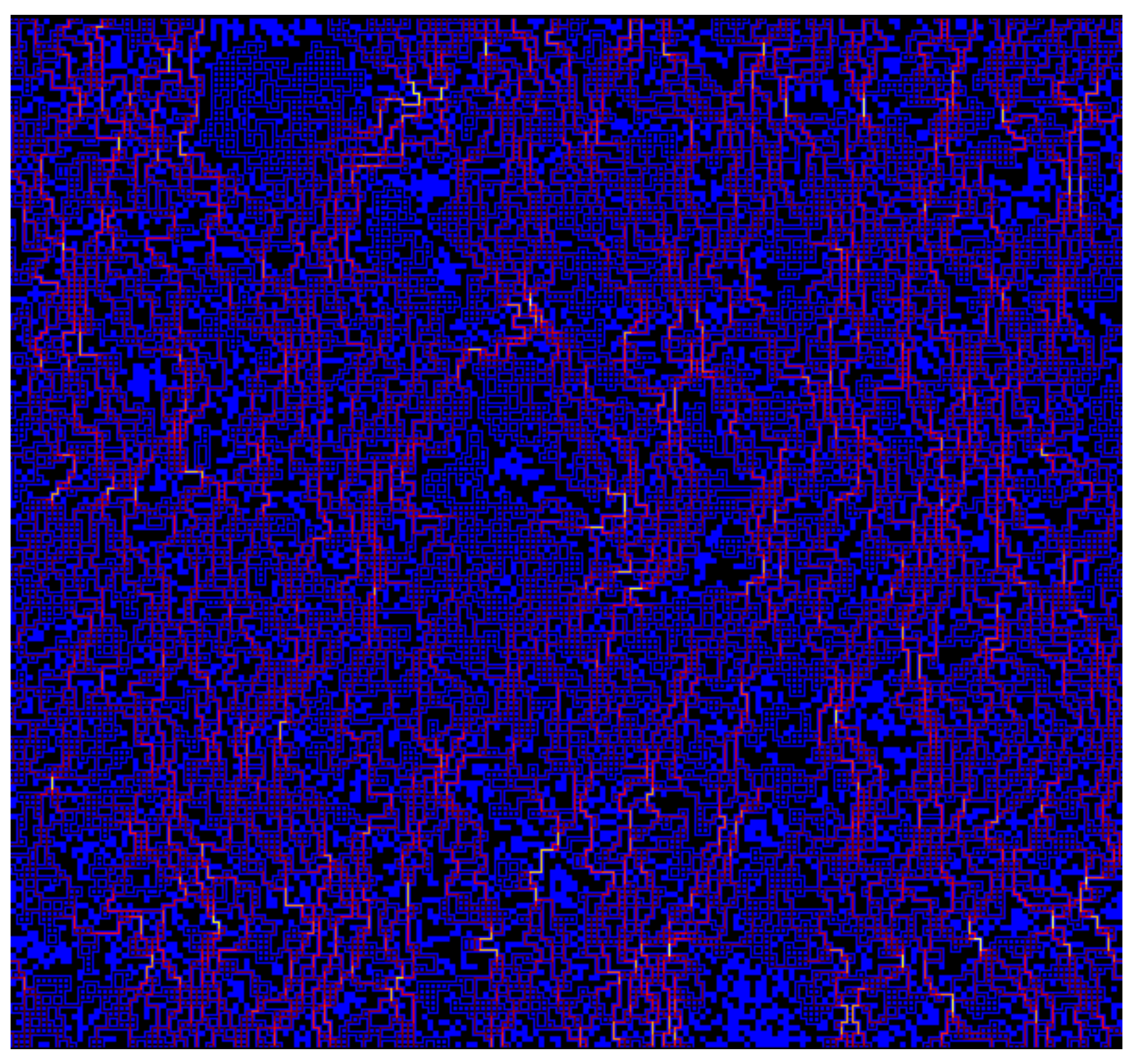
- For high *m* (low sample temperature) the process evolves via transient hot spots at low density cross sections. For small *m* (sample temperature close to melting temperature), whole conducting pathes melt and fluctuate sidewises.

- Compaction is accompanied by a cross-sectional depletion, i.e. by large pores parallel to the electrodes. Optimizing the density increases the final resistivity of the sample.

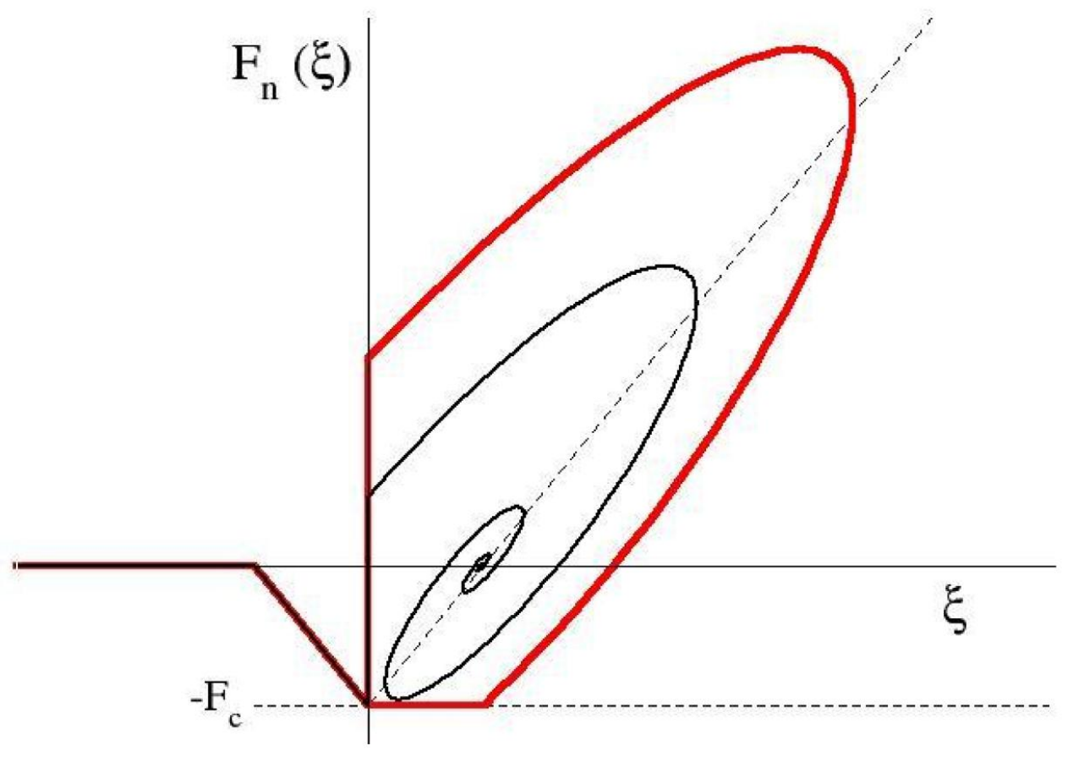
$m = 12$



$m = 24$



B) Molecular dynamics simulation & resistor network



- Particle trajectories are calculated with molecular dynamics using a spring dashpot model with cohesion, Coulomb fricti and rolling friction.

- Overlapping particles form the resistor network, including electrical and thermal resistance. Besides the electrical potential, the temperature is a dynamical variable.

- The electrical potential is recalculated each time the percolating cluster changes.

- The temperature evolves in time like $\dot{T}_i = \frac{1}{C}\sum_j \lambda\left(T_i - T_j\right) + \frac{1}{2}RI_{ij}^2$

- As initial configurations ballistic deposits are used.

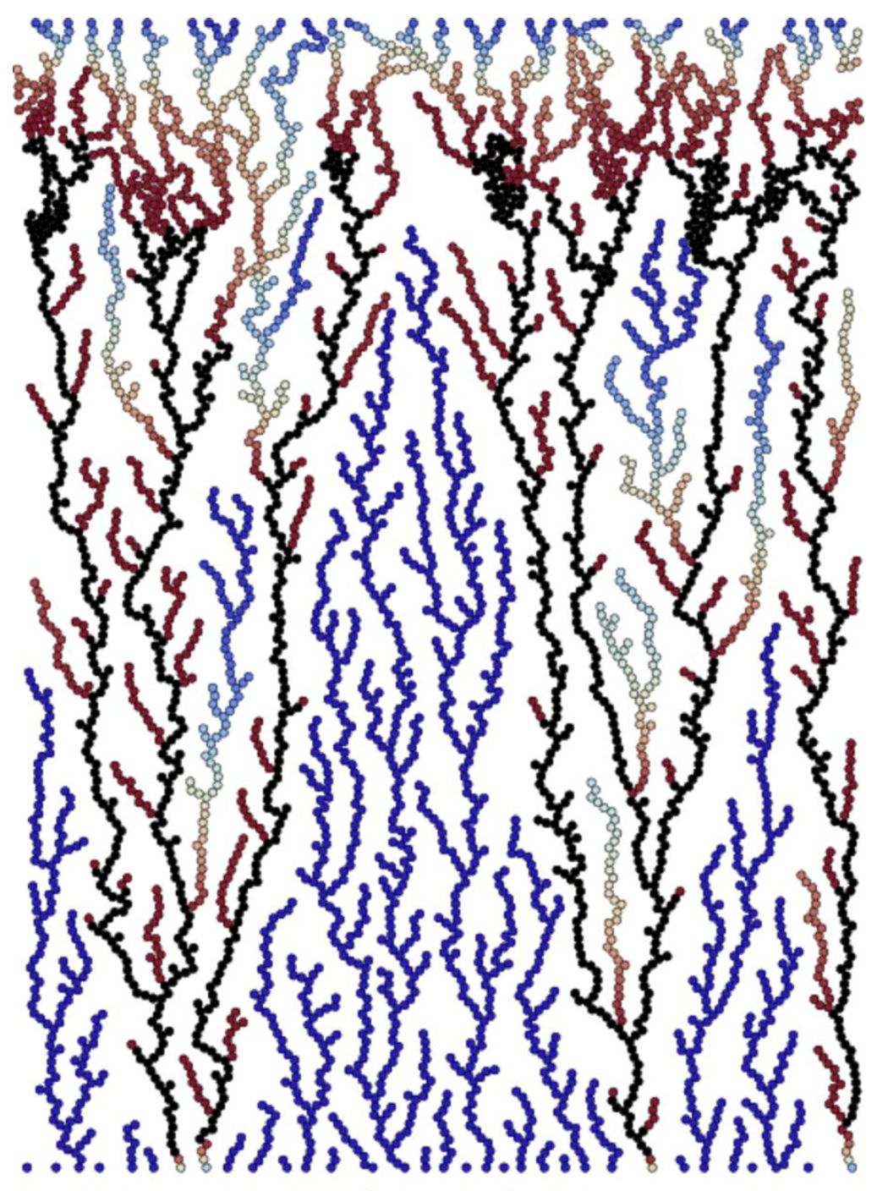
- The upper electrode is drive by the pressure σ_y while the lower electrode is fixed. The temperature of the electrodes is kept constant.

Time evolution

Time scales

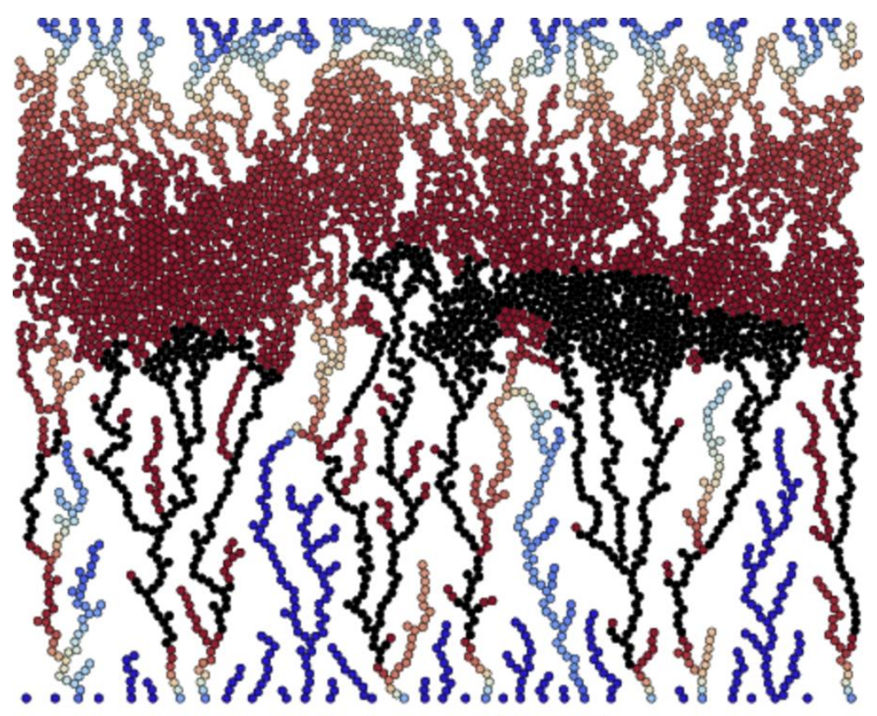
collision time $t_c = \sqrt{m^*/K}$, thermal time $t_{th} = C/\Lambda$, heating time $t_{he} = CT_mG/I^2$

Particle configurations and temperature distribution

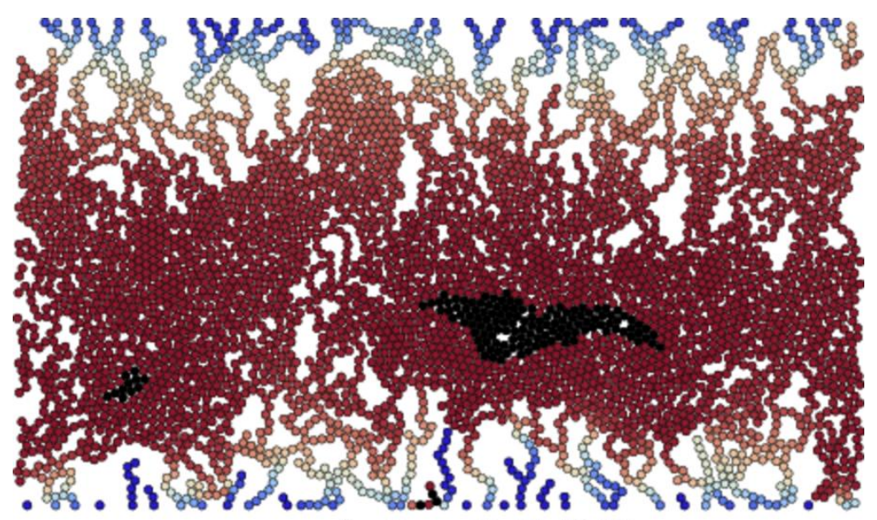


a) t=394

At first molten particles (black) are found in current bottlenecks (a). A self-regulating mechanism inhibits sufficient dense regions from melting, due to high electrical and thermal conductance the little Joule heat produced flows off quickly to the upper electrode.

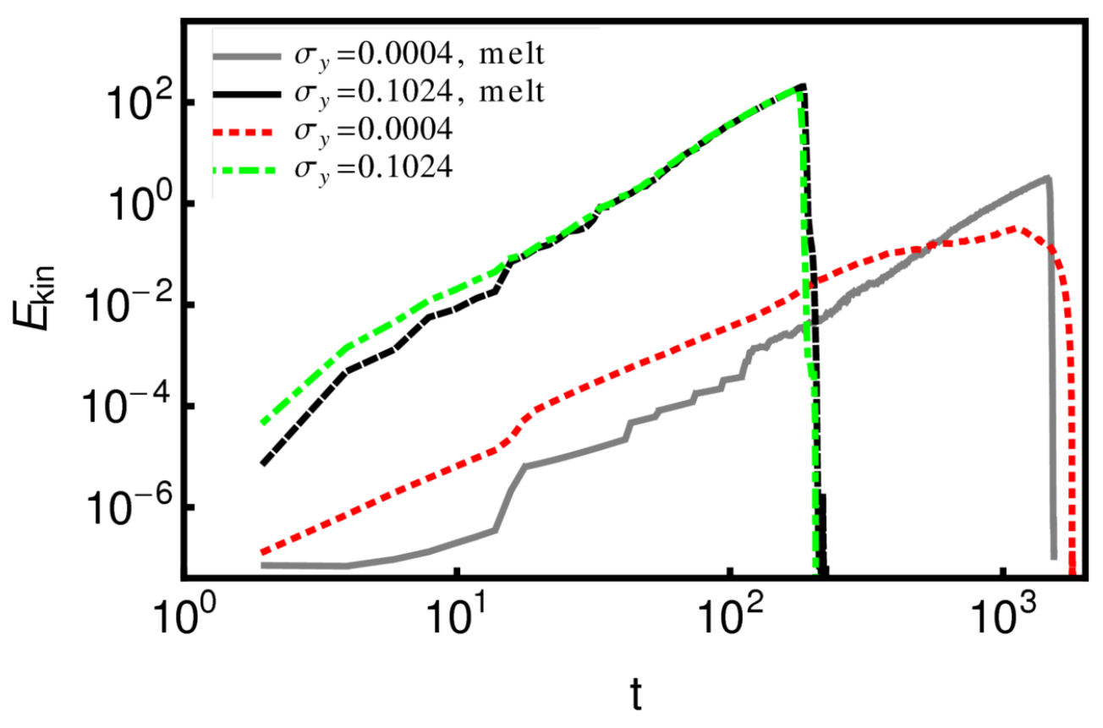


b) t=944



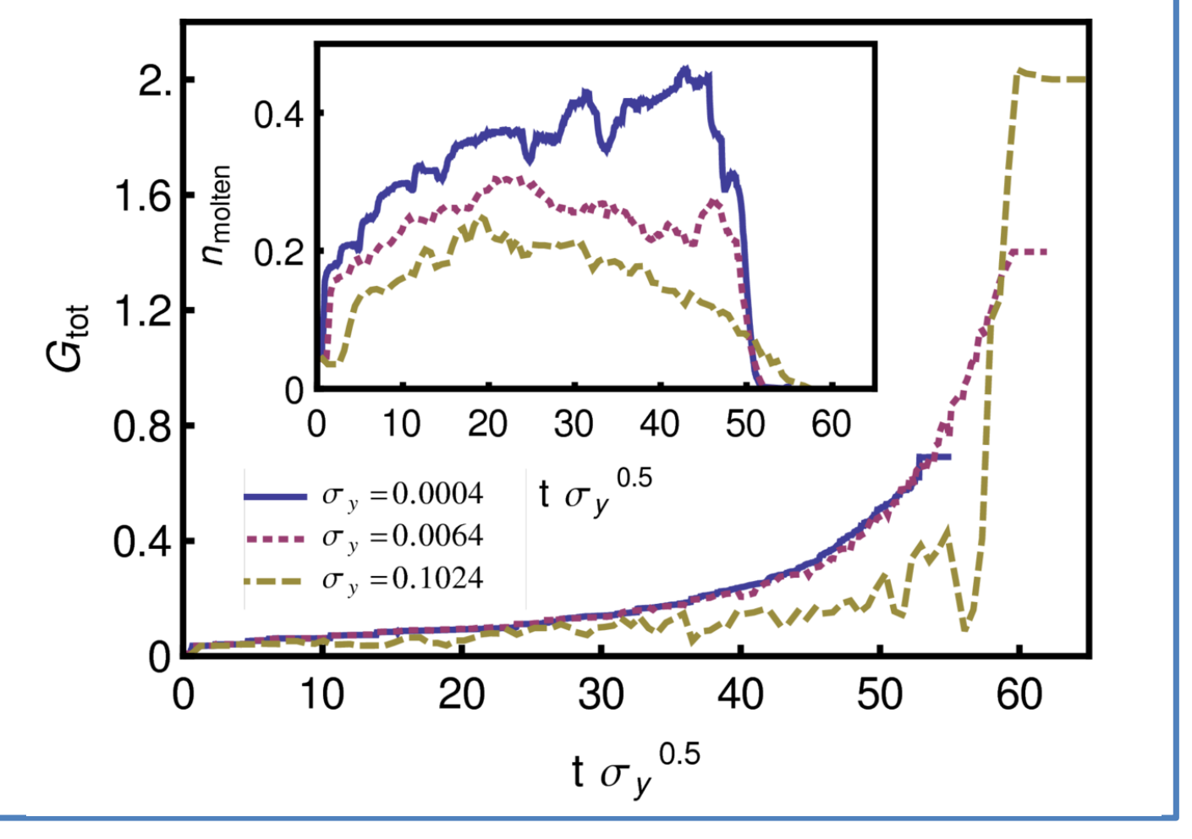
c) t=1122

Kinetic energy, total conductance and molten particles



- A smooth time-dependence for a normal pressure-driven densification (ND) is found, while a stepwise increase characterizes CAPAD. Each step can be identified with the sliding of a huge particle branch.

- At the beginning just a few particles close to the piston are accelerated resulting in a reduced kinetic energy.



- Applying a high pressure, a shock compaction occurs and a significant increase of the total conductance is observed, when the compaction front reaches the lower electrode.

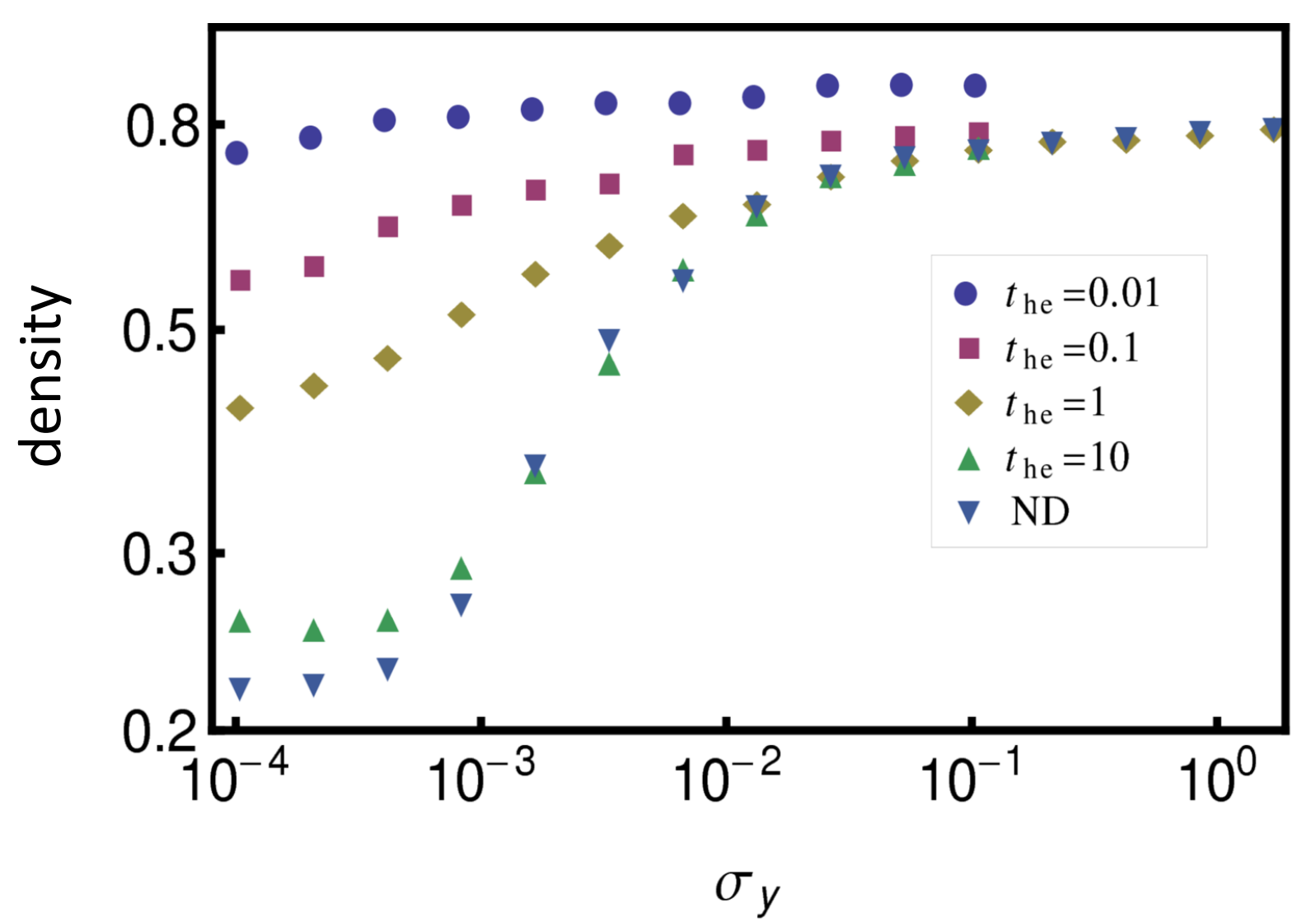
- The number of molten particles increases with time, but drops, when the conductance becomes large.

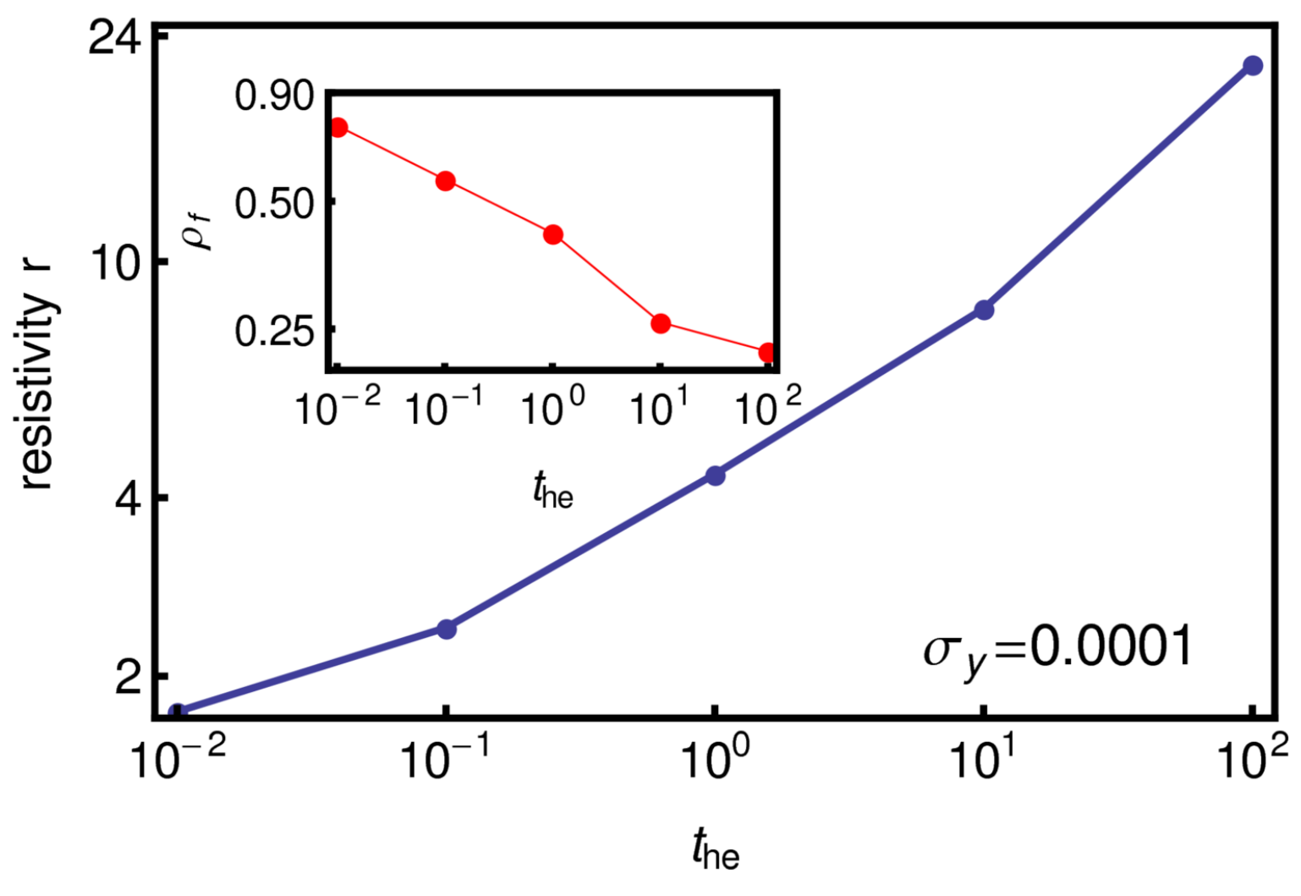
Final states: Resistance and density

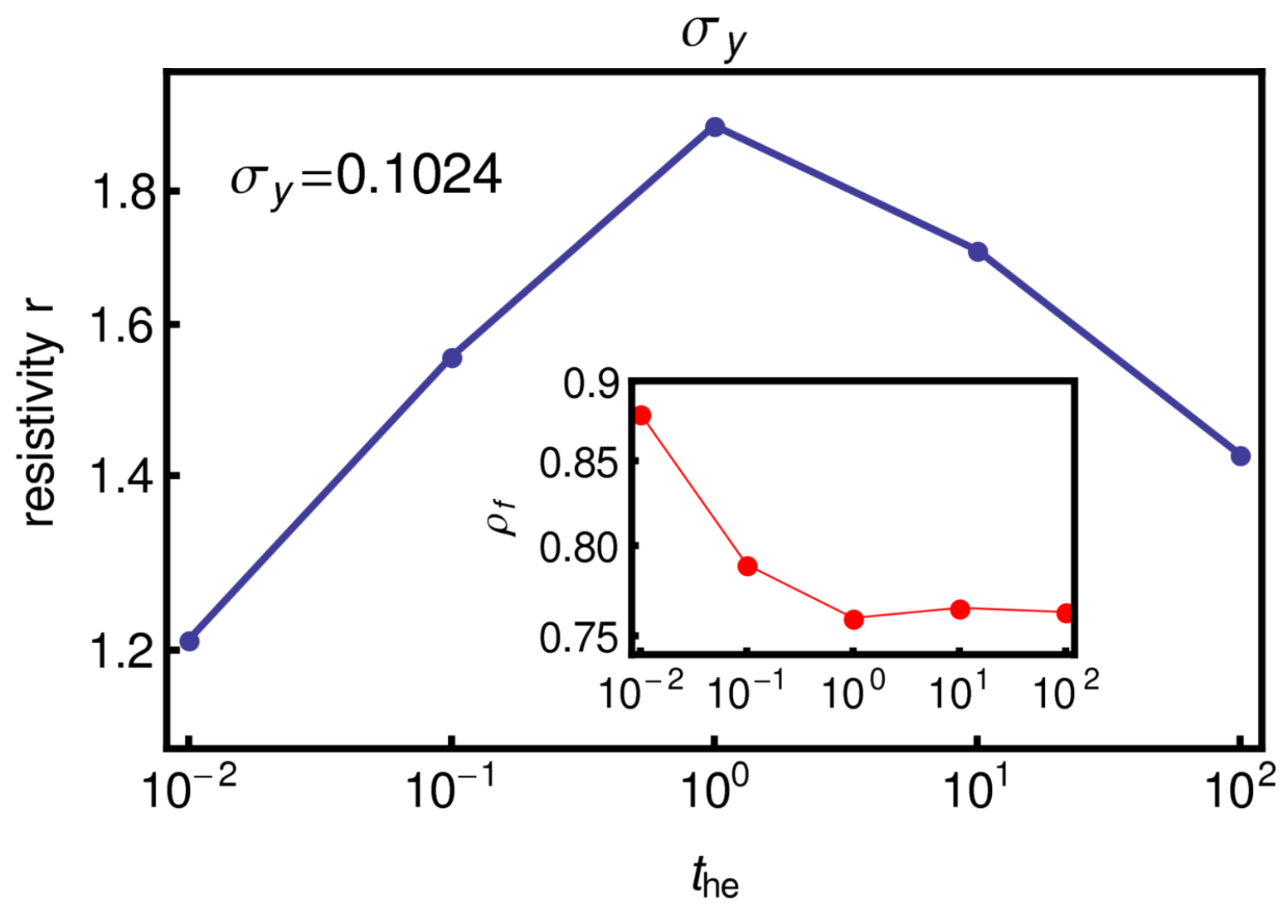
- The final porosity strongly depends on the heating time.

- For large heating times and high pressures CAPAD does not differ from ND, as far as the density is concerned.

- For small pressure and small heating times, Joule heating affects densification. In contrast to the lattice model, density and resistivity are anticorrelated.







References

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