On the Possible Mechanism of Energy Transmission by Mechanical Impact

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Abstract

The phenomenon of mechanical impact has been studied to determine the response of solids to the intensive mechanical disturbance. The process of blow is considered as sudden simultaneous change of velocities of all atoms of striking particle. The probabilities of lattice excitation and prerequisites to structural imperfections have been investigated. The calculations for cubic germanium, silicon, and diamond crystals were performed.

INTRODUCTION

At present, the phenomenon of mechanical activation of solids is used successfully in various technological processes. There are many kinds of grinding equipment (ball, vibration, planetary, attrition, roller, jet, pin mills and disintegrators), which are used for powder activation. Although mechanical strains in particular mills are different and depend on grinding conditions, one can distinguish a group of apparatuses with very close strain conditions, for example, jet, pin mills and disintegrators. This kind of apparatus is characterized by high velocities of impact at the free-hit mode and little time of interaction.

In connection with the fact that transformation of mechanical impact energy into the enthalpy of activation is the main problem while using the phenomenon of mechanical activation, the present work deals with the possible mechanism of energy transmission in the process of mechanical treatment in the above-mentioned kinds of mills.

METHOD AND RESULTS

Mechanical strains appearing during a blow directly act on the atomic structure of matter and, as it was noted for the first time in [1], cause the excitation of lattice vibrations. Considered below is the possible mechanism of energy transmission by mechanical impact through the exciting of the mechanically induced lattice vibrations.

Lattice vibrations of atoms in a monoatomic lattice are regarded as a set of identical independent quantum-mechanical harmonic oscillators [2]. The wave functions of these harmonic oscillators can be obtained from equation [3]:

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} - v(x)\right]\Psi_n(x) = E_n\Psi_n(x) \qquad (1)$$

Here, $\hbar$ – Plank constant, m – mass of atom. In the harmonic approximation, $v(x) = kx^2/2$, where $k = m\omega^2$ – force constant, ω – frequency of thermal vibration, n – main quantum number of oscillator. Solutions of this equation are the wave functions of harmonic oscillator:

$$\Psi_n(x) = \left(2^n n!\, a\sqrt{\hbar}\right)^{-\frac{1}{2}} \exp\left[-\frac{x^2}{2a}\right] H_n\left(\frac{x}{a}\right) \qquad (2)$$

Here, $H_n(x/a)$ is Hermite polynomial, $a = \hbar/(m\omega)$.

The energy E_n is the eigenvalue of the equation (1) and is determined from the relation:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \tag{3}$$

The process of blow is considered as a sudden simultaneous change of velocities of all harmonic oscillators. Then, each of the oscillators, described by the equations (2), (3) at the moment of time $t = 0$ begins moving with the velocity v. The probability of excitation of oscillator can be found by transition to a system of coordinates K^1, which is moving with the lattice. Then, $x^1 = x - vt$.

The wave function of initial state $\Upsilon_0(x^1)$ is connected with the wave function of the oscillator $\Upsilon_n(x^1)$ for $t > 0$ by the relation:

$$\Psi_n(x^1) = \exp\left[-\frac{imv}{\hbar}x^1\right]\Psi_0(x^1) \tag{4}$$

In order to obtain relation (4), the law of wave function transformation under Halileo conversion [4] was used. The probability of oscillator excitation or, in other words, the probability of transition W_{0n} from the initial state with the wave function $\Upsilon_0(x)$ and the energy E_0 to the excited state with the wave function $\Upsilon_n(x)$ and the energy E_n is given by the relation:

$$W_{0n} = \left[\int_{-\infty}^{\infty}\Psi_n(x)\exp\left[-\frac{imxv}{\hbar}\right]\Psi_0(x)dx\right]^2 \tag{5}$$

The calculation of integral (5) gives:

$$W_{0n} = \frac{1}{n!}\left(\frac{mv^2}{2\hbar\omega}\right)^n \exp\left[-\frac{mv^2}{2\hbar\omega}\right] \tag{6}$$

Thus, the consideration of mechanical impact as a process of sharp change of atomic harmonic oscillator velocities gives directly the probabilities of excitation of mechanically induced lattice vibrations. The value W_{0n} denotes the probability of transition to the n-th exciting level. The dependences of the probability W_{0n} of collision excitation for the first two values of n vs. $q = mv^2/(2\hbar\omega)$ are shown in Fig. 1. All the functions W_{0n} are dimensionless and normalized, so that $\sum_{n=0}^{\infty} W_{0n} = 1$. Here, W_{00} is the probability of the nonexcited state formation. The collision parameter q is also dimensionless. As can be seen from Fig. 1, the maximum values of these functions are observed

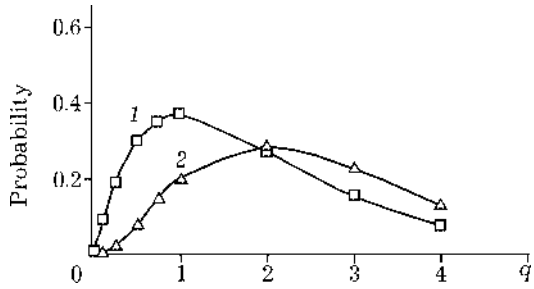

Fig. 1. The probability of collision excitation *vs.* $q = mv^2/(2\hbar\omega)$ parameter: *1* and *2* – functions W_{01} and W_{02}, respectively.

at the points $mv^2/2 = n\hbar\omega$. The conditions for excitation of vibration levels with the least expenditures of energy, *i. e.* transition when W_{01} are used, are of practical interest. The maximum value of W_{01} is observed when

$$mv^2/2 = n\hbar\omega \tag{7}$$

The relation (7) indicates that the maximum values of the probability of the lattice excitation and accordingly the maximum effect of mechanical action are observed for the velocities, at which the kinetic energy of blow per one atom is close to the energy of lattice vibration quantum.

Assuming that (7) is complied with, the amplitude of the vibration r_m caused by the mechanical blow can be calculated using the relation $mv^2/2 = m\omega^2 r_m^2/2$, hence, one can derive

$$r_m = v/\omega \tag{8}$$

This relation gives an expression of the atomic vibration amplitude r_m, caused by the mechanical blow, as a function of the impact velocity. At the definite critical values of the collision velocities v_{cr}, the amplitude r_m can reach some critical value r_{cr}, when the equilibrium atom position in the lattice is unstable, and the possibility of atomic displacements to interstice emerges. Further, the following relation is introduced:

$$a_{cr} = r_{cr}/R \tag{9}$$

Value of a_{cr} will be used later on as a criterion of the emergence of lattice imperfections caused by the mechanical blow.

Using (8), (9) the following relation can be obtained:

$$v_{cr} = a_{cr} w R \quad (10)$$

This relation expresses v_{cr} in terms of atomic frequencies and interatomic distances. Excluding w from (10) and using relation (7), the following expression can be obtained:

$$v_{cr} = 2\hbar / (a_{cr} m R^2) \quad (11)$$

DISCUSSION

Thus, assuming that the structural imperfections in a solid appear as soon as atomic vibration amplitudes exceed definite critical value, the equation, which relates impact velocity, atomic mass, interatomic distance and vibration frequency, has been found. Value of v_{cr} has the following meaning: v_{cr} is the velocity of collision, which is necessary to make an atom oscillate in the crystal lattice up to the amplitude of $r_{cr} = a_{cr} R$. This expression is helpful one, since it permits to estimate the effective regime of mechanical treatment, using atomic characteristics of crystals and a_{cr}. The latter value can be estimated by means of well-known Lindeman criterion [4], according to which in most cases solid melts, when the vibration amplitudes reach the value of about 10 % of the interatomic distance, that is a_{cr} = 0.1. To illustrate the obtained relations the calculations of v_{cr} have been made using $a_{cr} = 0.1$ for cubic germanium, silicon and diamond crystals, which have the same diamond-type lattice and different mechanical and thermal properties. The results of the calculations are presented in the Table 1. Since modern equipment, for example a disintegrator, permits to attain collision velocities of about 450 m/s, an estimation gives ground to assert that the regime of an effective mechanical treatment is accessible for germanium (v_{cr} = 180 m/s), and is real for silicon (v_{cr} = 410 m/s), yet it is unattainable for diamond (v_{cr} = 1680 m/s).

Further, from (7) and (10) one can deduce

$$w = \hbar / (0.005\, m R^2) \quad (12)$$

Here, w_{cr} is the frequency of atomic vibrations with the amplitude $r_{cr} = 0.1R$. The calculations showed that w_{cr} for Ge and Si is within the infrared spectra range, but $w_{cr} > w$ for any frequency of the diamond IR spectrum range. That is why the collisions with $v = v_{cr}$ excite effectively crystal lattice vibrations of Ge and Si with the amplitudes $r_m \sim 0.1R$ and result in the appearance of the structural imperfections. At the same time, the results of calculations for diamond can be interpreted as the impossibility to attain $r_m = 0.1R$ condition for any frequency from the infrared spectra range. By this is meant that the energy in the infrared spectra range is insufficient to oscillate atoms up to the necessary amplitude, and the $\hbar\omega_{cr}$ absorbing probability is negligible since $\hbar\omega_{cr}$ is beyond the limit of the infrared spectra range. Apparently, this fact is the cause of unique stability of the diamond crystal lattice in respect to mechanical and thermal influences.

Thus, the consideration of mechanical impact as a process of sharp change in velocities of atomic harmonic oscillators gives directly the probabilities of excitation of mechanically

TABLE 1

Physical and mechanical parameters of diamond, silicon and germanium

Parameter	Diamond	Silicon	Germanium	Ref.
Bulk modulus of elasticity, 10^{11} N/m^2	5.45	0.988	0.772	[5]
Shear modulus, 10^{10} J/m^3	93.88	11.35	9.39	[5]
Melting temperature T, ℃	3500	1420	937	[6]
Interatomic distance, Å	1.54	2.35	2.44	[7]
Frequency range of infrared (vibration) spectra, cm^{-1}	550–1250	100–530	65–300	[8]
Critical frequency w_{cr}, cm^{-1}	1433	233	97	
w_{cr}, 10^{13} s^{-1}	4.3	0.70	0.29	
Critical velocity v_{cr}, m/s	1680	410	180	

induced lattice vibrations, which strongly depend on collision velocity. The stage of the effective excitation of lattice vibrations is the first necessary step of the energy transmission to solids by mechanical impact. This energy of mechanically induced vibrations can be absorbed by lattice through the formation of structural imperfections if their amplitudes exceed some critical values. Otherwise, the energy of these vibrations is spent for the heat evolving and other radiation and emission effects. The results obtained for cubic germanium, silicon, and diamond crystals reproduce the distinct correlation between the conditions of the effective mechanical treatment and physical and mechanical properties of these crystals. It is established that the stability of crystal structures for the mechanical and thermal disturbances, within the limit of the proposed approach, is determined by the arrangement of the key parameter W_{cr} regarding the infrared spectra range.

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