Dynamics of nitrogen in niobium-based implantation phases

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The slow-neutron inelastic scattering spectra of the α and β implantation phases of the system Nb–N are investigated. The energies of the vibrations of the nitrogen atoms in the α phase ($\hbar\omega_{1,2}=58.6$ meV and $\hbar\omega_3=91.7$ meV) and the β phase ($\hbar\omega=74.4$ meV) are determined, along with the widths of the impurity bands, and the dependence of the energies of the impurity vibrations on the metal–impurity distance is constructed. It is shown that this dependence has a general character for Me–N systems, where Me is a transition metal from group IV or V. The interatomic interaction constants are determined in the investigated alloys (Me–N), and a complex structure of the gap modes is observed in the vibrational spectrum of the α phase. © *1996 American Institute of Physics.* [S1063-7761(96)01606-X]

1. INTRODUCTION

A study of the interaction of p-elements for implantation (O, N, C) with transition metals is of great interest in connection with their effect on the physico-chemical and mechanical properties of these materials. Studies of alloys by slow-neutron inelastic scattering allow one to obtain direct information about the interatomic forces in the crystal lattice. In Ref. 1 this method was used to investigate the dynamics of nitrogen in the α and β phases of the Ta–N system. A correlation was shown to exist between the vibrational energy of nitrogen and the Me–N distance, where Me denotes transition metals from groups IV and V. To obtain a more complete picture of the behavior of nitrogen in group V transition metals and generalize the results already obtained, we have carried out a study of the dynamics of nitrogen in various implantation phases of the system Nb–N.

In Ref. 2 we presented data on the energy and half-width of only one of the local modes of the alloy $NbN_{0.03}$, which did not allow us to analyze the dependence of the vibrational energy on distance. In the present paper we present data on the vibrational spectra of the nitrogen atom in the α and β phases of the system Nb–N, gleaned from slow-neutron inelastic-scattering spectra. The dependence of the energies of the impurity vibrations of nitrogen on the metal–impurity distance is constructed and the coupling constants of the Nb and N atoms are determined. An analysis is given of the changes in the vibrational spectrum of the α-phase of Nb–N in comparison with the spectrum of pure niobium over the entire region of transferred energies, the nature and structure of the features localized in the gap between the spectrum of the acoustic vibrations of the metal atoms and the band of impurity modes of the nitrogen atoms.

2. PREPARATION AND PHASE ANALYSIS OF THE SAMPLES

2.1. Preparation and analysis of Nb sample with 3 at.% N

A sample of the α-phase of NiN_x was prepared by saturating a piece of pure niobium foil with nitrogen from the gaseous phase at 1000 °C followed by annealing for 24 hours to homogenize the sample with subsequent quenching in water. The nitrogen content, determined from the amount of absorbed gas and the change in mass of the sample after saturation, was 3 at.%. Neutron-diffraction phase analysis did not reveal a second phase in the sample; however, the *bcc* lattice parameter $a=3.304$ Å corresponds to a nitrogen content of 1.2 at.%. Indeed, subsequent measurements of the neutron inelastic-scattering spectra showed that some of the nitrogen is found in the β-phase, the amount of which is estimated at $\sim 2\%$

2.2. Preparation and analysis of Nb–N sample with high nitrogen content

With the aim of obtaining the β-phase of Nb_2N, the alloy was prepared by multiple remelting of pure niobium and niobium mononitride in a plasma-arc furnace in an inert atmosphere. The phase composition of the sample was determined by neutron diffraction analysis. Studies have shown that besides the β-phase it contains *bcc*-niobium with lattice parameter corresponding to the α-phase with 0.8 at.% N. Here, however, the overwhelming portion of the nitrogen ($\geqslant 98$ at.%) is found in the β-phase of composition $Nb_2N_{0.8}$. The total amount of nitrogen in the sample was around 20 at.%.

The structure of the β-phase corresponds to the spatial group $P\bar{3}1m$ with lattice parameters $a=5.293$ Å and $c=4.96$ Å (Ref. 3). The sublattice of metal ions of the β-phase forms a hexagonal close-packed structure with $a_0=a/\sqrt{3}$ and $c_0=c$, in which nitrogen occupies the octahedral interstices. Results of structural analysis are given in Table I.

3. EXPERIMENTAL SETUP AND PROCESSING OF RESULTS

Measurements of the neutron inelastic-scattering spectra were performed on a DIN-2PI spectrometer mounted in the beam of an IBR-2 reactor.[4] The experiments were carried out at room temperature with energy acquisition by the neutrons in two working regimes of the setup—for an initial neutron energy of 10 meV and 18.8 meV with different speeds of rotation of the chopper–monochromator.

TABLE I. Neutron-diffraction data on the structure of β-$Nb_2N_{0.8}$.

Parameter	Atom	Site	Occupancy	x	y	z
Perm.gr. $p\bar{3}1m$	Nb	$6(k)$	0.5	1/3	0	1/4
$a=5.293$ Å	N	$2(d)$	0.134	1/3	2/3	1/2
$c=4.96$ Å	N	$1(a)$	0.066	0	0	0

The scattered neutrons were recorded by detectors placed within a range of scattering angles 70° − 135°. In the case of the Nb–N sample with 3 at.% N the resolution of the spectrometer in the energy transfer regions $\varepsilon = 39$, 59, and 92 meV was $\Delta E_R = 3.9$, 5.7, and 9.3 meV, respectively ($\varepsilon = E - E_0$, where $E_0 = 18.8$ meV and E are the energy before and after scattering of neutrons by the sample).

The measurements of the sample with high nitrogen content were carried out for a lower initial energy, and the resolution in the energy transfer regions $\varepsilon = 36$, 75, and 93 meV was $\Delta E_R = 2.3$, 4.7, and 6.3 meV, respectively. Since the transmittance of both samples was $\geqslant 90$ %, corrections for multiple scattering of the neutrons in the sample were not calculated. The experimental spectra were processed to the level of the generalized frequency spectrum $g(\varepsilon)$ in the incoherent approximation in a way analogous to that described in Ref. 5.

To reveal the deformations of the vibrational spectrum of the matrix atoms brought about by the introduction of nitrogen, we measured the neutron inelastic-scattering spectra of pure niobium under the same conditions as in the α-phase. Vibrational spectra of the Nb atoms of these samples are shown in Fig. 1.

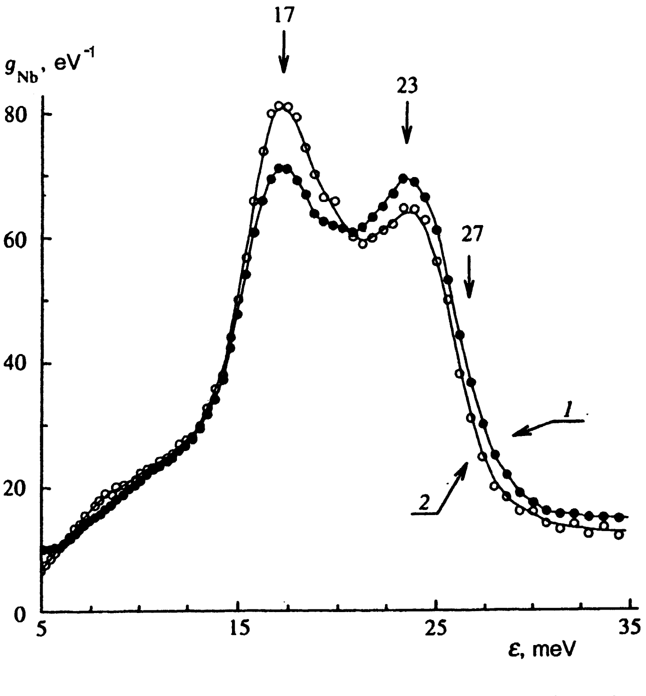

FIG. 1. Acoustic vibrational spectra of the niobium atoms in α-phase NbN_x (*1*) and in a nitrogen-free sample (*2*): $\varepsilon = \hbar\omega$ is the energy of the vibrational phonons. The positions of the features indicated by arrows and the limits of the spectra are given in meV.

To determine the vibrational spectrum of the nitrogen atoms $g_N(\varepsilon)$ in α-NbN_x from the neutron inelastic-scattering spectrum, we subtracted the pure niobium spectrum in order to account for the contribution of multiphonon and multiple processes of neutron scattering from the matrix atoms.

The frequency spectra in the region of gap and impurity modes of the α and β phases, obtained by processing the experimental data, were fitted to Gaussian curves by least squares fitting.

4. EXPERIMENTAL RESULTS

4.1. Vibrational spectra of the atoms of the matrix

Figure 1 shows a vibrational spectrum of the metal atoms in the Nb–N samples with 3 at.% (total amount) nitrogen. The fraction of vibrations of the implantation atoms in the energy region $0 \leqslant \varepsilon \leqslant 27$ meV is small and can be neglected. As indicated above, the 3 at.% N sample was two-phase; however, in the region of vibrations of the matrix atoms the overwhelming contribution (>98%) came from the α-phase. Therefore it may be assumed that the spectrum shown in Fig. 1 belongs to the α-phase of $NbN_{0.012}$. The same figure shows the vibrational spectrum of pure niobium, obtained under the same conditions. For the given experimental conditions in the energy transfer region $\varepsilon \geqslant 10$ meV the conditions of the incoherent approximation are well fulfilled. At smaller energy transfers the contribution of inelastic coherent neutron scattering can noticeably distort the actual density of vibrational states of the metal atoms.

It is clear from Fig. 1 that when nitrogen is introduced, the intensities of the two main peaks at $\alpha \simeq 17$ and 23 meV are redistributed and the boundary of the vibrational spectrum of the metal atoms is shifted by ~0.5 meV toward higher frequencies (the boundary of the vibrational spectrum of the metal atoms is defined as the midpoint of the descending side of the high-frequency limb of the spectrum $g(\varepsilon)$). Calculation of the mean-square frequency $\langle \varepsilon^2 \rangle$ of the experimental spectra of Nb and $NbN_{0.012}$ gives 360 meV^2 and 374 meV^2, respectively. Thus, introducing nitrogen into niobium leads on average to approximately a 3-percent strengthening of the Nb–Nb interaction per 1% N. Nitrogen has a similar effect on the Ta–Ta interaction in the α-phase.[6]

4.2. Impurity vibrations

Like hydrogen, the p elements O, N, and C for implantation in metals form bands of impurity states in the frequency spectrum of the crystal lattice, where the energies of these states, ω_{loc}, considerably exceed the boundary ω_D of the frequency spectrum of the matrix atoms ($\bar{\omega}_{\mathrm{loc}} \geqslant 2\omega_D$). In this case the structure of the spectra of the impurity vibrations is determined, as a rule, by the local symmetry of the interstitial site occupied by an implantation atom.[1,2,5,6] The features observed in the neutron inelastic-scattering spectra of the Nb–N samples with 3 at.% N and 20 at.% N in the energy transfer region $\varepsilon \geqslant 30$ meV are shown in Figs. 2 and 3, respectively, in the form of the function $g(\varepsilon)$. Results of least-squares fitting of the peaks corresponding to the vibrations of the nitrogen atoms in the investigated alloys are given in Table II.

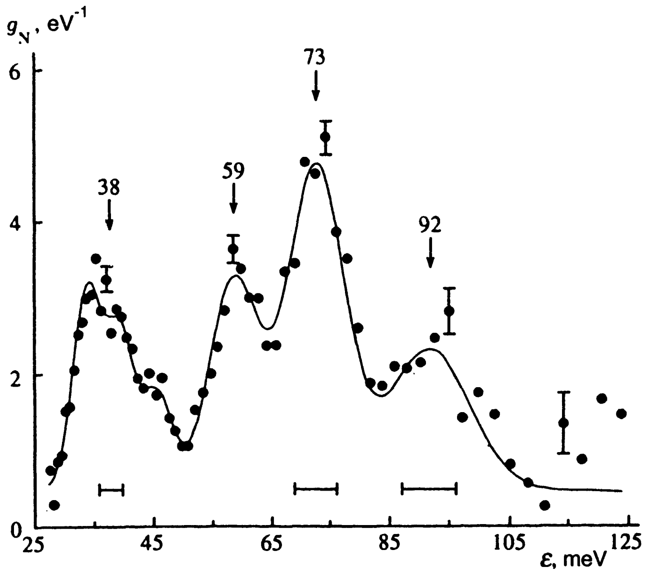

FIG. 2. Spectrum of a two-phase ($\alpha+\beta$) sample of Nb–N in the region of gap and impurity vibrations. The solid curve is the result of fitting of Gaussian curves to the spectrum of the gap modes and the spectrum of the frequencies $g_N(\varepsilon)$ of the nitrogen atom. The horizontal line segments indicate the half-width of the resolution function of the setup.

4.2.1. Vibrational spectrum of the nitrogen atoms in the α phase

In the spectrum of the two-phase sample of Nb with 3 at.% N the main features are observed at energies $\hbar\omega=\varepsilon=38$, 59, 73, and 92 meV (see Fig. 2). The feature $\hbar\omega_{1,2}=59$ meV corresponds to vibrations of the nitrogen atoms in α-NbN$_{0.012}$, which are polarized in the basis plane. The same value of $\hbar\omega_{1,2}$ in α-NbN$_x$ was previously reported in Ref. 2.

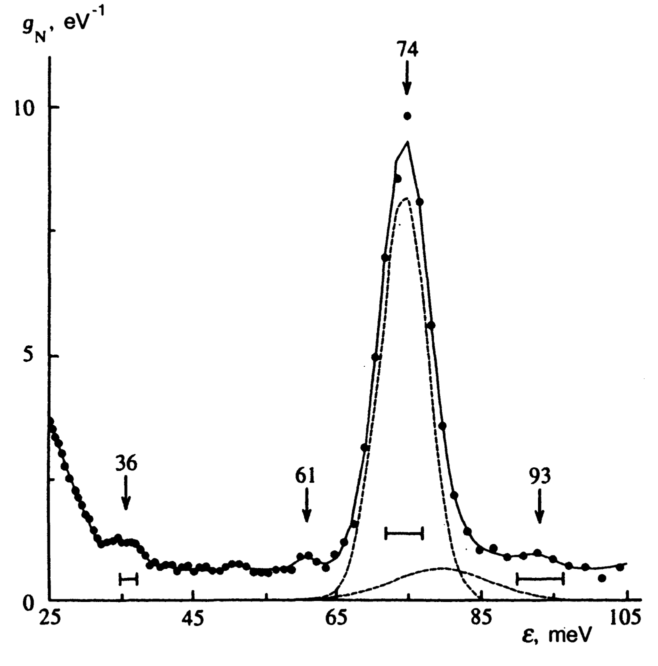

FIG. 3. Vibrational spectrum of the nitrogen atom in β-phase Nb$_2$N$_{0.8}$ ($\varepsilon=74$ meV). The features at $\varepsilon=61$ and 93 meV are associated with the vibrations of the nitrogen atoms in the α-phase. The solid curve corresponds to the least-squares description of the vibrational spectrum in the region of the gap modes and impurity modes for the case of a "split" peak at $\varepsilon=74$ meV. The dashed curves show the decomposition of the vibrational spectrum of the nitrogen atom in the β-phase into two Gaussians (see text). The horizontal line segments show the half-width of the resolution function of the spectrometer (model DIN2-PI). The incident energy of the neutrons was $E_0=10$ meV. The statistical error is indicated by the size of the points.

The frequencies $\hbar\omega_{1,2}$ of the vibrations of the nitrogen atoms in the α-phase of Ta–N have roughly the same values as in the α-phase of Nb–N, which has its *bcc* lattice parameter close to the lattice parameter of the α-phase of Ta–N.[1,2] Since, as was indicated in Ref. 1, there exists a correlation between the values of the energies of the vibrations of the nitrogen atoms and the metal–nitrogen distance, it may be asserted that the feature at $\hbar\omega_3=92$ meV belongs to the nitrogen vibrations in α-NbN$_{0.012}$ that are polarized along the c axis. The widths of the peaks at maximum after taking account of resolution are given in Table II and have values characteristic of the α-phases of transition metals with p implantation elements (see Refs. 1,2,5,6).

It follows from an analysis of the dependence of the vibrational energy of the nitrogen atoms on the metal–impurity distance, which is discussed below (Fig. 4), that the feature at $\hbar\omega_\beta=73$ meV in the spectrum in Fig. 2 is associated with the presence in the sample of a small amount of the β-phase. The feature at $\hbar\omega\simeq38$ meV has a complicated structure and will be discussed below.

In the high-concentration sample Nb + 20 at.% N, as the phase analysis showed, together with the β-phase there is also present some α-phase, containing 1.5 % of the total amount of nitrogen in the sample. This leads to the appearance in the vibrational spectrum, measured in this sample, of features at 60.9±1,2 meV and 93.1±2 meV (see Fig. 3), which within the limits of error coincides with the values of the values of the vibrations of the nitrogen atoms in the α-phase of the sample Nb+3 at.% N.

4.2.2. Vibrational spectrum of the nitrogen atoms in the β phase

In the region $\varepsilon\geqslant30$ meV in the spectrum of the sample of Nb with 20 at.% N the main peak is observed at $\hbar\omega\simeq74$ meV (Fig. 3). This feature corresponds to the vibrational spectrum of the nitrogen atoms in the β-phase of Nb$_2$N$_{0.8}$ since, as was indicated above, the overwhelming fraction of the nitrogen in the given sample is found in the β-phase. Within the limits of error, the value obtained coincides with the energy of the peak, $\hbar\omega_\beta$, in the high-frequency part of the vibrational spectrum measured in the sample of Nb with 3 at.% N (see Fig. 2). This confirms the conclusion made above that the peak $\hbar\omega_\beta=73$ meV in Fig. 2 corresponds to the vibrations of the nitrogen atoms in the β-phase of the Nb–N system.

In addition to the main peak $\hbar\omega\simeq74$ meV in the spectrum in Fig. 3, very insignificant (in magnitude) features are observed with energies 36, 61, and 93 meV. The two latter features are associated with the vibrations of the nitrogen atoms in the α-phase. Possible reasons for the appearance in the gap between the "continuous" spectrum of vibrations of the matrix atoms ($\hbar\omega_D\simeq30$ meV) and the impurity vibrations of the nitrogen atoms ($\hbar\omega_\beta\simeq74$ meV) of a feature at $\hbar\omega\simeq36$ meV will be discussed in the following section.

TABLE II. Metal-impurity coupling constants γ and vibrational energies $\hbar\omega_N$ of the nitrogen atoms in α and β implantation phases of NbN_x.

Sample	Implantation phase	Structure	$\hbar\omega_N$, MeV	Level width, meV	$\gamma, 10^4$ dyn/cm	R_{M-X},* Å	Lattice parameter, Å
Nb			58.6±0.6	8±3	8.5±0.2	2.336	a=3.304
+	α-$NbN_{0.012}$	bcc	91.7±3	13±6	20.9±1.4	1.652	
3 at.%							a=5.293
N	β-$Nb_2N_{0.8}$	hcp	72.5±1.0	9±3	13.1±0.4	2.157	c=4.96
Nb			60.9±1.2	3.6±3	9.2±0.4	2.335	a=3.303
+	α-$NbN_{0.008}$	bcc	93.1±2	6±4	21.6±0.9	1.651	
~20 at.%							a=5.293
N	β-$Nb_2N_{0.8}$	hcp	74.4±0.5	7±1	13.7±0.2	2.157	c=4.96

Note: *R_{M-X}, is the radius of the octohedral interstices.

5. DISCUSSION OF RESULTS

5.1. Influence of nitrogen on the deformation of the vibrational spectrum of the matrix atoms in the α phase

One of the manifestations of an implantation impurity in the α-phase is the deformation of the density of vibrational states of the matrix elements in the region of the acoustic vibrations, where this deformation is associated with a change in the strength of the metal–metal interaction. The effect of the implanted atom as an additional force center for the metal atoms "coupled" by the impurity is equivalent to an increase in the metal–metal coupling constant by $\gamma/2$, where γ is the metal–implantation atom coupling constant. In the mean-field approximation this leads to an increase in the metal–metal coupling constant by $x\gamma$, where x is the concentration of the impurity atoms.[7]

The studies carried out in this work show that implantation of nitrogen in a niobium lattice leads to an increase of the average metal-metal interaction by approximately 3% for every 1 at.% of impurity. Growth of the mean-square frequency of the matrix spectrum takes place despite lattice dilatation. A consideration of the energy required to shift an "average" Nb atom in the "frozen" lattice (analogous to the treatment in Ref. 7) leads to the expected stiffening of the spectrum by ~1% per 1 at.% N. This estimate, although it is obviously rough, indicates the existence of additional mechanisms leading to deformation of the vibrational spectrum of the matrix atoms in α-NbN_x. This may be primarily changes in the electronic subsystem of the metal caused by the implanted atoms. Such a correlation between the density of electronic levels on the Fermi surface and $\langle\varepsilon^2\rangle$ is observed for a number of implantation phases and substitution of group V transition metals.[8]

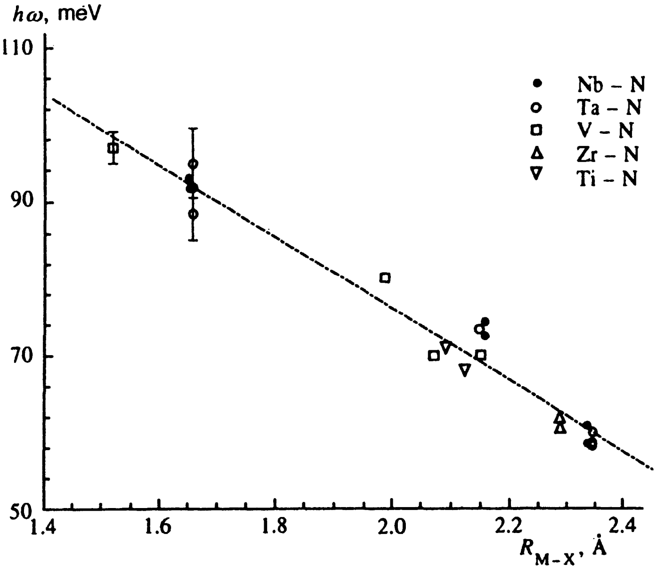

FIG. 4. Dependence of the vibrational energy of the nitrogen atom in the implantation phases of transition metals from the IV and V groups on the metal–impurity distance without taking account of local distortions. Errors extending beyond the thickness of the points are indicated by vertical bars. The dash-dot line corresponds to a linear approximation of the experimental data. The values of the vibrational energies are taken from the present paper and Refs. 1, 2, 5, and 6.

5.2. Coupling constants and dependence of the energy of the impurity vibrations on the metal–impurity distance

The experimentally determined energies of the vibrations of the nitrogen atoms in niobium allow us to make the following estimate of the metal–impurity interaction constants.

The relatively narrow intrinsic width of the peak at $\hbar\omega \simeq 74$ meV (Fig. 3) implies that the direct interaction of the nitrogen atoms is weak. Therefore, to first order we may consider the dynamics of the nitrogen atoms in $Nb_2N_{0.8}$ as independent impurity centers. This allows us to estimate the Nb–N interaction constant for the β-phase as well as for the α-phase in the improved Einstein approximation. The effect of the vibrations of the matrix atoms on the renormalization of the coupling constant of the impurity center with the metal atoms was taken into account, as in Ref. 1, by expanding the Green's function of the crystal-plus-defect at high frequencies. For the system Nb–N the correction amounts to $\simeq 8\%$. Results of our calculation of the Nb–N coupling constant are shown in Table II. The values obtained are similar to the values of the coupling constants of Ta–N in the corresponding phases.

The implantation atoms are rigidly coupled with the matrix atoms. In the α-phase the coupling constant between nearest neighbors for Nb–N is 2.5 times greater than, for example, the coupling constant for Nb–H, and almost seven times greater than the coupling constant f between nearest neighbors for Nb–Nb ($f \simeq 3.2 \cdot 10^3$ dyn/cm, see, e.g., Ref. 9). In the isotropic harmonic oscillator approximation the mean

Nb–Nb coupling constant is three times greater than the Nb–N coupling constant averaged over its octahedral environment.

The complication of accounting for the local distortions arising when an impurity is introduced in a lattice of metal atoms hinders determination of the dependence of the vibrational frequency of the implanted atoms (or their coupling constant with the matrix atoms) on the actual metal–impurity (Me–X) distance. However, it is extremely noteworthy that the experimentally determined energies of the vibrations of the nitrogen atoms in the α and β phases of the system Nb–N, as can be seen from Table II, correlate with the Me–N distance without taking account of local distortions. To first order, this is a linear dependence. Moreover, all of the data on the vibrational frequencies of the nitrogen atoms in the implantation phases (Ti, Zr, V, Nb, Ta)–N, and also the optical frequencies of the corresponding mononitrides, are adequately described by the same dependence as for Nb–N (see Fig. 4). This fact is apparently not accidental and testifies to the generality of the nature of the Me–N bond in alloys of group IV and V transition metals with nitrogen, in dilute solid solutions and implantation phases with high nitrogen content, and in mononitrides.

5.3. Structure of the impurity band in the β phase

A more detailed consideration of the shape of the feature at $\hbar\omega_\beta \simeq 74$ meV in the spectrum of $Nb_2N_{0.8}$ (Fig. 3) shows that the peak is asymmetrical. The best least-squares description of the nitrogen vibrational spectrum in the β-phase is achieved by the model of two Gaussians at $\hbar\omega' \simeq 74.2$ and $\hbar\omega'' \simeq 79.5$ meV with intrinsic half-widths $\Delta\hbar\omega' \simeq 6.5$ and $\Delta\hbar\omega'' \simeq 14.5$ meV, respectively. To estimate the goodness of fit to the experimental spectra we used the χ^2 criterion, which characterizes the mean-square fluctuation of the experimental values relative to the values calculated by the given model. For the single-Gaussian and double-Gaussian models, we obtained $\chi^2 = 1.53$ and 1.08, respectively. The number of degrees of freedom of the fit was about 40. For this many degrees of freedom, $\chi^2 = 1.53$ corresponds to the confidence parameter characterizing deviations of three standard deviations or greater.

There are numerous probable reasons for the splitting of the peak. It may be because the octahedral interstices are nonideal. The magnitude of this splitting estimated in the harmonic approximation in a frozen lattice amounts to $\Delta\hbar\omega \simeq 1$ meV, while the experimental value is equal to 5 meV. In principle, it is possible that the splitting arises because the sample has nonuniform composition. However, the most probable manifestation of such an effect would be a broadening of the peak. The observed splitting may be connected with an ordering of the nitrogen atoms over the various octahedral interstices of a structure of the type ε-Fe_2N. At the same time, it cannot be ruled out that the wide peak corresponds to two-phonon processes in which an acoustic and an optical phonon are annihilated. Calculation of such a contribution is difficult because for this it would be necessary to know the contribution of the vibrations of the nitrogen atoms to the low-frequency part of the spectrum. A more complete analysis of the structure of the vibrational spectrum of the nitrogen atoms in the β-phase would require measurements performed with better resolution than in the present experiment and a comparison with model calculations of the dynamics of the crystal lattice.

5.4. Gap modes in the vibrational spectra of the α and β phases

The introduction of nitrogen into a niobium lattice leads to a strong deformation around the implanted atom and to a renormalization of the Me–Me interaction between the niobium atoms nearest the impurity. In addition, the Nb–N coupling constant, averaged over two nearest neighbors, is, as was indicated above, three times greater than the Nb–Nb coupling constant. Therefore, the space of the defect in the *bcc* lattice of the α-phase is a rigidly bound molecule consisting of six metal atoms and a nitrogen atom. The same applies to the β-phase.

The vibrational spectrum of the quasimolecule with cubic symmetry in the force field of the unperturbed lattice of the remaining metal atoms consists of the local vibrations of the impurity and the relatively narrow band consisting of 15 localized modes near the boundary of the acoustic vibrations of the atoms of the crystal lattice.[10] Depending on the ratio of the masses and the coupling constants, the quasimolecular vibrations can show up in the gap between the local vibrations of the impurity and the acoustic vibrations of the atoms of the lattice as well as in the continuous spectrum. The positions of these modes are not badly reproduced even in the simplest approximation of a linear chain with variable mass and coupling.

From the estimates (analogous to Ref. 1), the localized modes of the niobium atoms nearest to the nitrogen atom in the α-phase fall on the boundary (or close to it) of the acoustic vibrations of the metal atoms in the alloy NbN_x (28 and 34 meV). The features in this energy region are indeed observed in the difference of the spectra of NbN_x and Nb in the continuous spectrum and in the band of the gap vibrations ($\varepsilon = 27$ and 34 meV, see Fig. 5) and, thus, may be associated with the quasimolecular vibrations. At the same time, the region of the gap vibrations has a quite complex structure—the feature with mean energy $\hbar\omega \simeq 38$ meV consists of at least three peaks: $\hbar\omega_b \simeq 34$ meV, $\hbar\omega_c \simeq 39$ meV, $\hbar\omega_d \simeq 46$ meV (Fig. 2). The energies of the last two peaks deviate considerably from the estimates derived above. Therefore it is also possible that these features are unlike the peaks at $\hbar\omega_a \simeq 27$ meV and $\hbar\omega_b \simeq 34$ meV.

Indeed, besides quasimolecular vibrations (if they are present), another possible reason for the appearance of additional features in the gap of the spectrum may be sidebands associated with two-phonon processes. In addition to this, the formation of pairs and other complexes of implantation atoms may also lead to gap modes. Finally, another reason for the appearance of peaks in the energy region under discussion may be the removal of degeneracy in the vibrational spectrum of the impurity due to occupation by the impurity of an interstitial site with lower symmetry than at the octahedral interstices.

The spectrum shown in Fig. 3 also exhibits a gap mode at $\hbar\omega \simeq 36$ meV, which may be associated with quasimo-

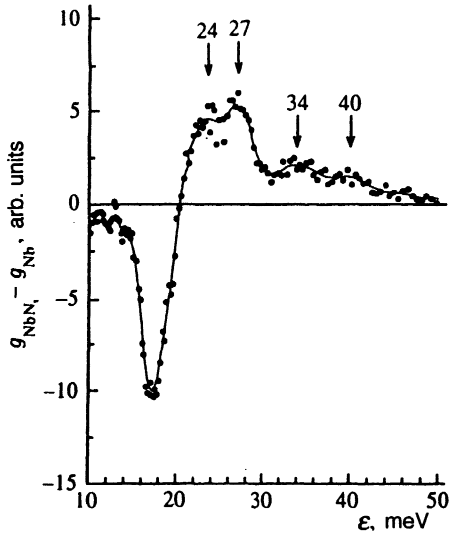

FIG. 5. Difference of the vibrational spectra of α-NbN_x and pure niobium. The notation is the same as in Fig. 1.

lecular vibrations in the β-phase (estimation of the position of the localized modes of the metal atoms in the β-phase gives $\hbar\omega \simeq 31$ meV). At the same time, the observed position of the gap mode in Nb_2N essentially coincides with the position of the analogous feature in the spectrum of the β-phase of Ta_2N ($\varepsilon \simeq 35$ meV, see Ref. 1) while the masses of the metals in these phases differ by a factor of two.

Thus, the question of the origin of the peaks in the gaps of the spectra of the β- and α-phases requires additional consideration both on the experimental and calculational–theoretical level.

6. CONCLUSION

In summary, we may formulate the main conclusions of this work. As a result of measurements of the neutron inelastic-scattering spectra of the α and β implantation phases of the system Nb–N, we have determined the vibrational frequencies of the nitrogen atoms in a *hcp* lattice of the β-phase ($\hbar\omega = 74$ meV) and the polarized (along the c axis) vibrations of the nitrogen atoms in the *bcc* α-phase ($\hbar\omega \simeq 92$ meV).

The dependence of the vibrational energies of nitrogen and niobium on distance has the same nature as in tantalum and other group IV and V transition metals.

The least-squares fitting shows that the vibrational spectrum of the nitrogen atoms in the β-phase in the optical region of the spectrum apparently consists of two peaks, and the splitting is equal to $\Delta\hbar\omega \simeq 5$ meV. To uniquely determine the reason for such a structure is difficult; it may be connected with the way nitrogen is distributed over the various octahedral sites of a structure of the type ε-Fe_2N or with multiphonon processes.

Gap modes are observed in the vibrational spectra of the α- and β-phases. Some of these modes probably belong to quasimolecular vibrations. Definite conclusions about the nature of these features can be drawn only after additional studies and model calculations of the dynamics of the atoms of real crystals have been carried out.

The deformation of the vibrational spectrum of the atoms of the niobium matrix caused by the introduction of nitrogen has been analyzed. To explain the stiffening of the spectrum that occurs despite dilatation of the lattice, it is apparently necessary to account for changes in the electronic subsystem of the alloy.

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