The influence of external pulse-vibrational loadings on the atomic-molecular motion in real soils

T Magkoev¹,², V Zaalishvili¹ and G Tuaev¹,²

¹ Geophysical Institute of Vladikavkaz Scientific Center, Markov Street, 93a, 362002, Vladikavkaz, Russia
² North Ossetian State University after K.L. Khetagurov, Vatutina Street, 44-46, 362025, Vladikavkaz, North Ossetia - Alania, Russia

E-mail: cgi_ras@mail.ru

Abstract. The connection between the effect of atomic-molecular vibrations on macroscopic phenomena in real soils is investigated. Granite and clay samples were used as an object of study. The experiment was carried out by IR spectroscopy method. Spectra from the samples were taken under various external loadings. The clearly nonlinear nature of the phenomena occurring in real soils was established. The results of the experiment were compared with the data for real soils obtained in field surveys using the GSK-6M explosive source. This procedure confirmed the relationship of atomic-molecular vibrations with manifestations on macroscopic objects.

1. Introduction
Modern fundamental science often “seeks” development paths in the relationships of seemingly completely different and unexpected directions. This trend has not become alien to modern geophysical science. At the beginning of the 20th century, Koblenz discovered the phenomenon of individuality and characterization of the silicates spectra. In the 1930s, Schaefer and Matossi investigated the spectra of more than 50 minerals [1]. In the 1960s, a large amount of research was conducted by Russian and foreign scientists [2, 3]. And such work continues to this day [4-17]. At the same time, despite quite numerous publications, the question of the nature of the interaction of an external mechanical (pulse-vibrational) loading on the behavior of a macrobody caused by atomic-molecular motion in a solid remains practically unexplored. It is the reaction of atomic-molecular bonds to one or another loading that largely determines the behavior of a solid on a macroscopic scale since the observed macroscopic manifestations are, to one degree or another, the result of multiple superposition of the movements of individual atoms and molecules. From these positions, the interconnection of the interaction phenomena of microparticles and macroparameters of real objects is one of the most important issues of modern geophysics, including engineering seismology and geoinformatics [18]. Moreover, the interrelation of the phenomena of the interaction of nanosized particles of the soil medium and the macroscopic parameters of real soils is one of the most important directions [12, 16, 17].
2. Methods

Figure 1. Infrared Fourier spectra of granite at various frequencies of external mechanical impact.

We used the physicochemical method for studying atomic and molecular vibrations in the matter - the method of infrared Fourier spectroscopy, which has recently been widely used in geology and geophysics. Two devices were used in the work: FSM-1202 Fourier spectrometer (Infraspec) and Bruker Alpha2 IR Fourier spectrometer.

The size of the samples is 10 x 10 x 1 mm$^3$. The samples were exposed to signals of different frequencies: 0, 5, $10^2$, $10^5$ Hz. The spectra obtained are shown in figure 1. The spectral band of vibrational frequencies in the 2000–3000 cm$^{-1}$ area corresponds to the Si=O bond in the investigated granite sample (inset to the right, in figure 1). Moreover, as can be seen from figure 1, the vibrational characteristics of the spectra outside the band of 2000–3000 cm$^{-1}$ are almost completely identical to each other at all frequencies of the applied external loading. This indicates that, under external loading, the interionic bonds in granite Si2+ - O2 undergo the greatest change. In this case, with an increase in the frequency of the external force, the amplitude of vibrations of these bonds increases. This can lead to a change in the lengths and angles of bonds in the granite lattice and the appearance of internal mechanical stresses in this connection. The invariance of the spectra, with the exception of the area corresponding to interionic vibrations (2000-3000 cm$^{-1}$), made it possible to establish that external intense loading leads to a significant fundamental change in the state of interatomic bonds, which, in our opinion, determines one or another of its macromechanical manifestations.

Figure 2 presents a graph showing the dependences of the vibration amplitudes on the loading frequency. Here we can talk about some sharp increase in the amplitude, after which there is energy saturation, and the rate of the amplitude change varies slightly. This indicates the presence of nonlinear effects arising in the structure of the rock.
Figure 2. The dependence of the amplitude of the vibrations of the intramolecular bond Si = O on the frequency of external mechanical impact.

In a first approximation, the dependence shown in figure 2, can be approximated by two linear sections, the intersection point of which, taking into account the above, can be considered the ultimate strength of the atomic lattice of granite. This dependence has a clearly nonlinear form, characterized by a critical point corresponding to the tensile strength of the atomic lattice of granite under variable mechanical loading.

This effect is observed not only in laboratory samples but also in real soils, which completely excludes the connection of the damping effect with the dimensions of the test object (figure 3, figure 4) (Zaalishvili, Magkoev et al., 2019) [18,19].

In this regard, it is precisely such models based on the study of the internal structure of real soils that can serve as an alternative to existing methods.

For convenience and possible predictions of the behavior of granite at other frequencies of external loading, the dependence shown in figure 2 can be represented in the following analytical form:

$$A = 0.2262 + 2.46537E-4 \sigma - 2.1986E-6 \sigma^2 + 2.19614E-11 \sigma^3$$ (1)

The analysis of field studies for loadings with a powerful non-explosive source GSK-6M (with two strikers and a total falling mass of up to 20 tons on the surface of the soil stratum of thick sand deposits (figure 3)) shows that a high-frequency area arises under intense loads in the near zone of the source. This area is characterized by a significant value.

This area attenuates rapidly with a distance from the source. In this case, in a remote (low-frequency) or linear area of the source influence, the waveform and the predominant vibration frequency remain practically unchanged.
Figure 3. Investigations of spectral features from the source GSK-6M: a - profile measurements on the site; b - record of ground vibrations from the second striker; c - record of ground vibrations from the first striker.

This clearly indicates the manifestation of distinct nonlinear effects in soils under intense loads in real soils. A comparison of the results obtained in the analysis of atomic-molecular motion with phenomena on a macro-object shows their good analogy (figure 2-4).

Figure 4. Dependence of the real spectrum area of vibrations on acceleration.
Similar experimental studies of this type were also conducted for clay samples. The samples were exposed to different frequencies: 0, 20, $10^2$, $10^3$, $10^4$, $10^5$ Hz. In this case, infrared spectra were recorded using a Bruker Alpha 2 IR Fourier spectrometer.

The experimental results are shown in figure 5.

![Infrared Fourier spectra of clay at various frequencies of external mechanical loading.](image)

**Figure 5.** Infrared Fourier spectra of clay at various frequencies of external mechanical loading.

Here, the vibrations in the range of $3000–3500$ cm$^{-1}$ correspond to the vibrations of OH groups. A decrease in amplitude depending on the frequency of exposure can be an indicator that water here is a certain damper of vibrations caused by the impact of the pulse-vibration type.

The reaction spectrum corresponding to clay soils is in the lower frequency range ($750-1250$ cm$^{-1}$) than the reaction spectrum of granite soils ($2000-3500$ cm$^{-1}$). This phenomenon, namely, the high-frequency spectral characteristics of granite, is explained by the incomparably stronger bonds of granite particles than clay.

3. Results

At the next stage, it seemed necessary to conduct an experiment in the field. These results were supposed to allow a direct comparison of the results of the load at the level of atomic-molecular bonds with the macromechanical action (impulse or vibration) on real soils.

In figure 6 is presented the dependence of the real spectrum area of soil vibrations for strong earthquakes on the frequency of external loading (acceleration). For hard or rocky soils, the real spectrum area of the corresponding vibrations (station Oni) increases (figure 6a), and in soft or clay soils (station Iri) it decreases with an increasing acceleration of vibrations (figure 6b).
It was previously established that the values of the ratio of the areas of the subspectral areas are similar to the ratio of the peaks of the corresponding soil vibrations (Zaalishvili, Magkoev et al., 2019). This made it possible to use the simplest and at the same time very stable characteristic of soil vibrations – the area of real vibrational spectra.

It was shown above that an intense external mechanical or pulse-vibrational loading on granite leads to a rather pronounced change in the vibration amplitude of the Si=O interionic bond without a significant change in its wave number. It was found that an increase in the frequency of external load leads to an increase in the amplitude of vibration bond Si=O. This dependence has a clearly nonlinear form, characterized by a critical point corresponding to the tensile strength of the atomic lattice of granite under varying or variable intense mechanical load (figure 2).

The results of the studies show that the atomic-molecular movements of nanoscale soil particles are similar to the phenomena observed under external loads or effects on real objects or macro objects. This is, without a doubt, a good reason for including the results of the research directly into practical activities. At the same time, the results of laboratory studies of atomic-molecular effects, in contrast to the results of small-scale laboratory studies in the form of different types of models, which are at the

Figure 6. The dependence of the real spectrum area of rocky (hard) (a - Oni) and soft (b - Ambrolauri) soils on the vibration frequency.
same time tens or even hundreds of times macroscopic objects and under pressure from critics in recent years, can be quite justifiably used in terms of reliability with the results of field studies.

4. Discussion
The final results of the research should be the relationship between the phenomena observed at the atomic-molecular level, with their manifestation at the macro level in one or another empirical-analytical form. This will make it possible to predict changes in the behavior of various media under external loadings, due to the characteristics of various processes and phenomena. This, in turn, necessitates a number of theoretical and experimental studies. So, the next most important stage should be an active comprehensive experimental research conduction with the aim of creating new theoretical views on the relationship of the state of the same objects and the phenomena occurring in them from the point of view of the micro- and macro-world. This will significantly develop our ideas about the cause-effect relationships of the formation and course of these phenomena themselves. Then, on the basis of numerous standard measurements, statistically valid quantitative relationships will be established between similar phenomena at micro and macro objects, which will create conditions for the development of an adequate physical and mathematical model of soil destruction under intense external pulse-vibration loading. This will make it possible to predict the behavior of macro-objects at the quantitative level based on the characteristics of atomic-molecular motion in a micro-object.

5. Conclusions
Using methods of X-ray photoelectron spectroscopy and infrared Fourier spectroscopy the relationship between the nature of interatomic vibrations in various types of soils and the features of their manifestation at the macro level was established for the first time. It is shown that an increase in the amplitude of vibrations of interatomic bonds leads to a nonlinear increase in the frequency of soil vibrations. The nature of this dependence allows us to estimate the limit of stability (destruction) of the soil.

The similarity of the relationships between the selected vibrational indices in the form of the areas of the real vibrational spectra of objects with the vibrational frequency of the load at the atomic-molecular and macro levels is defined. With an increase in the vibration frequency of the real spectrum area in hard soils grows and in soft soils decreases in both cases.

An analysis of the results of atomic-molecular studies shows that they can reasonably be used along with the results of field studies on real objects or on macro-objects.

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