Nonideally Packed Granular Media: Numerical Modeling of Elastic Nonlinear Properties

V. Yu. Zaitsev
Institute of Applied Physics, Russian Academy of Sciences, ul. Ul'yanova 46, Nizhni Novgorod, 603600 Russia
Received September 14, 1994

Abstract — This paper analyzes experimental findings, including those obtained by the author. They reveal that the nonlinear properties of real granular media strongly differ from those calculated using known models that ignore the nonideal character of packing (that is, intergranular contacts, which exist under widely differing initial loading conditions). The results of numerical calculations done with allowance for relieved contacts are given. The model is shown to explain the differences observed as being both qualitative and quantitative. It is shown that nonideal packing has the strongest bearing on higher-order nonlinearities.

INTRODUCTION

Recent years have seen a proliferation of studies on the acoustoelastic nonlinearity of granular media (see, for example, [1 - 7]). The reason is that the nonlinear properties of granular media are a manifest example of a rather common occurrence — the effect the microstructure of a material has on its elastic nonlinearity [4, 8]. At present, quite a number of such strongly nonlinear media have been identified [8, 9] whose properties fail to fit the classical theory of elasticity (as exemplified by, for example, the five-constant model [10]). Moreover, today, granular media are almost the sole case in which nonlinear elastic properties may be described in ways other than the phenomenological approach. Therefore, a consistent comparison of theoretical and experimental results is both essential in verifying and elaborating upon existing strongly idealized models and useful in developing such physical models for other structurally inhomogeneous media. Also, because many earth rocks similarly belong to the category of flowable granular materials, studies of this kind are attractive due to the likelihood of their diagnostic applications (in engineering seismology, seismic prospecting, etc.).

This paper presents an analysis of experimental findings on the linear and nonlinear elastic properties of granular media [11 - 16] that do not fit into known models [1 - 5], where the basic concept is what we will call the ideal packing of spherical granules, i.e., one with a constant number of contacts. To explain why the relations derived differ from the ideal packing model, Belyaeva et al. [16] proposed allowing for the effect of nonideal packing, i.e., one involving partly or even completely relieved contacts. To confirm this explanation, simple estimations were made. In what follows, the results of a more detailed analysis of the linear and nonlinear properties of nonideally packed granular samples are presented as an elaboration of the idea stated in [16]. In this paper, the analysis of the stress-strain relationship is not purely phenomenological. Rather, its basis is a hypothesis about the behavior of individual contacts, although, here, we invoke a simpler approach than the more rigorous treatment used in [5].

It is relevant to recapitulate the key corollaries of the model proposed in [5] for a granular medium in the form of an ideal packing of spheres. It was assumed that the spheres could be packed at random but with a constant number of contacts and compressed identically. It was further assumed that the behavior of an individual contact could be described using Hertz's law [10]. Consider small longitudinal deformations in a granular sample relative to some initial compression $d_0$. According to [5], it then follows that the elasticity of the sample increases as $d_0^{1/2}$ (or, equivalently, the velocity of longitudinal waves varies as the static pressure is raised to the 1/6 power). For the second and third harmonics, the forces arising when a weak harmonic wave $d_{cos}$ is superimposed on the static pressure $d_0$ (as was done, for example, in the experiments reported in [3, 16]) will, as follows from the model proposed in [5], vary as the amplitude of $d_0$ is raised to the second and third power, respectively.

We now turn to see how the above corollaries of the ideal packing model, which can be verified experimentally, match the results of known measurements.

The manner in which the velocity of a longitudinal wave in sand varies with the initial static pressure was investigated in detail in, for example, [11, 12]. Depending on the sand samples used, the power exponent of this quantity ranged from nearly 1/6 [11] to 1/4 [12]. The former figure fits the granular-medium model with a constant number of compressed contacts. Of course, such forms of packing, similar in properties to the ideal model considered in [5], can occur in some situations. More often, however, a power exponent greater than 1/6 has been reported [12 - 14]. This behavior can be
attributed to the increase in the rigidity of the sample with increasing pressure, as new contacts appear between particles owing to the contacts being exposed to very different loading conditions. To demonstrate, the average number $n$ of contacts per granule, as evaluated from the ideal packing model [5], will, according to [12], range from $n = 2.3$ at the lowest pressure on the sample (2 kgf/cm$^2$) to $n = 4.5$ at the highest pressure (50 kgf/cm$^2$). When $n = 12$, which is characteristic of the closest ideal packing and is often used for evaluation purposes, an overstated packed elasticity will result, a fact also noted in [13, 14]. Thus, the pressure dependence of sound speed in granular media reported in [11-14] is in fairly good agreement with our contention concerning the effect produced by the variable number of contacts. It should be admitted, though, that one cannot assess higher-order nonlinearities from such measurements directly.

Experimental findings about the nonlinear acoustic properties of granular media, especially those obtained in the field, are rather lacking. One apt example is the abnormally high quadratic and cubic nonlinearities observed under natural conditions and reported in [15]. Within the ideal packing model [5], we were able to explain the high nonlinearity of loose soil established in [15] and derive estimates comparable in order of magnitude with the measured ones. However, a more rigorous comparison shows that the ratio of the cubic and quadratic variables measured in [15] is three or four times greater than the estimate derived in [5]. As the results of numerical modeling will prove shortly, this can similarly be attributed to relieved contacts.

Lastly, in [16], where the experiments were concerned with the generation of harmonics in granular media, special attention was given to the difference between the results measured and the theoretical relations derived from the ideal-grain-packing model [5]. In [16], the following salient features that we associate with the nonideal packing of granules were observed. At the first (fundamental) harmonic of force, the elasticity of the sample was significantly lower (compared to what one might expect for ideal random packing), the linear elasticity increased at a faster rate with static pressure, and the rigidity of the samples showed a rather noticeable decrease or increase with increasing wave amplitude, which likewise cannot be explained in terms of the model proposed in [5]. At the second harmonic, the amplitude increased by as much to 50% and, its behavior with the specified displacement of the sample boundary deviated from strictly quadratic at the first harmonic. At the third harmonic, the amplitude increased tenfold to hundredfold, sometimes the sign of the phase reversed with increasing amplitude of the displacement at the fundamental $d_{0}$, and the amplitude varied with $d_{0}$ in a strongly noncubic manner (sometimes even exhibiting almost quadratic behavior).

**EXPERIMENTAL RESULTS**

We now consider the results of consecutive numerical modeling of the above effects using the hypothesis from [16] with regard to the effect of loosely compressed intergranular contacts. In describing an isolated contact, we will use, as before: Hertz’s theory [10]. Now, instead of the relation $F = \frac{x^2}{2}$ stemming from the ideal packing model proposed in [5] and describing the connection between the strain suffered by a granular sample and the compressive force applied, we obtain a somewhat different relation. For the samples used in [16], which were compressed in a rigid cup by a piston vibrating harmonically as $x = d_{0} + d_{0} \cos \omega t$, we may write

$$F = \sum_{i} v_{i} Q_{0i} \frac{\xi^{2}}{d_{0}} \theta_{i} \left( \frac{\xi}{\mu_{i}} + \frac{\xi}{\cos \omega t} \right) \left( \frac{\xi}{\mu_{i}} \right)^{1/2} \left( \frac{\xi}{\mu_{i}} \right) \cos \omega t \quad \theta_{i}(x) = \begin{cases} 1, & x > 0 \\ 0, & x \leq 0 \end{cases}$$

where $\xi = d_{0}/d_{0}$ is the normalized amplitude of vibrations at the fundamental; $Q_{0i}$ is proportional to the number of contacts in the sample, with their compression determined by the initial deformation $d_{0}$ of the sample (in what follows, we call them the main fraction of contacts); and $v_{i}$ is the number of contacts in the $i$th slightly compressed fraction, whose degree of compression is characterized by $\frac{\mu_{i} d_{0}}{\mu_{i}}$ ($\mu_{i} \leq 1$). To the particles in the main fraction that are compressed by an amount equal to $d_{0}$, there corresponds $\mu_{0} = 1$. Slightly compressed contacts ($0 \leq \mu_{i} \leq 1$) may turn out to be completely relieved if the amplitude is sufficiently large during the part of the period where $(\mu_{i} - \xi \cos \omega t) < 0$. The negative values of $\mu_{i}$ also have meaning: they correspond to the particles that are completely relieved at first and begin to deform at $|\xi| > |\mu_{i}|$ during the part of the period when $(\mu_{i} - \xi \cos \omega t) > 0$.

If all $\mu_{i} > 0$ at low vibrational amplitudes $\xi < \mu_{i}$ (that is, when "clapping" contacts are nonexistent), the bracketed term $\left[ 1 + \frac{\xi}{\mu_{i}} \right] \cos \omega t \frac{\xi^{2}}{d_{0}}$ in (1) may be expanded in a power series of $\xi$. Then, the elastic force may also be expanded into a harmonic series as

$$F = F_{0} + F_{w} + F_{2w} + F_{3w} + \ldots,$$

where

$$F_{0} = \sum_{i} v_{i} \mu_{i}^{3} (Q_{0i} d_{0}) \cos \omega t,$$

$$F_{w} = \sum_{i} v_{i} \mu_{i}^{3} (Q_{0i} d_{0}) \times \left( \frac{\xi}{\mu_{i}} + \frac{(\beta - 1)(\beta - 2)}{8} \left( \frac{\xi}{\mu_{i}} \right)^{3} \cos \omega t + \frac{(\xi)^{2}}{\mu_{i}} \cos \omega t \right),$$

$$F_{2w} = \sum_{i} v_{i} \mu_{i}^{3} (Q_{0i} d_{0}) \frac{\beta(\beta - 1)}{4} \left( \frac{\xi}{\mu_{i}} \right)^{2} \cos \omega t,$$

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\[ F_{3a} = \sum_i \nu_i \mu_i^3 (Q_{3a} \Omega_i^3) \]
\[ \times \frac{\beta(\beta - 1)(\beta - 2)}{24} \left( \frac{\xi}{\mu_i} \right)^3 \cos 3\alpha_i. \]  

(5)

Here, \( \beta = 3/2 \) is the exponent of the Hertzian nonlinearity. Note that, according to the expressions (3) and (5), derived for low vibrational amplitudes at which clapping contacts are nonexistent, the initial phase of the third harmonic is shifted through \( \pi \) rad from that of the fundamental. Also, the terms with \( \mu_i < 1 \) appearing in (1) bring about certain changes in the level of force harmonics. As follows from (3) - (5), the contribution of the nth fraction of relieved contacts to the nth force harmonic is \( \mu_i^{2n-2} \) times as great as the contribution of the main contact fraction for which \( \mu_i = 1 \) by definition. It follows, then, that relieved contacts have a negligible effect on the fundamental for which \( n = 1 \), and \( \mu_i^{2n-2} < 1 \) for \( \mu_i < 1 \). However, they strongly affect the amplitudes of the higher harmonics for which \( n \geq 2 \), and, accordingly, for \( \mu_i < 1 \), the factor \( \mu_i^{2n-2} \gg 1 \). Also, despite the increased level of the higher harmonics, their amplitudes vary in the usual manner, i.e., as \( \xi_i^\alpha \). In contrast to the simply relieved contacts, the clapping contacts can (as will be demonstrated by numerical results) significantly change not only the amplitudes but also the functional form of the relations.

Harmonic levels are an integrated characteristic of the stress–strain curve of a sample over a complete cycle of vibrations. For this reason, they should depend in a rather coarse manner on \( \nu \) and \( \mu_i \) in (1), which we use to depict the actual packing of grains. Therefore, as is often done in modeling integrated dependences of nonuniform distributions, we will limit ourselves to the simplest version of the ideal packing model – the two-component model. In addition to the main contact fraction compressed by an amount equal to \( \delta \) (for them, \( \mu_i = 1 \)), this model contains one fraction of partly relieved contacts (for which \( \nu < \mu_i < 1 \)). Through an appropriate choice of \( \nu \) and \( \mu_i \), we will try to describe the effects observed in an experiment in the best possible way.

For a clearer interpretation of the results derived in numerical modeling and experiments, we will examine the special traits that should be expected in the behavior of the harmonics outside the power expansions (3) - (5) as the medium changes to the clapping contact condition owing to the increase in the amplitude of the fundamental to \( \xi_i^\alpha > \mu_i \). Contacts for which \( \mu_i < 1 \) exhibit purely clapping-type nonlinearities. In the case at hand, the granules interact in compliance with Hertz's law, and their nonlinearity index is \( \beta = 3/2 \). Therefore, all the nth elastic force harmonics on the clapping contacts must be proportional to \( \xi_i^{2n} \) rather than \( \xi_i^n \), and the initial phase of, for example, the third harmonic must coincide with the phase of the fundamental (in contrast to the power-series nonlinearity (5)).

In the case of contacts for which \( \mu_i > 1 \), either the power-series or the clapping nonlinearity can make a greater contribution, depending on the amplitude \( \xi_i \). The resultant behavior of the harmonics may be far more complicated than in the limiting cases mentioned above. With respect to the relationships especially important for comparison with the experiment, the most striking differences should be expected in the behavior of the third harmonic, in which case the contributions coming from the various nonlinearities are in antiphase. This assertion is illustrated by the curves given in Fig. 1a, which shows the contribution, numerically calculated on the basis of equation (1), made by one contact fraction with \( \mu_i = 0.01 \) to the elastic force at the third harmonic (naturally, the relations for other values of \( \mu_i \) will behave in a similar way). For comparison, the dashed curve represents a similar relation derived from the approximate cubic expansion (5) for the same grain fraction. These curves closely coincide in region I of relatively small amplitudes, \( \xi_i < \mu_i \). Further on, as the amplitude increases so that \( \xi_i > \mu_i \), the harmonic first increases, reaches a maximum at around \( \xi_i = 2\mu_i \) and then decreases owing to the increase in the antiphase contribution from the clapping nonlinearity (region II in Fig. 1) until it crosses zero and its phase changes sign. Given sufficiently large amplitudes \( \xi_i > 3\mu_i \) (region III in Fig. 1a), the level of the third harmonic is mainly determined by the clapping nonlinearity, and its amplitude, instead of obeying a cubic law, varies as \( \xi_i^{2/3} \). This change in behavior from \( \xi_i^2 \) to \( \xi_i^{2/3} \) can be clearly seen in Fig. 1b, where the amplitudes of the first to third harmonics are plotted in logarithmic coordinates. The abrupt dip seen in the logarithmic curve for the third harmonic occurs because the amplitude crosses zero (see Fig. 1a). In comparison, the dashed curve corresponding to a lower level represents the cubic behavior of the third harmonic, calculated by equation (5) for the main grain fraction (\( \mu_i = 1 \)) with the same value of \( \nu \).

As they appear, clapping contacts do not cause the phase of the second harmonic to change sign. Therefore, its amplitude gradually changes from the \( \xi_i^2 \) behavior in region I to the \( \xi_i^{2/3} \) behavior in region III (see Fig. 1b).

As to the amplitude of the fundamental in region II, where clapping contacts are in effect, the energy of the fundamental is intensively transferred to the higher harmonics. This slows down the increase in \( F_{3a} \) with increasing amplitude \( \xi_i \), which, given a sufficiently great proportion of clapping contacts, may look like a decrease in the elasticity of the sample. As the amplitude continues increasing in region III, the clapping contacts make an ever-increasing contribution, proportional to \( \xi_i^{2/3} \), to the total elastic force \( F_{3a} \), which shows up as increased rigidity of the sample. Note that, according to the power series expansion (3), one should expect solely a negative nonlinear correction to the
level of the fundamental, with its relative value being no greater than 0.1% for amplitudes $\xi < 0.2$. Therefore, in view of the accuracy achieved in the experiments in [16], this frequency could have passed unnoticed. Actually, in [16], we observed nonlinear effects as both an increase and a decrease in the elasticity of the sample (and their combinations), depending on the form of packing actually observed [or, according to (1), depending on the number of fractions and the values of $v_i$ and $\mu_i$].

To demonstrate that such strong nonlinear corrections are attributable to the effect of clapping contacts, Fig. 2 shows the experimental graphs of the elastic-force fundamental harmonic derived in [16] for plastic grains ($d_g = 25 \mu m$), rescaled in terms of the rigidity coefficient $K = F_n/\xi$. The dashed curve represents the function $K(\xi)$ evaluated on the basis of the expansion (3) for the main fraction alone, and the solid curve represents the one evaluated on the basis of equation (1) for a two-component model using $\mu_0 = 1$, $\mu_1 = 0.07$, and $v_1/v_0 = 6$ (in arbitrary units). On the scale used for the graph, the nonlinear power-series correction for the dashed curve is almost unnoticeable. Calculation for the simplest two-component model near the transition to the clapping mode clearly demonstrates the tendency toward a decrease in the effective elasticity, even at $\xi < 0.1$. The further decrease occurring in $K$ at $\xi > 0.1$ could be described using a greater number of fractions for which the values of $\mu$ range from 0.1 to 0.15.

Now, we turn to the relative levels of the force harmonics, which, in the experiments reported in [16], displayed the most striking differences from those calculated for the ideal packing model [15]. For the lead and plastic granules investigated in [16], the amplitudes of elastic-force harmonics plotted on a logarithmic scale against the normalized vibrational displacement and the ones numerically calculated for the ideal-packing model (dashed curves) and a nonideally packed two-component model (solid curves) are shown in Figs. 3a and 3b. Experimental curves plotted in terms of normalized variables appear to be very similar at different compressions. Therefore, in order not to overcrowd the figure, only the points taken at one of the initial compressions are shown in Figs. 3a and 3b. As can be seen, even in the two-component model, the effect of slightly compressed contacts offers a good explanation for the strongly increased level of the higher harmonics compared to those calculated for the ideal-packing model.
The experimental and calculated curves for the nonideally packed model differ by a factor of 1.5 to 3 at the second harmonic and by a factor of 10 to 50 at the third harmonic (see Fig. 3). The dip seen in the curve calculated for the third harmonic (see Fig. 3a) is traceable to the same cause as in Fig. 1b and can be readily removed by allowing a third fraction in the model defined by equation (1).

We will now dwell in more detail on the behavior of the amplitude at the third harmonic of the elastic force, where the nonideal packing shows up most strongly. In qualitative terms, its behavior in the case of plastic-grain samples differs markedly from the one in the case of lead-grain samples, being a cubic function of the amplitude $\xi$ in the former case and an almost quadratic function of the amplitude $\xi$ in the latter. Comparison between the behavior of the third harmonic and the manner in which it is produced by relieved contacts (see the discussion above and Fig. 1) shows that the conditions under which these contacts operate markedly differ in the case of lead grains from those in the case of plastic grains. More specifically, comparison of Figs. 1 and 3 reveals that, in the experimentally obtainable range of normalized vibrational displacements $\xi < 0.2$, the vibrations of the partially relieved contacts in the plastic samples corresponded mainly to region I and to the start of the transition to region II (using the notation of Fig. 1). In the lead samples, on the other hand, regions I and II corresponded to very small amplitudes (about $\xi \leq 0.05$), whereas, over the greater part of the amplitude range investigated, the prevailing condition was that of region III. Therefore, in numerical calculations, the coefficient $\mu_1$ characterizing the compression of relieved contacts was chosen to be 0.07 for the plastic samples and 0.01 for the lead samples. The ratio $v_0/v_1$ of contacts in the main and relieved fractions were assumed in calculations to be equal to 1/6 and 1/4, respectively. (They were chosen so as to match the level of the second harmonic and to account for the likely increase or decrease in the rigidity of the sample at the fundamental, which was mentioned earlier.) The choice of these variables was not very critical for the behavior of the third harmonic. Indeed, they could be varied by as much as 25 - 35% without radically affecting the calculated results qualitatively or quantitatively. In particular, with the variables changed as noted above, calculation consistently yielded a nearly cubic behavior for the third harmonic, as shown in Fig. 3, which is attributable to the joint action of compressed and clapping contacts.

The increase in the level of the second harmonic by a factor of 1.5 to 2.5 (compared to the value expected for the ideal-packing case) also showed good agreement with the calculated result. Moreover, allowance for the effect of clapping contacts (assuming the values of $v$ and $\mu$ given above) for the lead sample did lead in calculations to a power exponent in the range 1.7 - 1.9, instead of the strict quadratic relation, as was noted in the discussion of experimental findings in [16].

The relative level and behavior of the harmonics as obtained by numerical calculations with allowance for nonideal packing show a far better agreement with experimental values than with those associated with the ideal-packing model. Through the choice of $\mu_1$ and $v_1$ it would be possible to obtain a closer fit between experimental and calculated values. Notably, it would be possible to describe more accurately the range of amplitudes $\xi$ for the plastic sample where the third harmonic almost reached the level of the second harmonic in the experiment. (The minimum difference between the numerically calculated levels of harmonics was given by a factor of 3 to 5 instead of 100 to 200 for calculations based on the ideal packing model.) There seems to be no particular sense in refining the variables any further. The point is that the model itself, consisting of only two fractions of contacts, is rather crude, and the differences noted above can be minimized by using a greater number of components. What appears to be more surprising is the fact that the model proved accurate enough in describing the effects observed. From the comparison given above, it follows that the greater proportion of the relieved contacts in the test samples did operate under approximately the same conditions.
which were regions I and III (see Fig. 1) in the case of plastic and lead grains, respectively. This implies that the actual broad distribution of contacts in terms of initial pressure is bound to have two rather well-pronounced maxima; i.e., it must be almost bimodal.

CONCLUSION

In summary, allowance for the effect of relieved intergranular contacts has made it possible to explain all the qualitative differences noted in experiments in [16] and elsewhere [11 - 15] from the corollaries of the ideal-packing model and to obtain a fairly good fit with experimental values even with a nonideally-packed-grain model – the simplest two-component approximation conceivable. Relieved contacts have been found to have an especially strong effect on higher-order nonlinearities.

ACKNOWLEDGMENTS

I would like to thank I. Yu. Belyaeva and E.M. Timanin for their interest in this study and valuable suggestions.

This study was financially supported by the Russian Foundation for Fundamental Research (project no. 94-02-03508-a) and the International Scientific Foundation (project no. R8Y000).

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