PHONON DRAG OF DISLOCATIONS IN KCl CRYSTALS WITH VARIOUS DISLOCATION STRUCTURE STATES

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The pulsed technique has been used to study a dislocation resonance under the ultrasound absorption in KCl crystals with the residual strain $\varepsilon = 0.17 \div 1.8\%$, in the frequency range of 7.5 – 232.5 MHz, and at room temperature. The analysis of the data obtained testifies that a variation of the dislocation structure parameters gives rise to a substantial modification of the frequency and amplitude localizations of the dislocation resonance, whereas the damping factor B remains unchanged. The theoretical estimations of the factor B are in good agreement with the obtained experimental results.

1. Introduction

Studies of the nature of dynamic dislocation drag mechanisms that govern the mobility of dislocations at their overbarrier motion in crystals is an important issue of solid-state physics. As was shown in review [1], in the range of high velocities ($v = 10^1 \div 10^3$ m/s), a dislocation has substantial energy losses as a result of its interaction with various elementary excitations in the crystal (electrons, phonons, and so forth). This gives rise to the appearance of braking forces that act on the dislocation, with their total effect being expressed in terms of the damping B. It should be noted that the dynamic characteristic, B, is used not only for the analysis of mechanisms that restrict viscous [1] and thermal fluctuation [2] motions, but also in the cases where a moving dislocation overcomes obstacles with the help of only mechanical forces and taking inertia forces into account [3].

Earlier, for the sake of identifying the mechanisms of high-mobility dislocation drag, both the absolute values of B and the temperature dependences $B(T)$ were measured for many dielectric and metal crystals with the use of various experimental techniques. A detailed analysis of the results obtained and the methods of researches is given in reviews [1, 4].

In addition, there also appeared works [5–7], in which the influence of residual strain on the phonon drug of dislocations in acoustic crystals was first regularly studied to find the functional relation $B(\Lambda)$, where Λ is the dislocation density; in particular, KCl [5] and LiF [6] crystals were studied by the high-frequency pulse technique and Zn crystals [7] in the framework of the shock-loading method. Two reasons commanded that the dependence $B(\Lambda)$ should be determined. On the one hand, it was a necessity of studying the influence of dislocation structure parameter variations induced by a specimen deformation on the phonon drug of dislocations. On the other hand, it was a desire to verify the validity of the theory [8] which predicted a new mechanism of dynamic drag caused by the interaction between dislocations. The specified experimental techniques [5–7] were considered at that time as such which provided the most correct estimations for the damping coefficient B. Experimentally [5–7], it was revealed that the coefficient B depends on the dislocation density Λ, although this dependence was found to be rather weak. The profile of the experimental curve $B(\Lambda)$ was connected by the author of works [5–7] with a probable manifestation of the theoretically proposed drag mechanism [8]. The problem of the dislocation dynamics seemed to be solved to a certain extent, if judged from the viewpoint of experimental researches. However, a comparison made in work [4] between available, at that time, experimental data and the theory of the dynamic drag of dislocations [1] gave rise to a distrust to the majority of experimental data, including those of works [5–7].

The authors of work [4], having analyzed a large body of experimental data concerning the phonon drug of dislocations in the framework of theory [1], revealed that those data did not agree with one another, as well as with the theoretical estimations of B. The discrepancy among the absolute values of B obtained for identical crystals in a number of works and using different techniques exceeded two orders of magnitude. The situation with experimental data on the temperature dependences $B(T)$ was unsatisfactory as well; the extreme contradiction with one another was inherent to them. Moreover, it was found that not only conventional methods – in particular, the low-frequency internal friction method –

but also the basic method of shock loading [7] produced overestimated, in comparison with the theory [1], results for B, so that urgent methodological improvements were required.

Those circumstances stimulated the authors of works [9–11] to fulfill a careful verification of methods aimed at studying B. In particular, having analyzed the methodological bases of the shock loading method, the authors of work [9] came to a conclusion that, when calculating B, the amplitude and the duration of a voltage pulse in a specimen have to be measured directly rather than calculated theoretically, proceeding from model considerations. Not long after, the authors of work [10], on the basis of their own methodological developments and taking the results of work [9] into account, succeeded in applying this method to correctly examine the temperature dependence $B(T)$ for a number of insulators.

While studying the dependence $B(T)$ in copper with the use of the method of low-frequency internal friction, the authors of work [11] showed that considerable errors could mainly arise, when estimations for B were obtained in the framework of the "low-frequency" measurement techniques, because the level of the ultrasound absorption by dislocations at such frequencies is governed by not only a viscous, but also a relaxation component.

Concerning the high-frequency pulse technique [5, 6] – here, the coefficient B is determined by analyzing the decaying branch of the dislocation resonance – the authors of work [4] assert that it allows correct estimates for B, by the order of magnitude, to be obtained. At the same time, this technique also requires certain methodological improvements, in particular, more reliable methods of treatment of experimental results are needed [12].

Later on, after the experimental technology had been improved, the pulse technique was used not only to establish the reliable enough temperature dependences $B(T)$ for a number of ionic crystals [12–14], but also the functional relation $B(\Lambda)$ for NaCl [15] and KBr [16] crystals at $T = 300$ K. The temperature behavior $B(T)$ was also found for NaCl [15] and KBr [16] crystals, provided that the dislocation density was varied.

In this work, in order to specify the results of work [5] and to obtain a reliable functional dependence $B(\Lambda)$, new methodological approaches, which had been successfully approbated in works [13–16], were used to carry out reference acoustic measurements of dislocation resonance losses of ultrasound in KCl crystals under conditions that their dislocation structure was modified.

2. Experimental Technique

In this work, the damped dislocation resonances were studied by the pulse technique on longitudinal waves in the frequency range $22.5 - 232.5$ MHz. Single crystals of KCl with a residual strain of $0.17 - 1.8\%$ were examined at $T = 300$ K. The interval of preliminary specimen strains was specially selected to be much wider than that in work [5] and to provide a pronounced observation of the dislocation resonance inversion shift effect with respect to the frequency and the amplitude, which was observed for the first time in works [5, 6].

An original experimental complex [17] was used. It allowed the simultaneous precision measurements of acoustomechanical characteristics of crystals to be carried out at temperature and deformation rate variations, making use of acoustic waves with various amplitudes and frequencies.

For a confrontation of the results obtained with the data of work [5] to be more correct, the experiments were carried out using $\langle 100\rangle$-oriented specimens $18\times18\times30$ mm^3 in size. The specimens were cleaved off from the same massive single crystal as was used earlier for the fabrication of specimens to study [5]. The specimens prepared in such a way were finely ground and polished in order that the nonparallelism of their working surfaces after the treatment should not exceed 1 μm/cm. To eliminate the results of a mechanical treatment, the specimens were annealed for 15 h at 630 °C. Then they were slowly cooled down to room temperature.

For the insertion of "fresh" dislocations, the crystal was preliminarily squeezed along its long axis on a test machine of the "Instron" type, at a deformation rate of 10^{-5} s^{-1} in the $\langle 100\rangle$-direction, in which the specimen was sounded. In so doing, we used an original specially designed device which ensured that the working surfaces of the specimen would remain plane-parallel. The techniques of selective etching and metallographic analysis of crystals were the same as in work [5].

To separate the dislocation part of the total absorption, which was measured for a strained specimen, the background measured for the same specimen before deformation rather than the average background (found by averaging over several specimens) was subtracted. An advantage of such a procedure for the separation of the dislocation contribution is that the spread of experimental points becomes substantially narrower, which allows the amplitude and frequency localizations of the dislocation resonance to be determined more accurately and, hence, the damping coefficient B to be found more exactly.

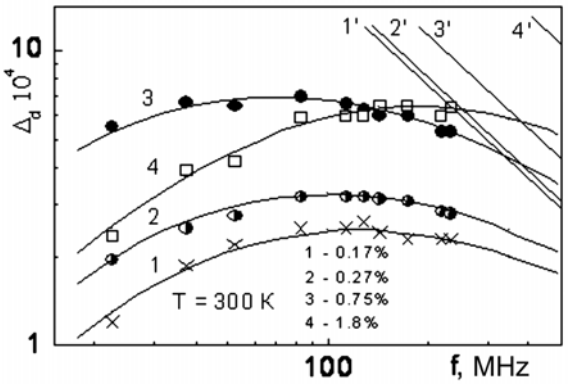

Fig. 1. Frequency dependences of the dislocation-induced resonance ultrasound absorption in KCl crystals deformed at T = 300 K to the strain $\varepsilon = 0.17$ (*1*), 0.27 (*2*), 0.75 (*3*), and 1.8% (*4*)

3. Experimental Results and Their Discussion

In Fig. 1, the typical experimental dependences of the dislocation decrement on the frequency, $\Delta_d = \Delta_d(f)$, for preliminarily strained KCl crystals are depicted. The curves for strains $\varepsilon = 0.44$, 1.15, and 1.54% have a similar shape and, therefore, are omitted. One can see that the strain change gives rise to the inversion in the behavior of frequency spectra.

When a deformation starts, resonance curves *1* and *2* increase their height and shift toward the low-frequency range. If a deformation grows, the rate of resonance shift firstly slows down, then the resonance stops and starts to move in the opposite direction. The inversion effect at a growth of the residual specimen strain is demonstrated more exactly in Fig. 2 by experimental curves 2 and 3 plotted for the resonance frequency f_m and the maximal decrement Δ_m, respectively. It is evident that the indicated resonance parameters change synchronously when the strain increases, but in the opposite directions.

From Fig. 1, one can see that the frequency dependence of the dislocation losses, $\Delta_d = \Delta_d(f)$, behaves like a damped dislocation resonance [18]. According to the theory [18], the equation which describes the decaying branch of the resonance curve $\Delta_d = \Delta_d(f)$ looks like

$$\Delta_\infty = \frac{4\Omega G b^2 \Lambda}{\pi^2 B f}, \qquad (1)$$

where Δ_∞ is the value of dislocation decrement for the frequencies $f \gg f_m$, Λ is the dislocation density, Ω is the orientational factor, G is the shear modulus of the actual slip system, b is the absolute value of the Burgers vector, and B is the damping constant. With the help of the measured resonance curves (Fig. 1), it is easy to use Eq. (1) to calculate the constant of dislocation braking B, if the values of Δ_∞ and Λ are previously determined from the high-frequency asymptotics and by calculating etched patterns, respectively. For this purpose, in work [5], the obtained experimental curves were replotted in the coordinates $\Delta_d = \varphi(1/f)$, and the phonon drug coefficient B was found by formula (1) from the slopes of rectilinear sections of the obtained curves. As a rule, the experimental values of the constant B found in such a way agreed well with theoretical estimations [4]. However, in the cases where the number of experimental points, owing to their shift along the frequency axis, was not enough in the decaying branches of the resonance curves $\Delta_d = \Delta_d(f)$, the indicated treatment gave rise to substantial calculation errors for the damping coefficient B.

In such cases, another technique for the treatment of experimental data, which had been successfully applied in works [12–16], turned out more reliable. Namely, the experimental results were extrapolated into the limiting frequency range by the theoretical curve, whose high-frequency asymptotics was used to determine the absolute value of B. The experimental data together with the corresponding fitting curves are depicted in Fig. 1. One can see that the experimental points are described well by the normalized frequency profile which was calculated in work [19] for the case of the exponential distribution of dislocation segments over their lengths. Note that, according to recommendations made in works [12–16], when fitting a theoretical profile to experimental data, the fitting procedure should always include only experimental points in the decaying branch of the dependence $\Delta_d = \Delta_d(f)$ and in the resonance region.

Certainly, to ensure correct estimations of B-values, it is necessary to make an exact account of the other parameters in formula (1) as well. In this work, we used the value $\Omega_{100} = 0.4$ for the orientational factor and $G_{110} = 1.582 \times 10^{10}$ Pa for the shear modulus which were calculated by us with regard for the elastic moduli C_{ik} measured earlier in work [12] for annealed non-deformed KCl single crystals. The indicated characteristics were calculated by the formulas $G_{110} = \frac{1}{2}(C_{11} - C_{12})$ [20] and $\Omega_{100} = (C_{11} - C_{12})^2/(4C_{11}G_{110})$ [21]. The value $b_{110} = 4.46 \times 10^{-10}$ m was calculated by the formula taken from work [20] with the substitution of $a = 6.295 \times 10^{-10}$ m, the value taken from work [22], for the lattice constant.

In this work, as well as in work [5], a special attention was payed to a decrease of measurement errors of the parameter Λ which, according to the opinion of authors of work [1], confine the estimation accuracy for B.

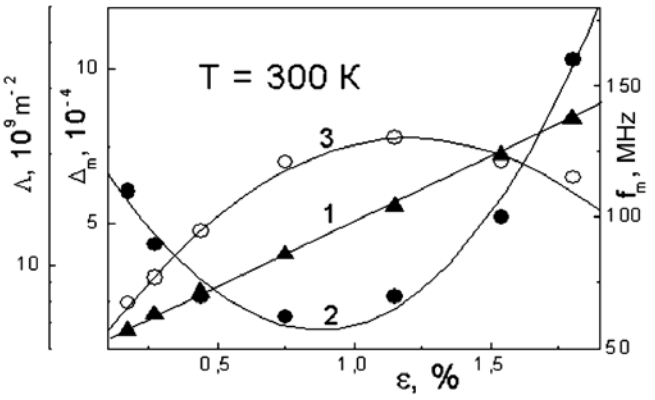

Fig. 2. Strain dependences of the dislocation density Λ (*1*), the resonance frequency f_m (*2*), and the decrement Δ_m (*3*) in the resonance curve maximum

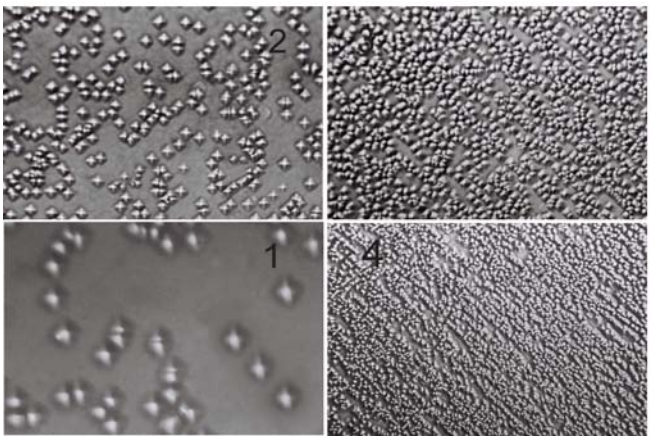

Fig. 3. Etched pits on the faces of KCl cubic crystals: (*1*) non-deformed crystal, the strain $\varepsilon = 0.27$ (*2*), 1.15 (*3*), and 1.8% (*4*)

For this purpose, in this work, we used a methodological technique which was proposed for the first time in work [5] and consists in the following. If the preliminary deformation of a crystal is carried out with a low deformation rate of 10^{-5} s^{-1}, the crystal surface, being etched after the loading, becomes uniformly covered with etched pits, with no slip band being formed. This state of dislocation structure is explicitly illustrated by the corresponding micrographs in Fig. 3 for non-deformed and deformed KCl crystals. We may assert that low-rate plastic deformation of KCl specimens, at least until the strain $\varepsilon = 1.8\%$, does not result in the appearance of slip bands, which considerably reduces the errors of Λ-value determination. The remark of the authors of work [1] is confirmed only in the cases, when the preliminary strain is carried out under the conditions of high-rate deformation, which gives rise to the appearance of slip bands.

For the selected specimen geometry and deformation direction, the slip in KCl crystals occurs in four equally stressed slip systems $\{110\}\langle 110\rangle$. In such systems, as experiments showed, when the loading continuously grows to the strain $\varepsilon \leq 1\%$, one slip plane is actuated firstly; then, at $\varepsilon > 1\%$, the second plane, which is perpendicular to the first one. The two other planes manifest themselves much later, at $\varepsilon \approx 10\%$.

In this work, as well as in work [5], the dislocation density was determined by the selective etching technique applied to as-cleaved lateral surfaces {100} which were parallel to the crystal squeezing axis. In order to determine the Λ-value, there were selected about 40 fields, which corresponded to different sections of crystal face. The calculation of etched patterns was carried out with the help of a Photoshop software. The average Λ-value was determined with an accuracy of not worse than $15 - 20\%$. The dependence of the dislocation density Λ on the residual strain in KCl crystals is presented by curve 1 in Fig. 2. One can see that the Λ-value increases proportionally to the strain ε.

Using the plot obtained for the dependence $\Lambda(\varepsilon)$ (Fig. 2), the measured frequency resonance curves $\Delta_d = \Delta_d(f)$ (Fig. 1), and the calculated values of parameters G_{110}, b, and Ω_{100}, we determined the shape of the function $B(\Lambda)$ which is presented by curve *1* in Fig. 4. In contrast to the results of work [5], the absolute values of the damping coefficient B remained expectedly almost invariable, when the parameters of a dislocation structure varied at the fixed temperature $T = 300$ K. In the opinion of the authors of work [11], the absence of any effect of a preliminary treatment of the researched crystal on the Λ-value is a natural result, if one supposes that the constant of viscous damping is determined by the interaction between dislocations and elementary crystal excitations, in particular, phonons. The obtained independence of B- and Λ-values for KCl crystals qualitatively agrees with similar data obtained earlier for NaCl [15] and KBr [16] crystals.

In this work, we confronted the absolute values of B obtained experimentally and calculated in the framework of the theory [1]. According to the results of work [1], the contributions of the phonon wind and "slow" phonon relaxation mechanisms to the dislocation drug can be calculated by the formula

$$B = \left[4 + \left(\frac{|n|}{G} - 6\right)^2\right] \frac{\hbar}{b^3} \left(\frac{\kappa_{\rm D} b}{2\pi}\right)^5 \times$$

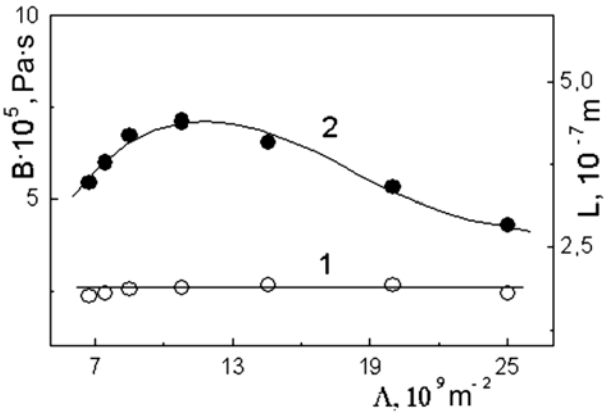

Fig. 4. Dependences of the coefficient of dislocation braking by phonons (*1*) and the dislocation segment length (*2*) on the dislocation density

$$\times \left[f_1\left(\frac{T}{\theta}\right) + \lambda_\theta \frac{\theta}{T} f_2\left(\frac{T}{\theta_0}\right)\right], \qquad (2)$$

where $\hbar = \frac{h}{2\pi}$, h is Planck's constant, $\kappa_{\rm D}$ is the Debye limit in the phonon spectrum, n is the Murnaghan modulus, b is the Burgers vector modulus, $\lambda_\theta = \Delta f_1(1)/[1 - \Delta f_2(1)]$, Δ is a phenomenological parameter that is determined from experiment, $f_2(1) = 0.92$, and θ is the Debye temperature.

When using the plots of the functions $f_1(T/\theta)$ and $f_2(T/\theta)$, and the values of the quantities $|n|/G = 35$ and $\beta = 2\kappa_{\rm D} r_0 = 30$ (here, $r_0 \approx 3b$ is the effective radius of the dislocation core) taken from work [1], as well as the values of the parameters $\Delta = 0.5$ and $\theta = 235.77$ K found earlier [12], and $T = 300$ K, Eq. (2) brings about the absolute value for the damping coefficient $B = 0.8 \times 10^{-5}$ Pa · s. The obtained theoretical estimation for B agrees satisfactorily with the average value $B = 2.57 \times 10^{-5}$ Pa · s found experimentally.

To elucidate the nature of an inversion shift of the dislocation resonance with respect to the amplitude and the frequency, we experimentally studied the dependence of the average effective length of a dislocation segment L on the dislocation density Λ. The quantity L was calculated, according to work [18], by the relation

$$L = \sqrt{\frac{0,084\pi C}{2B f_m}}, \qquad (3)$$

where C is the linear tension of a bent dislocation, which was estimated as $C = 2Gb^2/[\pi(1-\nu)]$. The Poisson's ratio $\nu = 0.158$ was calculated by the formula $\nu = C_{12}/C_{11} + C_{12}$ [20]. Using the found values for the quantities $C = 2.379 \times 10^{-9}$ N and $Gb^2 = 3.15 \times 10^{-9}$ Pa·m^2, as well as the plots of the dependence of the resonance frequency on the strain $f_m(\varepsilon)$ (Fig. 2, curve *2*) and $B(\Lambda)$, we found the dependence $L(\Lambda)$ exhibited in Fig. 4 (curve *2*).

One can see that if the dislocation density in the crystal grows continuously, the quantity L firstly increases and then, having achieved its maximal value, starts to decrease monotonously. Such a behavior can evidently be explained in the framework of the dislocation interaction model [23]. According to this model, a crystal strain gives rise to the unfixturing of existing "growth" dislocations and the emergence of new sources which generate long dislocation loops. An increase in the number of such high-mobility dislocations leads to an increase of the maximal decrement Δ_m and a decrease of the resonance maximum frequency f_m with increase of a deformation (see Fig. 2).

However, starting from the strains $\varepsilon \approx 0.9\%$, dislocations also emerge in the other slip planes and exert a fixing action upon dislocations in the primary plane. As a result of this interaction between dislocations, the quantity L starts to decrease, which manifests itself in a reduction of the dislocation-induced ultrasound losses and a shift of the damped dislocation resonance toward the high-frequency range.

After the dependences $L(\Lambda)$ and $\Lambda(\varepsilon)$ have been found, it becomes possible to estimate a contribution of the mechanism associated with the interaction between dislocations which was proposed in work [8] to the dislocation braking. The value of the braking coefficient B^* related to this effect can be estimated by the relation $B^* = B(1 + \Lambda L^2/\beta^2)$ [8], where B is the braking coefficient for a crystal with low dislocation density, and β is a numerical coefficient close to 1. From this formula, one can see that the quantity B^* can be appreciable only provided that $\Lambda L^2 \gg 1$. According to our data, for the most favorable combination of the parameters $\Lambda = 1.3 \times 10^{10}$ m^{-2} and $L = 4.41 \times 10^{-7}$ m, which takes place at the strain $\varepsilon = 1\%$, the increment $\Lambda L^2 \ll 1$. It is evident that, under the given experimental conditions, the dislocation drug by phonons prevails in KCl crystals. Concerning a weak dependence of B on the parameter Λ which was reported in previous work [5], a new analysis of the data presented in works [5, 6] demonstrated that it was completely related to a treatment of experimental data which was not correct enough.

4. Conclusions

1. A gradual increase of the residual crystal strain was found to induce the effect of inversion shift of the

damped dislocation resonance with respect to both the frequency and the amplitude, which can be explained in the framework of the dislocation interaction model.

2. A considerable variation of the dislocation density in KCl crystals, which is caused by their deformation at a fixed temperature, was shown not to affect the absolute value of the coefficient of a dislocation braking by phonons B, but it results in the appearance of a nonmonotonous $L(\Lambda)$-dependence.

3. By applying the technique of low-rate crystal deformation which enhances the accuracy of calculation of etched pits and by using a more rational procedure of treatment of experimental data, rather correct estimations for B were obtained. On their basis, the functional dependence $B(\Lambda)$ was determined.

4. The determination accuracy of the absolute value of B becomes substantially higher, if a series of crystals with different dislocation densities rather than one crystal are used in experiments. In this case, the accuracy concerned becomes almost independent of the error made while calculating the dislocation density.

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ФОНОННЕ ГАЛЬМУВАННЯ ДИСЛОКАЦІЙ У КРИСТАЛАХ KCl З РІЗНИМ СТАНОМ ДИСЛОКАЦІЙНОЇ СТРУКТУРИ

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Р е з ю м е

Імпульсним методом в області частот 22,5–232,5 Мгц при $T = 300$ К досліджено дислокаційний резонанс в монокристалах KCl із залишковою деформацією $\varepsilon = 0{,}17$–$1{,}8\%$. На основі аналізу отриманих даних було встановлено, що в умовах варіювання параметрів дислокаційної структури істотно змінюються лише частотна і амплітудна локалізації дислокаційного резонансу, але величина коефіцієнта в'язкості B залишається незмінною. Відзначено, що отримані результати добре узгоджуються з теоретичними оцінками параметра B.