

In: D. E. Wolf, P. Grassberger (Eds.) “Friction, Arching, Contact Dynamics”
World Scientific (Singapore, 1997) p. 265-273

Force Distribution and Comminution in Ball Mills

Volkhard Buchholtz and Thorsten Pöschel

Institut für Physik, Humboldt-Universität zu Berlin, Invalidenstr. 110, 10115 Berlin
email: volkhardsumma.physik.hu-berlin.de, thorstenip02.physik.hu-berlin.de

The motion of granular material in a ball mill is investigated using molecular dynamics simulations in two dimensions. In agreement with experimental observations by Rothkegel¹ we find that local stresses – and hence the comminution efficiency – are maximal close to the bottom of the container. This effect will be explained using analysis of statistics of force chains in the material.

1 Introduction

Milling is one of the most important techniques in mechanical engineering and much effort has been done to optimize the comminution efficiency of milling techniques with respect to energy, space and time consumption².

Mainly because of their simple construction and application ball milling is a wide spread milling technology, particularly in mining. Ball mills are (usually large) cylindrical devices of length and diameter up to several meters which revolve along their axis. The material to be comminuted moves inside the cylinder. There are two different methods: autogeneous comminution where the material is pure and heterogeneous comminution where the material is mixed with heavy spheres from steel of typical diameter of several centimeters to increase efficiency. Throughout the paper we will deal with autogeneous comminution. Unfortunately the efficiency of ball mills is not very high and, therefore, engineers did much scientific work to increase their efficiency. There exists much experimental knowledge on the operation mechanisms of ball mills and on the comminution of granular matter in these mills. An overview can be found in ref.².

There are still effects, however, which have not been understood yet. The present paper deals with the spatial distribution of stress in the material. At first glance one could assume that the largest stresses will be observed close to the surface of the material where the granular particles have the largest values of relative collision velocity. Hence one could assume that large part of particle comminution occurs close to the material surface. To increase efficiency of the mill one would have to tune the rotation velocity so that the average collision velocity becomes maximum.

Experimental investigations, however, show opposite results: Rothkegel and Rolf measured directly the spatial distribution of intensive impacts¹ in a ball mill. In an experiment using a small almost two-dimensional mill they used instrumented balls which flash whenever the acting force at a particle contact is larger than a

threshold. The statistics of the spatial distribution of the flashes led to a surprising result: the spatial distribution of intensive particle contacts which in realistic ball mills might lead to particle comminution has its maximum deep inside the material close to the bottom of the cylinder. This result was new and there was no satisfying explanation for the measured stress distribution yet.

In the following section we present the results of a two dimensional molecular dynamics simulation of a ball mill. It will be shown that the spatial stress distribution is closely related to the properties of force chains in the material. The occurrence of such force chains, and even of entire networks of such chains has been reported before, see e.g. refs.³⁻⁸.

2 Molecular dynamics model

The rotation velocity of ball mills is high enough to keep the granular particles in the continuous flow regime (for explanation of the regimes see⁹) and on top of the material grains are thrown through the air caused by intensive forcing due to rapid revolution of the mill. Therefore static friction does not play an important role for the dynamics of the material and, hence, we can apply a sphere model in the MD simulations. We just want to remark that in other cases when static behavior of granular material becomes essential for the dynamics one has to apply more complicated grain models of non-spherical shape. For detailed discussions of the differences in the dynamics of spherical and non-spherical objects see references¹⁰⁻¹².

For our simulation we apply a spherical MD model for granular materials by Cundall and Strack¹³ and Haff and Werner¹⁴ which was used by many authors in simulations of rapidly moving granular material.

Two particles i and j with radii R_i and R_j , positions \vec{r}_i , \vec{r}_j and velocities $\dot{\vec{r}}_i$ and $\dot{\vec{r}}_j$ feel a force

$$\vec{F}_{ij} = F_{ij}^N \vec{n} + F_{ij}^T \vec{t} \quad (1)$$

only when contacting, i.e. if the condition $|\vec{r}_i - \vec{r}_j| < R_i + R_j$ holds. The force consist of a component F_{ij}^N acting in normal direction \vec{n}

$$F_{ij}^N = Y \cdot (R_i + R_j - |\vec{r}_i - \vec{r}_j|) - m_{ij}^{eff} \cdot \gamma_N \cdot (\dot{\vec{r}}_i - \dot{\vec{r}}_j) \cdot \vec{n} \quad (2)$$

and a component F_{ij}^T acting in tangential direction $\vec{t} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \vec{n}$

$$F_{ij}^T = \text{sign}(v_{ij}^{rel}) \cdot \min(m_{ij}^{eff} \gamma_T |v_{ij}^{rel}|, \mu |F_{ij}^N|) \quad (3)$$

$$\text{with} \quad (4)$$

$$v_{ij}^{rel} = (\dot{\vec{r}}_i - \dot{\vec{r}}_j) \cdot \vec{t} + R_i \cdot \omega_i + R_j \cdot \omega_j \quad (5)$$

$$m_{ij}^{eff} = \frac{m_i \cdot m_j}{m_i + m_j} \quad (6)$$

m_i and ω_i are the mass and the rotation velocity of the i -th particle. $Y = 8 \cdot 10^6 \text{ g s}^{-2}$ is the Young Modulus, $\gamma_N = 800 \text{ s}^{-1}$ and $\gamma_T = 3000 \text{ s}^{-1}$ are the damping coefficients in normal and tangential direction, and $\mu = 0.5$ is the Coulomb friction

coefficient. The parameters have been chosen to give realistic results in comparison of the simulation results with the behavior of a typical granular material.

Eq. (5) describes the relative velocity of the particle surfaces at the contact point. This velocity consists of the tangential part of the relative velocity of the particles and of a term which originates from rotation of the grains. m_{ij}^{rel} stands for the effective mass.

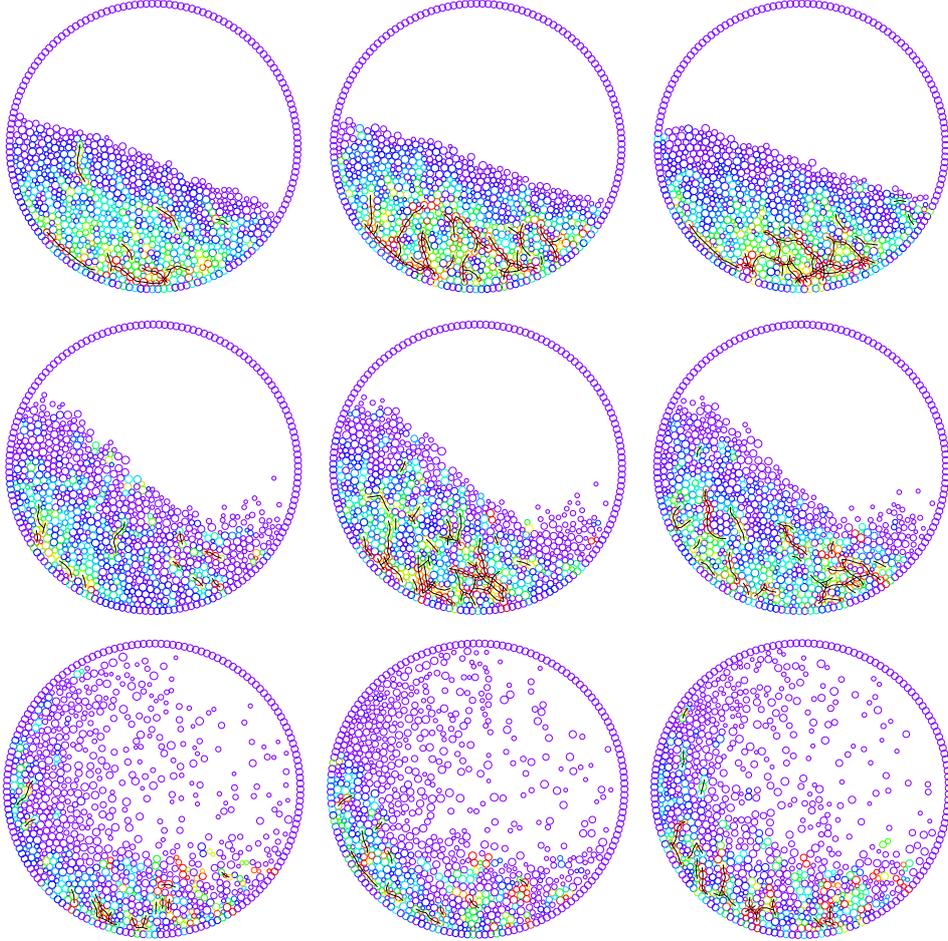


Figure 1: Snapshots of the simulation for different velocity. The color codes for the local pressure P_i (cf. eq. (7)). Black lines connecting adjacent particles mark automatically detected force chains. The ball mill revolves with angular velocity $\Omega_I = 2Hz$ (top), $\Omega_{II} = 10Hz$ (middle), $\Omega_{III} = 19Hz$ (bottom).

The Coulomb friction law is taken into account by equation (3) saying that two grains slide on each other if the tangential force is larger than μ times the normal force. Otherwise they roll mainly. For the detailed discussion of this and other models for molecular dynamics simulation of granular material see¹⁵.

Based on the force (1) Newton's equations of motion have been integrated using

a Gear predictor-corrector scheme of fifth order, e.g.¹⁶. This method was used in many simulations of granular material and has been proven to be very numerically stable.

3 Results of the simulation

The model described in the previous section was used to simulate a two-dimensional ball mill of diameter $D = 8 \text{ cm}$ filled with $N = 800$ spherical grains. The radii of the grains are distributed in the interval $[0.05, 0.11] \text{ cm}$. To study the influence of the rotation velocity of the cylinder we performed simulations for three different velocities $\Omega_I = 2\text{Hz} = 2/(2 \cdot \pi)$ revolutions per second, $\Omega_{II} = 10\text{Hz} = 10/(2 \cdot \pi)$ revolutions per second, $\Omega_{III} = 19\text{Hz} = 19/(2 \cdot \pi)$ revolutions per second.

At $\Omega = \Omega_I = 2\text{Hz}$ the flow at the surface is already continuous and the surface is characterised by an inclined line (see fig. 1, top). For $\Omega = \Omega_{II} = 10\text{Hz}$ the material surface is still almost compact and consists of two sections a steep and a flat one (fig. 1, middle). This velocity regime is experimentally known to have the best comminution efficiency². Large rotation velocity $\Omega = \Omega_{III} = 19\text{Hz}$ leads to free flight of the grains at the surface (fig. 1, top).

Fig. 1 shows snapshots of simulations with $N = 800$ grains for the three mentioned rotation velocities $\Omega_I, \Omega_{II}, \Omega_{III}$. The color codes for the local pressure P_i acting on the i -th particle

$$P_i = \sum_j F_{ij}^N. \quad (7)$$

The index j runs over all neighbors of the i th particle. Grains feeling a pressure $P_i > 1000g \text{ cm s}^{-2}$ are drawn bold lined. Obviously most of the hardly stressed particles are located near the walls inside the bulk of material, which agrees well with the experimental findings by Rothkegel and Rolf¹.

The hypothesis we want to discuss in the following is, that the self organized formation of *force chains* is responsible for the spatial stress distribution and, hence, the relevant physical reason for comminution processes in ball mills. Without the existence of such force chains, ball mills would not work or at least would work much less efficient. In the following we will discuss the properties of these force chains.

Force chains are defined by a set of simple conditions: Particles are called members of the same force chain if:

1. they feel a pressure (eq. (7)) of more than $1000g \text{ cm s}^{-2}$,
2. each member particle of the chain touches at least one other member, and
3. for all members k of the chain having two neighbors i and j , which belong to the force chain as well, the condition

$$\left| \frac{\vec{r}_k - \vec{r}_i}{|\vec{r}_k - \vec{r}_i|} \cdot \frac{\vec{r}_k - \vec{r}_j}{|\vec{r}_k - \vec{r}_j|} \right| < 0.85, \quad (8)$$

holds, i.e. these three particles lie almost on a line.

These three conditions can be checked using a computer algorithm. In fig. 1 neighboring particles have been connected by a black line provided that either of them belong to the same force chain. Obviously most of the hard stressed (and therefore bold drawn) particles are members of force chains. We conclude that an essential part of the static and dynamic pressure in the ball mill propagates along force chains. Particles which belong to a force chain feel pressure which are up to 100 times larger than the local average pressure

$$P_i^{(av)} = \frac{1}{K} \sum_{k=1}^K P_k, \quad (9)$$

where the index k runs over all K neighbors of the particle i which are within a certain neighborhood $|\vec{r}_i - \vec{r}_k| \leq 4 \cdot \bar{R}$ and which do *not* belong to any force chain.

The occurrence of force chains in granular systems is not new. They have been observed before in other granular systems in experiments³⁻⁶ and computer simulations^{7,8}. It can be shown that one of the (at least) three phases of an idealized granular system is characterized by the occurrence of force chains⁸.

Fig. 2 (left) shows the frequency of force chains of lengths L where L is the number of particles which join the chain. The frequency decreases almost exponentially with increasing length. For the highest rotation velocity Ω_{III} (fig. 2, bottom) the frequency distribution breaks down for longer chains, which is mostly due to less compact bulk of material and finite size of the system.

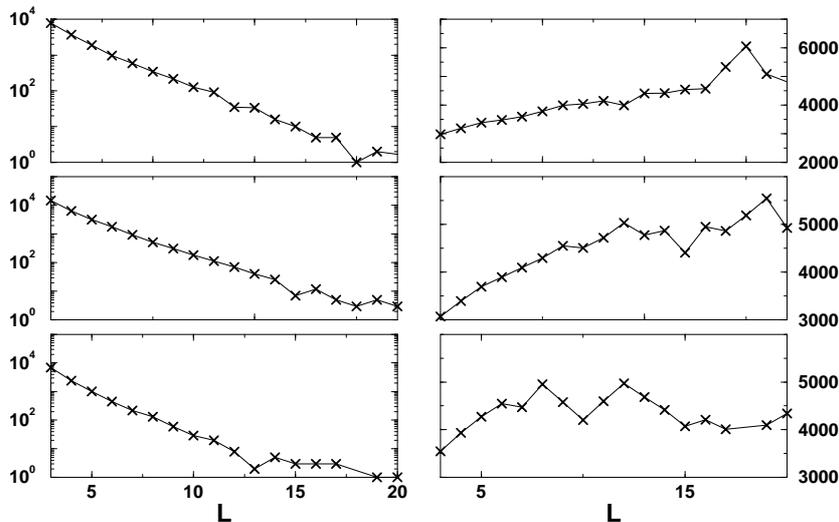


Figure 2: Left: Frequency of force chains of length L . Right: Average of the maximal pressure inside one force chain as a function of the length L of the force chain. Top: $\Omega_I = 2Hz$, middle: $\Omega_{II} = 10Hz$, bottom: $\Omega_{III} = 19Hz$.

The right hand side of fig. 2 shows the correlation of the length of a force chain and the pressure which acts on the particles which belong to this chain. Of particular interest is not the *average* but the *maximum* pressure inside a chain. The

maximum pressure is criterion whether a grain will be comminuted in a mill. As soon as one of the particles of a chain has broken the load discharges and the force chain vanishes and reappears elsewhere. Therefore here we are mainly interested in the *maximum* pressure. For low velocities Ω_I and Ω_{II} (fig. 2, top and middle) the average value of the maximal force in a force chain of length L grows monotonously with the length, i.e. a force chain acts similar as a beam in a framework: all the weight and momenta from particles above the chain are supported by the chain and propagated through the chain. Therefore one finds in most cases that the lower the position of a grain the higher the load.

In contrast, the corresponding plot (fig. 2, bottom) for high velocity Ω_{III} shows no characteristic dependence of the maximal force on the length of the force chain, i.e. for this case the force chains do not act as described in the previous paragraph. Thus we conclude that the mechanism of stress propagation in force chains is much less efficient in the case of high rotation velocity.

In fig. 3 the average number of particles per force chain which feel a pressure P_i larger than a given threshold P is plotted versus the length of the force chain. This number is directly related to the breaking probability which can be described using Weibull statistics¹⁷. Again one can see that longer force chains lead to a higher probability of comminution. For the highest rotation velocity Ω_{III} the distributions are significantly lower again.

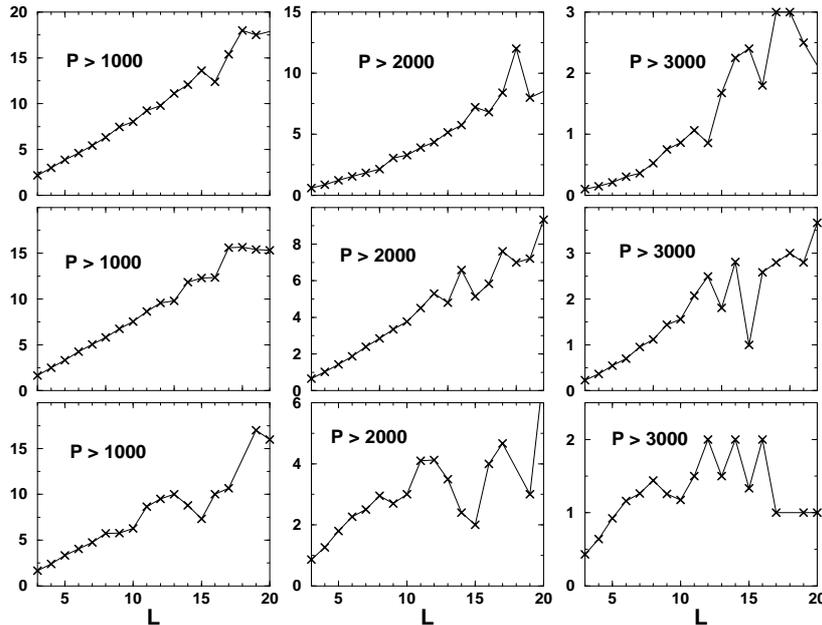


Figure 3: Average number of grains per force chain, which feel a local pressure P_i larger than a given threshold P . Top: $\Omega_I = 2 \text{ Hz}$, middle: $\Omega_{II} = 10 \text{ Hz}$, bottom: $\Omega_{III} = 19 \text{ Hz}$. The longer the chain the more particles feel pressure $P_i > P$ and, hence, the higher the comminution probability.

The time averaged spatial distributions of the pressure P_i for $\Omega_I = 2 Hz$ are shown in fig. 4 (left part of figure). The color codes for the local pressure P_i , where blue means low pressure and red color stands for high pressure. The upper plots include only particles which do *not* belong to a force chain, whereas the lower figures include only particles which *do* belong to a force chain.

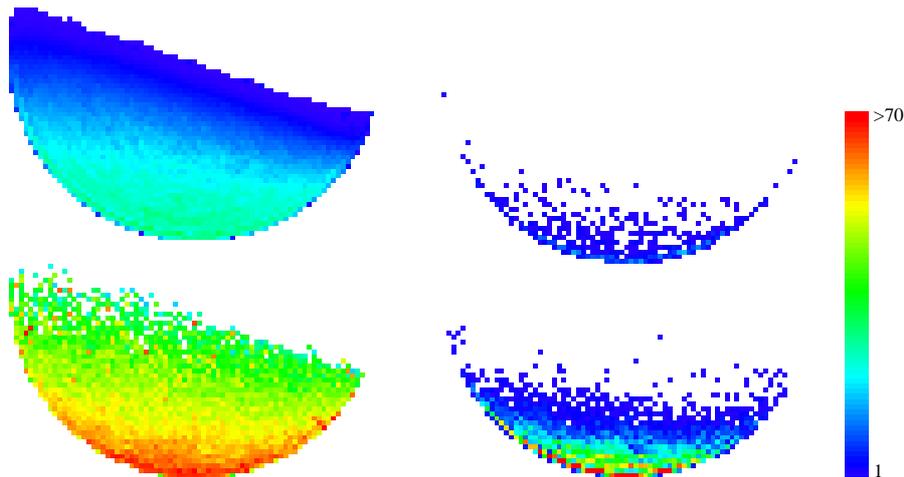


Figure 4: Left: Time averaged spatial distribution of the local pressure for $\Omega_I = 2 Hz$. The color codes for the pressure P_i , blue color means low pressure and red color stands for high pressure. The upper figure includes only particles which do not belong to a force chain, the lower figure includes only particles which do belong to a force chain. Right: Time averaged spatial distribution of the number of grains feeling a pressure $P_i > 3000 cm g s^{-2}$. The color code for the right figures is given by the color bar. Again in the upper figure only grains which do not belong to a force chain have been considered, whereas in the lower figure only grains which belong to a force chain join the averaging procedure.

The right hand side of figure 4 shows the time averaged spatial distribution of the number of particles, which feel a pressure $P_i > 3000 g cm sec^{-2}$. These results compare directly to the experiment by Rolf and Rothkegel¹ (see above). The maxima of the spatial distribution are located at the bottom of the cylinder near the wall which coincides with the results of the experiment.

Figures 5 and 6 are equivalent to fig. 4 where the angular velocity of the mill is $\Omega_{II} = 10 Hz$ and $\Omega_{III} = 19 Hz$, respectively. The color scaling is the same for all left side figures and the color code for the right figures is given by the color bar.

From these figures we conclude the surprising result that direct impacts of particles with high relative velocities at or close to the surface do *not* lead to high stresses. Therefore they are almost neglectable for the comminution process. Regions of high pressure can be found near the walls deep inside the material. Particles which do not belong to a force chain feel everywhere in the material a low pressure, only particles which are a member of a force chain feel larger stresses, i.e. only particles which belong to a force chain have a high probability to break. Fig. 6 shows that the mechanism of force chains is of low efficiency for rather high rotation ve-

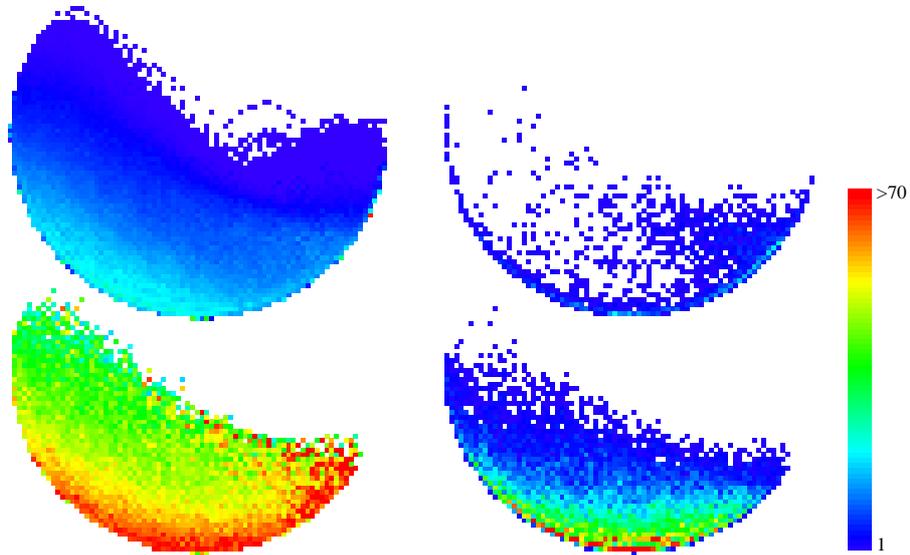


Figure 5: Equivalent figure to fig. 4 for $\Omega_{II} = 10Hz$. For explanation see fig. 4.

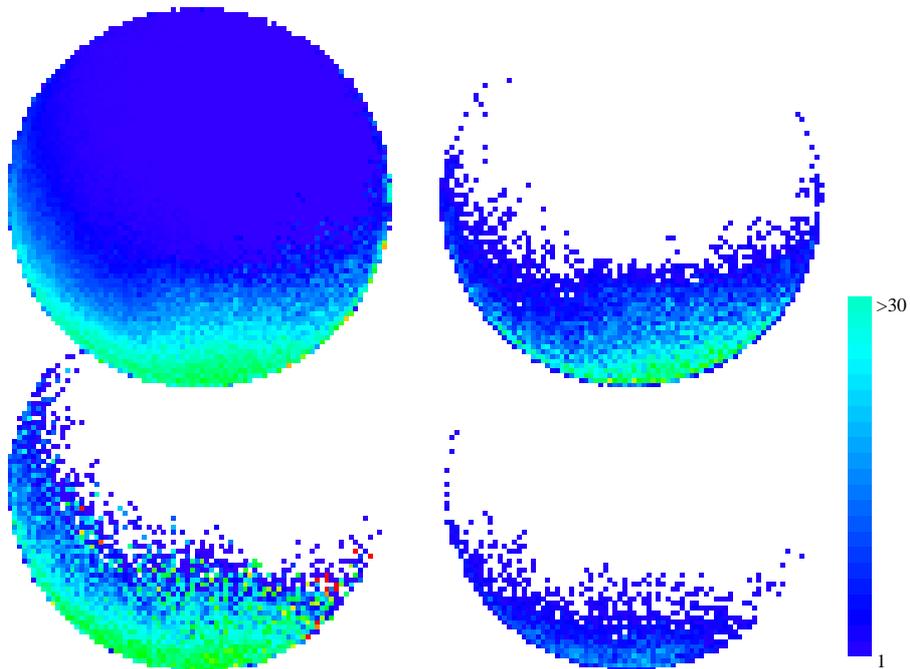


Figure 6: Equivalent figure to fig. 4 for $\Omega_{III} = 19Hz$. For explanation see fig. 4.

locities. The pressure is much lower than in the other figures 4 and 5, which leads to a diminution in the breaking rate as observed experimentally².

For $\Omega = \Omega_{III}$ (fig. 6) the rates resulting from impacts of particles at the surface overcomes the rates resulting from the force chains. Nevertheless the rates are clearly lower than for slower spinning mill.

4 Conclusion

Using two-dimensional molecular dynamics simulation of spherical granular particles we investigated the motion of granular material moving in a ball mill which spins with different angular velocity. The numerical results which agree with experimental data by Rolf and Rothkegel¹ lead to an explanation for the experimentally observed spatial distribution of pressure in such a ball mill. A network of force chains which permanently changes its structure has been observed in the rotating cylinder. Detailed and separate analysis of the statistical properties of these chains and of the pressure acting on particles which either *do* belong to a chain, or which *do not* belong to a chain lead to the conclusion that force chains play an important role for comminution processes in granular materials. Force chains lead to concentration of the dynamic and static load of a large amounts of grains in the bulk of the material to few grains close to the bottom of the container. These particles finally feel very large pressure. The described mechanism of the action of force chains is able to interpretate experimental data while other explanations fail¹.

References

1. Rothkegel, B.: *Örtliche Verteilung der Stoßenergien ≥ 22 mJ und die zugeordneten Bewegungszustände von Modellmahlkörpern in einer Modellkugelmühle*, Dissertation TU-Berlin, Verfahrenstechnik, 1992.
2. Bernotat, S. and K. Schönert: Size reduction (pp. 5-1). In: *Ullmann's Encyclopedia of Industrial Chemistry*, VCH Verlag, Weinheim (1988).
3. Duran J., T. Mazozi, S. Luding, E. Clément, and J. Rajchenbach: Discontinuous decompaction of a falling sandpile, *Rhys. Rev. E* **53**, 1923, 1996.
4. Behringer, R.: The Dynamics of Flowing Sand, *Nonlinear Science Today* **3**, 1, 1993.
5. Dantu, P.: Contribution à l'Etude Mécanique et Géométrique des Milieux Pulvérulents, *Ann. Ponts Chuasses* **4**, 144, 1967.
6. Liu, C. H., S. R. Nagel, D. A. Schecter, S. N. Coppersmith, S. Majumdar, O. Narayan, and T. A. Witten: Force Fluctuations in Bead Packs, *Science* **269**, 513, 1995.
7. Wolf, D. E.: Modelling and Computer Simulation of Granular Media, in *Computational Physics*, edited by K. H. Hoffmann and M. Schreiber, Springer, Heidelberg (1996).
8. Esipov, S. E. and T. Pöschel: The Granular Phase Diagram, *J. Stat. Phys.*, *in press*.
9. Rajchenbach, J.: Flow in Powders: From Discrete Avalanches to Continuous Regime, *Phys. Rev. Lett.* **65**, 2221, 1990.

10. Pöschel, T. and V. Buchholtz: Static friction phenomena in granular materials: Coulomb law versus particle geometry, *Phys. Rev. Lett.* **71**, 3963, 1993.
11. Pöschel, T. and V. Buchholtz: Molecular dynamics of arbitrarily shaped granular particles, *J. Phys. I France* **5**, 1431, 1995.
12. Buchholtz, V. and T. Pöschel: Avalanche statistic of sand heaps, *J. Stat. Phys.* **84**, 1373, 1996.
13. Cundall, P. A. and O. D. L. Strack: A Discrete Numerical Model for Granular Assemblies, *Géotechnique* **29**, 47, 1979.
14. Haff, P. K. and B. T. Werner: Computer Simulation of the Mechanical Sorting of Grains, *Powder Technology* **48**, 239, 1986.
15. Schäfer, J., S. Dippel, and D. E. Wolf: Force schemes in simulations of granular materials. *J. de Phys. I* **6**, 5, 1996.
16. Allen, M. P. and D. J. Tildesley: *Computer Simulations of Liquids*, Clarendon Press, Oxford (1987).
17. Weibull, W.: The phenomenon of rupture in solids Ingeniöretenskapsakademiens Handlingar, 149 (1938).