ENERGY DISSIPATION DUE TO PARTICLE SIZE AND SHAPE IN A SHEARED GRANULAR MIXTURE

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Abstract We study the energy dissipation in sheared granular mixtures consisting of particles with different sizes and shapes. Specifically, we generated energy dissipation spectra from DEM simulations of binary mixtures of cubical and spherical particles and of large and small particles in a slowly rotating tumbler. Mixtures of spherical particles of varying diameter have a single spectral peak while mixtures of cubical and spherical particle have two broader peaks. We developed an analytic model for these spectra by considering the particles as damped driven oscillators. The functional forms of the driving forces account for the sizes and shapes of the particles.

1 INTRODUCTION

The properties and behaviors of granular materials are intimately related to its response to forces and dissipation of energy. For example, energy dissipation in sheared wet (and dry) granular materials is mostly due to breakage and reformation of capillary bridges [1]. In incoherent vibrated granular materials, dissipation rates due to different interactions vary with density [2]. The amount and mechanistic origins of energy consumption in stirred mills also relates particle shape to grinding performance [3]. Previously, we have proposed that differences in dissipation rates for different particle shape types drives granular segregation [4]. In particular, avalanching cubical particles have been found to dissipate energy faster than round ones leaving them with lower translational energy which leads to vertical stratification according to shape.

One of the outstanding challenges in granular materials is the understanding and making use of the relationship between bulk behavior and individual particle geometry [e.g., 5, 6 and references therein]. However, the consideration of energy dissipation in this context is minimal or negligible. For example, so far most studies understanding pattern formation in flowing granular materials, e.g., segregation, directly relate pattern parameters (e.g., rise time) to individual particle geometry [7-11]. Considering that practically most granular materials are dissipative, investigations focused on relative energy dissipation (and their associated spectra) can complement these studies, improve our understanding of the mechanistic origins of these phenomena, and widen the range of experimental techniques. Spectral features have long been used to analyze and characterize spatial and temporal properties of diverse physical systems, e.g., elementary particles, proteins, turbulent flows, stars, etc [12]. In particle physics, particle lifetime and decay rates may be determined from spectral line width. In protein, nuclear magnetic resonance lines represent spatial protein structures. In turbulence, the laminar-turbulence transition may be indicated by the changes in peak number and continuity or discreteness of the spectrum.

Here, using the spectra, we analyze the energy dissipation in binary granular mixture partially filling a rotating horizontal cylindrical tumbler. This classical configuration for sheared granular materials is found in diverse applications [10-11, 13-15] and exhibits behaviors that are still not yet fully understood, such as radial [16, 17] and axial segregation [18-20]. Although our previous work [4] and those of others have started examining the role of energy dissipation in granular materials, to our knowledge, this is the first time that the energy dissipation is studied in this context in detail.

In Section 2, we describe the granular material system, and the parameters and results (energy dissipation spectra) of the DEM simulation. In Section 3, we propose an explanation for gross features of the dissipation spectra. We summarize the work in Section 4.

2 ENERGY DISSIPATION SPECTRA FROM DEM SIMULATION (*)

We simulate the shearing flow in a rotating drum using the Discrete Element Method (DEM) for various combinations of particle sizes and shapes. Our specific objective is to explain the features observed in the energy dissipation spectra of sheared granular materials and to relate these to differences in particle size and shape.

The energy dissipation spectra are calculated for DEM particle simulations of a binary granular mixture inside a rotating horizontal tumbler (which was 10 cm in diameter and 2 cm deep). This configuration is the same as the one used in previous works [4, 21-23]. The first set of mixtures considered here consists of particles differing only in shape (cubical and round particles). The other set consist of particles differing in size (large and small spherical particles). The DEM time-step is 10^{-5} seconds. We use a soft contact model to determine collisional forces, where particles are allowed to overlap and the amount of overlap Δx and normal v_n and tangential v_t relative velocities determine the collisional forces via a linear spring dashpot model. Periodic boundary conditions are used in the axial direction to represent a long cylinder, thereby eliminating axial segregation due to end-wall effects allowing us to focus on radial segregation. The gravity vector points in the negative y-axis direction. The parameter values are similar to those used previously [4, 21-23]: diameter of particles is taken from a uniform distribution with mean of 2mm and spread of 0.1mm, density of particles is $\rho = 2595\, kg/m^3$. The particles are either round or cubical (blocky) in shape. We use a super-quadric representation of shape, which has a parametric form that allows continuous description of corners [24-26]:

$$\left(\frac{x}{d}\right)^n + \left(\frac{y}{d}\right)^n + \left(\frac{z}{d}\right)^n = 1. \tag{1}$$

The shape factor n defines the amount of blockiness of a particle ($n = 2$ corresponds to a sphere of diameter $2d$ while $n =\infty$ corresponds to a cube with side length $2d$). The simulations explore the constant mixture ratio of 50:50 of nearly spherical (i.e., more round) particles (n = 2.03) and more cubical particles, with the n of the more cubical particles varying from 2.55 up to 10.05 for different simulation runs. The tumbler rotation speed is 3 rpm which produces granular flow that can be classified as being in the continuous flow regime with a Froude number $F = \omega^2 R/g$ approximately 5.0 x 10^{-4}. As previously established [4], the average surface speed of the two different particle shape-types indicated that rounder particles travel faster than more cubical particles on/in the surface shear layer. The cubical particles lose more energy and therefore travel more slowly within the surface shear layer enabling them to become buried by the faster moving round particles which flow more rapidly to the opposite side of the container (at the bottom of the granular slope). The steady state particle distribution is a central core of more cubical particles surrounded by the round particles.

We evaluate the power, P, or the rate of energy dissipation by the particles in the mixtures by summing all the dissipated energy E for each particle during each collision. The energy spectra is the energy dissipated in completed collisions (in the form of a plot of $\langle P \rangle$ versus E). This is constructed for (i) a mixture of round and cubical particles, (ii) a mixture of purely spherical particles different diameter (d = 2mm and 2.5mm) and, (iii) for comparison, a mono-disperse case ($d = 2$mm) composed entirely of spheres. Figure 1a shows that the energy spectrum for the mono-disperse spheres has a single peak at approximately E = 5 x 10^{-9} J and the maximum energy dissipated energy value is approximately 10^{-7} J. For the mixture of purely spherical particles the spectra for each particle size (not shown) are structurally similar to Fig.1a. The smaller particles have larger spectral amplitude and total energy dissipation indicating they dissipate energy faster than larger particles. Figures 1b and 1c show the spectra for cubical particles and for round particles, respectively, calculated from the flow of the round-cubical mixture. Note the following important observations:

1) relative to the mono-disperse case (Fig. 1a), the energy dissipation spectrum becomes much broader with energy dissipated over a much wider range of energy values (with larger maximum energy dissipated) from E = 10^{-10} J to E = 10^{-5} J; and

2) the spectrum for the cubical particles has two peaks of almost equal probability, with the first peak at approximately E = 5 x 10^{-9} J and the second peak at E = 5 x 10^{-7} J.

The correlation between the emergence of spectral peaks and the presence of certain features of a system often make the case for using the spectra as an analytic tool. In this case, the emergence of a second peak suggests that blockiness opened another energy dissipation mode.

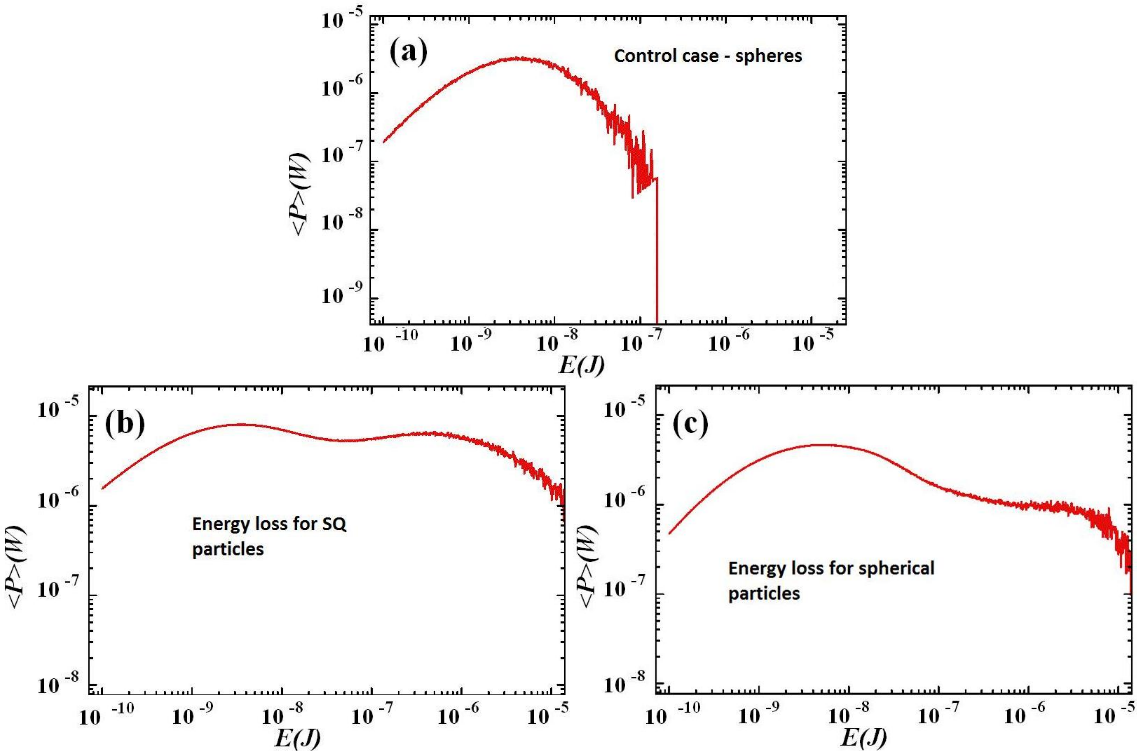

Figure 1: Energy spectra for avalanching flow of mono-disperse $d = 2$mm spherical particles. b) Energy spectra for cubical fraction ($n = 10$) in the mixture of round and cubical particles, and c) for round particles in the mixture of round and cubical particles. Note both axes are logarithmic scale.

3 ANALYSIS OF THE ENERGY DISSIPATION SPECTRA

3.1 Response function, force, and power

So far, there is no granular materials theory that can explain the micromechanical origin of these spectral features. In fact, use of dissipation spectra is still uncommon in current theories of granular segregation [see reviews, e.g., 7-11]. However, it has long been established in different contexts that the pairing between spectral features and spatial or temporal signals contain rich and useful information [27, 28]. Thus, we develop a theoretical model relating the features (the gross features, at least) of energy dissipation spectra to particle size and shape.

Although the dissipation spectra generated in the DEM simulation describes the whole granular mixture inside the container, they are derived from the summation of the energy dissipation for each particle per collision. Therefore we focus on the dissipation spectra and movement of a single particle rolling without slipping on the inclined granular bed (Fig. 2a).

The conceptual idealization used to construct the theoretical model involves considering the motion of a single surface particle as it moves down an undulating underlying surface (consisting of the rest of the granular bed). From the test particle perspective, the detailed dynamics of the rest of the bed are not important, only the apparent structure of the surface at the time when the particle reaches that location. We model the granular bed as a surface of length L inclined at angle θ while we model the particle as a damped harmonic oscillator driven by time (t)-dependent driving forces $f(t)$ (Fig. 2b). The damped harmonic oscillator is one of the simplest models of a dissipative elastic system. Although more sophisticated models [e.g., 22, 29] may sometimes be more realistic, the analytic tractability and simplicity of the oscillator allow us to focus on the main challenge of incorporating particle size d and shape factor n into the theory.)

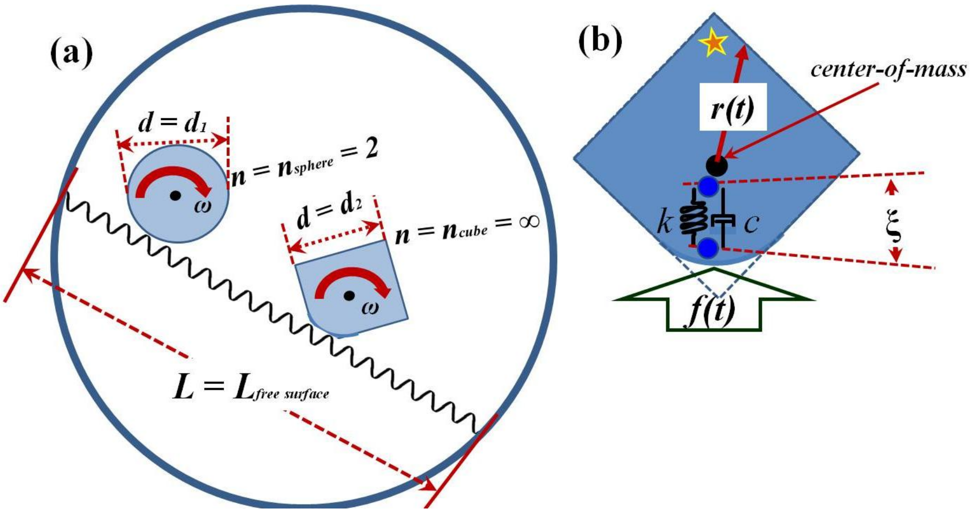

Figure 2: a) Granular particles of size d and shape factor n rolling on a granular bed. The granular bed is composed of other particles, has a surface of length L, and is inside a rotating horizontal cylindrical tumbler. b) The particle as a damped harmonic oscillator driven by force $f(t)$.

We define the dissipative interaction as any contact that deforms the particles. We distinguish $f(t)$ according to where on the surfaces of the particle a particular contact occurs, namely, $f_n(t)$, for forces applied to the corners and, $f_c(t)$, for forces applied to the smooth edges in between. Obviously, round particles do not have corners and so only have the smooth surface of constant curvature. Defining ξ as the deformation (normal to the surface), m as the mass, c as the damping coefficient, and k as the spring constant, $\gamma = \frac{c}{2\sqrt{km}}$ as the damping factor, and $\omega_0^2 = \frac{k}{m}$ as resonant angular frequency, the oscillator is described by this equation (Fig. 2b):

$$\frac{d^2\xi}{dt^2} + 2\gamma\omega_0\frac{d\xi}{dt} + \omega_0^2\xi = \frac{1}{m}[f_n(t) + f_c(t)] = \frac{1}{m}f(t). \quad (2)$$

We relate ξ to $f(t)$ using response function χ (define here in time and angular frequency space) [see e.g., 30, 31]:

$$\xi(t) = \int_{-\infty}^{\infty} dt'\chi(t-t')f(t), \quad (3)$$

$$\chi(t-t') = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \tilde{\chi}(\omega) e^{-i\omega(t-t')}, \tag{4}$$

$$\tilde{\chi}(\omega) = \frac{1}{-\omega^2 + i2\gamma\omega_0\omega + \omega_0^2}. \tag{5}$$

Accordingly, the energy dissipation rate or power, $P(t)$, in time and Fourier or angular frequency space, ω or $\nu = \omega + \omega'$ (* means convolution):

$$P(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} [-i\omega\tilde{\chi}(\omega)] e^{-i(\omega+\omega')t} \tilde{f}(\omega)\tilde{f}(\omega'), \tag{6}$$

$$= \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} e^{-i\nu t} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [-i\omega\tilde{\chi}(\omega)] \tilde{f}(\omega)\tilde{f}(\nu-\omega).$$

$$\tilde{P}(\nu) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} [-i\omega\tilde{\chi}(\omega)] \tilde{f}(\omega)\tilde{f}(\nu-\omega). \tag{7}$$

$$= \left[-i\nu\tilde{\chi}(\nu)\tilde{f}(\nu)\right] * \tilde{f}(\nu).$$

3.2 A simple example

We consider a simplified case to demonstrate the plausibility of our approach and perspective. We can see from Eq. (7) that the driving force $\tilde{f}(\nu)$ crucially defines the spectral features. We use the following *gedanken* experiment to describe the information it contains:

"Imagine one particle has a force detector. This particle is one of the grains inside a rotating container. Assume that the only information being detected by the observer is solely the magnitude of the instantaneous net force, $f(t)$, as a function of time, t, deforming the surface of the particle. The $f(t)$ is weak (i.e., zero) and steady while the particle is in the plug region because the particle is approximately immobile relative to its neighbors. Once the particle traverses the active region, $f(t)$ strengthens and fluctuates (Fig. 3a). The gross features of $f(t)$ can be described as windowed fluctuating signal. The signal features, namely 1) duration (window size), and 2) fluctuations (waviness) are dependent on the particle size and shape. Although the physical origins of these signal features are not perfectly compartmentalized, we propose these approximate correspondences: the duration is due to the finite time the particle spends in the active region; and the fluctuations are due to the geometry, elasticity, and damping of the particle."

Considering the principles of signal processing, the identification of these signal features of $f(t)$ naturally reveals the basic components of $f(t)$ and the mathematical operations that combined them. First, $f(t)$ is the sum of signals $f_c(t)$ and $f_n(t)$, which are then multiplied by a window function $W(t,\tau)$ (Fig. 3a). The counterparts of these elements and operations in the Fourier (angular frequency ω) space are also well established [e.g., 27, 28]. The signals $f_c(t)$ and $f_n(t)$ transform into the peaks and, through convolution, the window function gives width to these peaks (Fig. 3b).

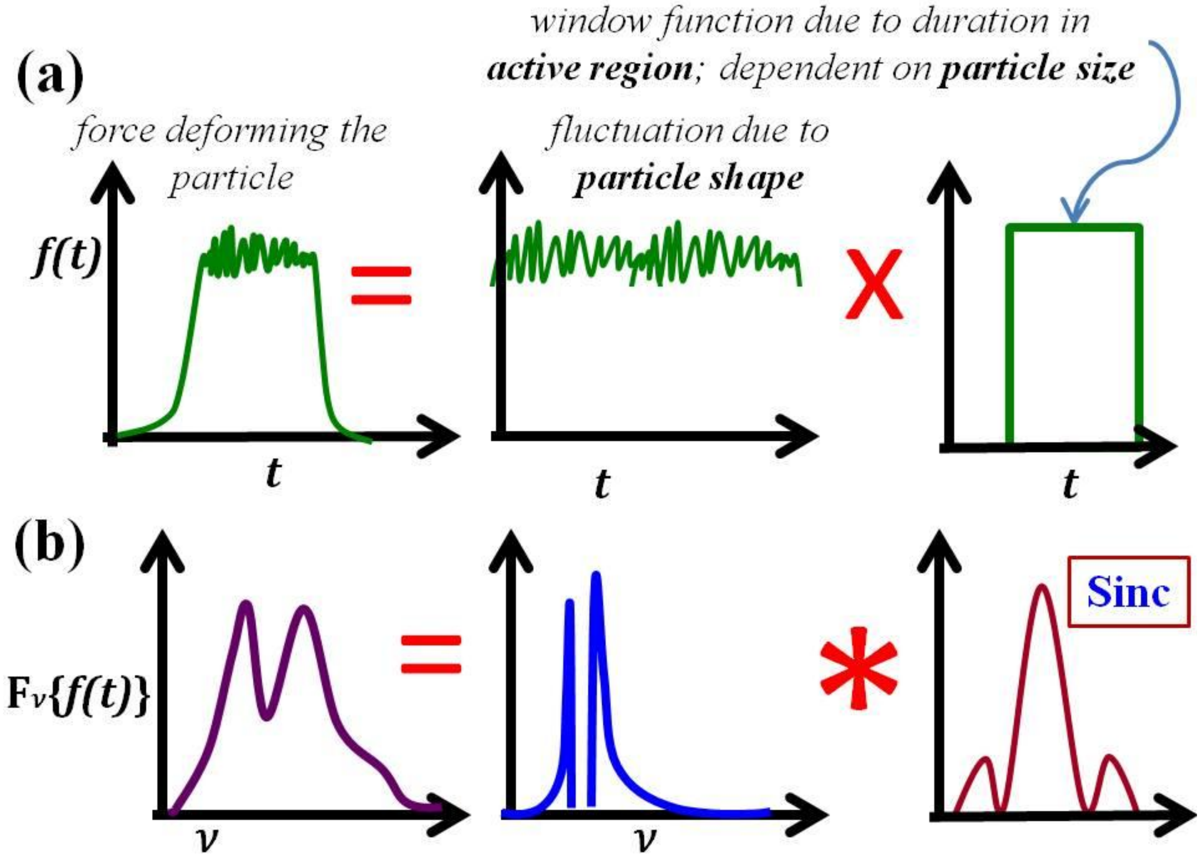

Figure 3: a) Caricature of the force $f(t)$ deforming the particle and its component. b) Force $f(t)$ and its component in Fourier (angular frequency) space (* means convolution).

We assume that the forces $f(t)$, $f_n(t)$, and, $f_c(t)$ are time-dependent functions that can be represented by sinusoidal functions, i.e., their Fourier transforms exists. Furthermore, for simplicity in this example, we lump together $f_{\mathrm{n}}(t)$ and $f_{\mathrm{c}}(t)$ into one fluctuating function:

$$f_{\mathrm{n}}(t) + f_{\mathrm{c}}(t) = f_{\mathrm{d}}(t) = F\cos(\nu_d t) \qquad (8)$$

Next, we describe the window function. Lastly, let the particle enter the active region at time $t = t_a$ and exits it at time $t = t_b$. Compared to larger particles, smaller particles tend to stay longer in the active region and have more chances for dissipative interactions. With proportionality constant β and a characteristic length L of the granular material configuration (e.g., length of the active region in the direction of the inclined surface (Fig. 2a)), one simple window function, $W(t, t_a, t_b)$, we could use is a rectangular function describe by two Heaviside or step functions, H:

$$W(t, t_a, t_b) \equiv H(t - t_i) - H(t - t_o) = H(t) - H(t - \tau), \qquad (9)$$

$$\tau = t_{\mathrm{b}} - t_{\mathrm{a}} = \beta \frac{L}{d}. \qquad (10)$$

Thus, the driving force for this case is as follows:

$$f(t) = f_{\mathrm{d}}(t) W(t, \tau). \qquad (11)$$

The Fourier transform $\tilde{f}(\nu)$ of Eq. (11) is:

$$\tilde{f}(\nu) = \pi F_d[\delta(\nu - \nu_d) + \delta(\nu + \nu_d)] * \tau \operatorname{sinc}(\nu\tau/\pi)e^{-i\nu\tau/2} \qquad (12)$$

$$= \tau\pi F_d\big[\operatorname{sinc}((\nu - \nu_d)\tau/\pi)e^{-i(\nu-\nu_d)\tau/2} + \operatorname{sinc}((\nu + \nu_d)\tau/\pi)e^{-i(\nu+\nu_d)\tau/2}\big],$$

where sinc function is a standard shorthand $\operatorname{sinc}(\theta) = \sin(\pi\theta)/\pi\theta$ (third panel, Fig. 3b). Equation (12) is to be substituted into Eq. (7) to obtain power. However, we could already make some important observations by simply examining Eq. (12).

The broadness of the spectra is dependent not only on the width but also on the shape of the window function [27]. The choice of a simple window function limits the comparison between the model and experiment at this point. Nonetheless, we can make the qualitative comparison between Eq. (12) and Fig. 1 (expressing angular frequencies ω in terms of energies E, i.e., $\nu_0 = \sqrt{2E_0/I_{sphere}}$ and $\nu = \sqrt{2E/I_{sphere}}$). The location of the spectral peaks, ν_d, is determined by particle shape, e.g., blockiness n. On the other hand, the sharpness of the peaks is mainly due to size. Particles that spend more time in the active region will have sharper and higher peaks, as shown by the modulation of Eq. (12) by τ. This is consistent with the observation in the DEM simulation that the smaller particles have larger spectral amplitude and energy dissipation.

More work is needed before we can fully assess and apply this theoretical model. This study at least contributes to the consideration of the spectroscopic perspective into the problem. Future works include actual spectral analysis of force signal detected by an individual particle and exploring various window functions.

4 SUMMARY

We studied the energy dissipation spectra generated from DEM simulations of binary granular mixtures, consisting of particles differing in sizes and shapes, inside a slowly rotating tumbler. We also studied the monodisperse case consisting of spheres. The monodisperse case has a single spectral peak. Compared to the monodisperse case, the spectra for cubical particles and for spherical particles are broader with energy dissipated over a much wider range of energy values. The spectra for the cubical particles have two peaks. In terms of particle size, the spectra for smaller particles have higher spectral amplitude indicating faster energy dissipation. We proposed a theory relating the peaks and widths of the spectra to the properties and motion of individual particles. The appearance of second spectral peaks is attributed to the blockiness of cubical particles opening another mode of energy dissipation at higher energy or angular frequencies. Furthermore, a property that causes particles to spending more time in the active region, say being small or being blocky, results to more dissipation.

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