Effect of change of phonon and electron spectra during amorphization on the change of T_c of the alloy $Zr_{70}Be_{30}$

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The heat capacity (between 2 and 500 K), magnetic susceptibility (2–300 K), and superconducting transition temperature of the $Zr_{70}Be_{30}$ system are measured in the amorphous and metastable crystalline states. The parameters that characterize the changes in the phonon and electron spectra of the alloy upon amorphization are determined from the experimental data, and the contributions of the changes to T_c are analyzed. The expression obtained for T_c by solving the Éliashberg equation with a kernel comprising the sum of peaks with significantly different characteristic frequencies is used in analysis. It is shown that for $Zr_{70}Be_{30}$ the contribution made to T_c by the change of the phonon spectrum on amorphization is comparable with the contribution due to the change of the electron spectrum. The role of the optical phonons in the establishment of T_c is considered.

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INTRODUCTION

Great importance is attached, in the study of the superconducting transition temperature T_c of transition metals undergoing amorphization, to a comparative experimental investigation of the normal and superconducting properties of the amorphous system and of its single-phase analog. It is known that amorphization of binary systems with close atomic masses is accompanied by a smearing of the system's phonon spectrum—the phonon-state density increases at both low and high frequencies, and edge of the spectrum shifts into the high-frequency region (see, e.g., Refs. 1 and 2). Upon amorphization, the electron spectrum of the system also undergoes a smearing accompanied by a change of the density of the electronic states on the Fermi surface (see, e.g., Refs. 3 and 4). The deformation of the phonon and electron spectra alters the electron-phonon interaction. For most investigated systems, the decisive role in the change of T_c of transition-metal alloys undergoing amorphization is played by the change of the electron spectrum (of the density of the electronic states on the Fermi surface) and of the electron-phonon interaction. Notwithstanding the strong increase of the density of the phonon states in the low-frequency region, on the whole the change of the phonon spectrum on amorphization is small and is not decisive in the change of T_c.

We have previously investigated the amorphous system $Zr_{75}Rh_{25}$ and its metastable single-phase crystalline analog with $E9_3$ structure, and analyzed also the data on the $La_{78}Zn_{22}$ system.[5] It was established as a result that the main changes of T_c are due to restructuring of the electron spectrum and of the electron-phonon interaction. The increase in the density of the electronic states on the Fermi surface was accompanied in the case of $Zr_{75}Rh_{25}$ by a weakening of the matrix element of the electron-ion interaction $\langle J^2\rangle$, and in the case of $La_{78}Zn_{22}$ by an increase of the electron-ion interaction. The main contribution ($\sim 80\%$) to the almost doubling of T_c in these systems on amorphization was made by the changes of just the electron spectrum and of the electron-ion interaction.

When assessing the universality of the statement that the deformation of the electron spectrum and the change of T_c of transition-metal alloys play a decisive role in amorphization, however, it must be recognized that this statement is based on an analysis of amorphous systems made up of atoms with close masses, and thus having so to speak "compact" phonon spectra. It is of quite definite interest to investigate an amorphous system consisting of atoms with greatly differing masses. For a diatomic system with greatly differing masses, the phonon spectrum should reveal clearly pronounced regions of acoustic and optical vibrations that differ greatly in energy, and the presence of high-frequency optical vibration can enhance their role in the change of the superconducting properties.[6] We note that from measurements of the heat capacity in a wide temperature range it is possible to assess the changes of the phonon spectrum at low and high frequencies ($\langle\omega^2\rangle$) on amorphization.

We have therefore investigated the causes of the change T_c on amorphization in the $Zr_{70}Be_{30}$ system. The choice of this system is due to the large mass difference of the constituent atoms ($M_{Zr}/M_{Be}\approx 10$) and to the presence, besides the amorphous phase, of a metastable crystalline phase[7] having the same composition, so that the amorphous and crystalline phases can be directly compared. The $Zr_{70}Be_{30}$ system in the stable crystalline state is two-phase and consists of $\alpha-Zr$ and Be_2Zr.

We report in this paper the results of measurements of the heat capacity, of the magnetic susceptibility, and of T_c of the superconducting system $Zr_{70}Be_{30}$ in the amorphous and in the metastable crystalline states, and compare the normal and superconducting properties of this system with the properties of systems of atoms having close masses.

PREPARATION AND DESCRIPTION OF SAMPLES

The $Zr_{70}Be_{30}$ alloys were prepared of electrolytically pure Zr (99.99%) and pure Be (99.5%). The samples were melted in an induction furnace in a suspended state under low helium pressure, and were quenched through a metering

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unit from the liquid state on the outer surface of a rotating copper disk. The quenching rate was $\sim 10^6$ deg/sec. The ribbons prepared in this manner, 1.5–2 mm wide and 0.03 mm thick, had an amorphous structure. The samples for the measurement of the heat capacity and of the magnetic susceptibility were prepared by pressing the ribbons into pellets of 5 mm diameter, 2 mm height, and 0.2 g weight. The measurements were performed simultaneously on four pellets. After the measurements, the amorphous pellets were annealed at a rate of 4 deg/min to a temperature 355 °C, at which the transition into the single-phase metastable crystalline state was observed. The transition was revealed by the jump of the electric resistance $R(T)$. The complete set of investigations of the heat capacity, magnetic susceptibility, and T_c was repeated on these samples. Further annealing of the samples transformed the metastable crystalline state into a stable two-phase system. This transition was also distinctly revealed by the electric resistance.

The sample structure was investigated by x-ray and electron diffraction. The general form of the x-ray diffraction curve is that typical of the amorphus metal and shows absence of long-range order. The first broad maximum at $2\theta = 38.5°$ and the width of the maximum at half height was $\Delta(2\theta) = 6.5°$ (Cu$K\alpha$ radiation). This gives an effective distance $d_{\text{eff}} \approx 2.86$ Å between the nearest neighbors.[8]

Analysis of the x-ray and electron diffraction patterns of the samples after annealing points to the appearance of a metastable crystalline phase, identified as an orthorhombic B_f-structure of the CrB type.[7]

The content of the Zr and Be atoms was determined by chemical analysis.

EXPERIMENT

The heat capacity of the samples was measured in the temperature range from 2 to 500 K without a field and in a magnetic field of induction ~ 5.9 T in the range 2-7 K. The technique of the heat-capacity measurement is described in detail in Refs. 9 and 10. The random error in the determination of the molar heat capacity was 2% in the 2–5 K region and 1% at 5–100 K. The measurements above 100 K were made with a differential scanning calorimeter, and the error did not exceed 2% at a systematic error less than 1.5%. The measurement procedure is described in Ref. 11.

The magnetic susceptibility was measured with a vibrating-string magnetometer in the field of a superconducting solenoid with induction ~ 7 T. The construction of the instrument is similar to that described earlier in Ref. 2. The systematic measurement error was 3%. The random error in the measurement of the susceptibility was 3%. The temperature of the transition into the superconducting state was determined from the measurements of the heat capacity, the electric resistance, and the induction. The resistance was measured by a dc four-contact method.

MEASUREMENT RESULTS AND REDUCTION OF THE EXPERIMENTAL DATA

Figure 1 shows the behavior of the low-temperature heat capacity (2–7 K) without a field and in a field ~ 5.9 T, plotted in the coordinates C/T and T^2. These data were used to calculate the Debye temperatures temperatures and the coefficients of the electronic heat capacity $\gamma(0)$. From the jump of the specific heat in the absence of field we determined the superconducting transition temperature T_c, the transition width, and for the amorphous phase also the relative jump of the heat capacity $\Delta C/\gamma T_c$.

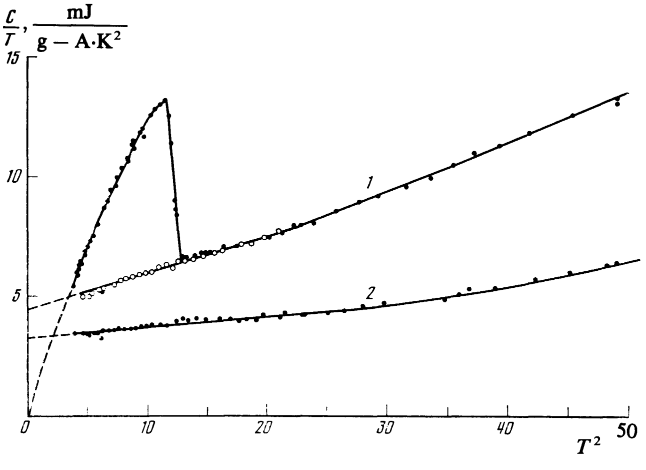

FIG. 1. Heat capacity of amorphous (1) and metastable crystalline (2) samples of $Zr_{70}Be_{30}$ without a field (●) and in a field ~ 5.9 T (○) in the temperature range 2–7 K.

The measured heat capacity in the range 100–500 K is shown in Fig. 2 in coordinates $(C_v - 3R)/T$ and $1/T^3$. The high-temperature parameters, namely the Debye temperature Θ_{ht} and the summary term $(A + \gamma_{\text{ht}})$, were determined from the expression[13]

$$\frac{C_v-3R}{T}=-\frac{3R\Theta_{\text{ht}}^2}{20T^3}+(A+\gamma_{\text{ht}}),$$

where C_v is the total heat capacitance at constant volume, obtained by subtracting from C_p the contribution due to the thermal expansion, γ_{ht} is the coefficient of the electronic

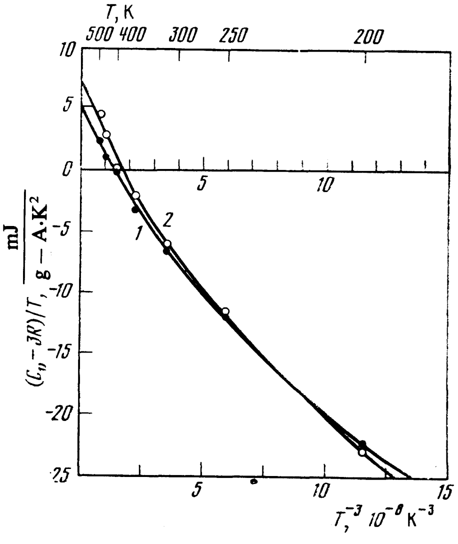

FIG. 2. High-temperature heat capacity of amorphous (1) and metastable crystalline (2) sample in the coordinates $(C_v - 3R)/T$ and T^{-3}.

heat capacity at high temperatures, and A is the anharmonicity parameter. The electronic heat-capacity coefficient at high temperatures was calculated from data on the magnetic susceptibility and the low-temperature heat capacity, as in Ref. 5.

The magnetic susceptibility was measured on the same samples as the heat capacity. In the entire investigated temperature range from T_c to 300 K the magnetic susceptibility of the sample in the amorphous state is 6% higher than in the crystalline state and does not depend on the temperature. This confirms the result which follows from the heat-capacity measurements, that the electronic density of states is increased by amorphization.

The experimental data are shown in Table I. It can be seen from it that the amorphization of the $Zr_{70}Be_{30}$ system changes a number of physical properties: T_c is almost doubled. $\gamma(0)$ and γ_{ht} increase substantially, and $\Theta(0)$ decreases sharply. It must be noted that in contrast to alloys with close component masses, where amorphization increases Θ_{ht}, in this case Θ_{ht} decreases. These changes point to a softening of the entire phonon spectrum, while the increase of $\gamma(0)$ and γ_{ht} indicates that the density of the electronic states on the Fermi surface increases. The heat-capacity jump $\Delta C/\gamma T_c$ in the superconducting transition exceeds the value 1.43 given by the BCS theory, thus indicating that the coupling is intermediate.

The data obtained made it possible to track the changes of the electron and phonon spectra in the course of amorphization and to reveal the role they play in the change of T_c. To this end, in the case of systems with strongly differing atom masses, it is necessary to know the phonon state density function. For lack of experimental or theoretical data on the phonon spectra of the investigated system, we have attempted to determine approximate phonon spectra from the temperature dependence of the heat capacity.

Strictly speaking, the determination of the spectral density $F(\omega)$ of the phonon states of a solid from its heat capacity is an incorrectly posed problem since the formal solution of the corresponding integral equation is unstable.[14] A stable solution can be obtained only by imposing on the function $F(\omega)$ additional conditions, such as a bounded energy interval on which the function $F(\omega)$ is sought, as well as a smooth, non-negative, and normalized $F(\omega)$.

A function $F(\omega)$ satisfying these additional conditions and ensuring a minimum deviation of the ensuing heat capacity from that measured in experiment was sought in the form of a finite trigonometric series:

$$F(\omega)=\sum_{k=0}^{n} A_k\cos(k\pi\omega/\Omega), \tag{1}$$

where Ω is the end-point frequency.

The heat capacity C_{calc} was calculated as the sum of three contributions: phonon, electronic, and anharmonic:

$$C_{calc}=C_{ph}(T)+C_{el}(T)+C_a(T).$$

The phonon heat capacity C_{ph} was determined in the harmonic approximation:

$$C_{ph}(T)=3R\int_0^{\Omega}\frac{(\omega/T)^2e^{\omega/T}}{[e^{\omega/T}-1]}F(\omega)\,d\omega.$$

Here R is the gas constant and T the temperature.

The electronic heat capacity C_{el} was calculated with allowance for the temperature dependence of the influence of the electron-phonon interaction on the electronic heat capacity[15]:

$$C_{el}(T)=\gamma(0)T\{1+\lambda_T(T)\},\quad \lambda_T(T)=\lambda_M\varkappa(T)/(\varkappa(0)-1), \tag{2}$$

$$\varkappa(T)=2\int_0^{\infty}\alpha^2F(\omega)z(T/\omega)\,d\omega/\omega, \tag{3}$$

$z(T/\omega)$ is the universal function introduced in Ref. 15, and $\alpha^2F(\omega)$ is the Éliashberg function.

TABLE I. Parameters of the $Zr_{70}Be_{30}$ system in the amorphous and metastable crystalline states.

Form of	T_c (from heat capacity)	T_c (from electr. resistance)	ΔT_c, K	$\frac{\Delta C}{\gamma T_c}$	$\Theta(0)$, K ± ± 1,5 %	$\gamma(0)$, $\frac{mJ}{g\text{-}a\cdot K^2}$ ± ± 2%	λ_M, [16]
$Zr_{70}Be_{30}$, amorphous	3,5	3,5	0,15 (therm.) 0,08 (electr.)	1,60	234	4,44	0.62
$Zr_{70}Be_{30}$, metastable crystalline	–	1,8	0.5 (electr.)	–	354	3,26	0.51
Relative change, %	–	94	–	–	–34	36	22

System	Θ_{ht}, K ± 3%	γ_{ht}, $\frac{mJ}{g\text{-}a\cdot K^2}$ ± ± 10%	$(A+\gamma_{ht})$, $\frac{mJ}{g\text{-}a\cdot K^2}$ ± ± 5%	A, $\frac{mJ}{g\text{-}a\cdot K^2}$ ± ± 10%	$\chi\cdot 10^6$, $\frac{emu}{g}$	$N(\varepsilon_F)$, $\frac{state}{eV\cdot at}$
$Zr_{70}Be_{30}$, amorphous	546	2,74	5.20	2,46	1,71	0,56
$Zr_{70}Be_{30}$, metastable crystalline	586	2,19	7,25	5.06	1,62	0.46
Relative change, %	–7	25	–28	–51	6	20

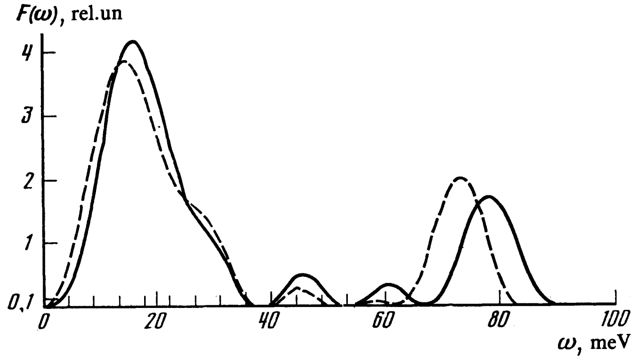

FIG. 3. Approximate phonon spectra of $Zr_{70}Be_{30}$ in the amorphous (dashed curve) and in the metastable crystalline (solid) states.

It must be noted that since the phonon contribution to the total heat capacity predominates in a wide temperature range, the changes introduced into the electronic component C_{el} of the heat capacity by choosing the function $\alpha^2(\omega)$ exert no substantial influence on the form of the function $\tilde{F}(\omega)$. In the actual calculation we used the approximation $\alpha^2(\omega) = \text{const}$.

The anharmonic heat capacity C_a was calculated in the form

$$C_a(T) = AT[C_{ph}(T)/3R]^2.$$

This form of $C_a(T)$ ensures a correct asymptotic anharmonic heat capacity at high temperatures and its smooth vanishing at low ones.

It was found that the expansion (1) with an end-point frequency Ω equal to 1000 K and with $n = 12$ harmonics can describe the heat capacities of both the amorphous and metastable crystalline phases of $Zr_{70}Be_{30}$ in the temperature 2–500 K with a mean square deviation $\sim 3\%$. The approximate phonon spectra obtained in this manner for the $Zr_{70}Be_{30}$ system in the amorphous and metastable crystalline states are shown in Fig. 3. It can be seen that the spectra of these systems are characterized by acoustic- and optical-vibration regions that differ greatly in their frequency locations. In amorphization one observes a strong softening of the phonon spectrum in the low-frequency region as well as a softening of the spectrum as a whole, so that the region of the optical vibration shifts towards lower frequencies. This is in full accord with the experimentally decreased decreases of the low-temperature $\Theta(0)$ and of the high-temperature Θ_{ht}.

DISCUSSION

Of greatest interest in the analysis of our experimental data is the determination of the contributions made to the change of T_c by the restructuring of the electron and phonon spectra and by the electron-phonon interaction in the amorphization. Traditionally, such an analysis is carried out on the basis of the McMillan equation[16] for T_c.

To determine the characteristic phonon frequencies and the electron-phonon interaction constant

$$\lambda = 2\int_0^\infty \frac{\alpha^2(\omega)F(\omega)\,d\omega}{\omega}$$

we used as the model the obtained approximate phonon spectrum $\tilde{F}(\omega)$. The quantities contained in the McMillan formula were calculated in analogy with Ref. 5 and are listed in Table II. The four approximations chosen by us for $\alpha^2(\omega)$ allow us to take into account the possible distinguishing features of disordered transition-metal alloys.[17,18]

To determine the scale of the change of T_c as a result of the change of $\langle\omega\rangle_\omega$, $\langle\omega^2\rangle_\omega$, $N(\varepsilon_F)$, $\langle J^2\rangle$ (the mean square matrix element of the electron-ion interaction), and μ^* we estimated the partial contributions to δT_c by the method of variation of the parameters:

$$\delta T_c = \delta x \partial T_c / \partial x. \tag{4}$$

Table III lists the partial contributions to δT_c in percent.

Owing to the strong softening of the phonon spectrum on amorphization, the pre-exponential factor in McMillan's formula makes a negative contribution to the change of T_c. The decrease of $\langle\omega^2\rangle_\omega$ leads to an increase of λ and accordingly of T_c, while the changes in the argument of the exponential turn out to be decisive compared with the decrease of $\langle\omega\rangle_\omega$ in the pre-exponential factor. As a result, the restructuring of the phonon spectrum upon amorphization of the $Zr_{70}Be_{30}$ system leads to an increase of T_c, while the contribution of the phonon restructuring to the change of T_c is substantial and amounts to 25–40%, depending on the choice of $\alpha^2(\omega)$. The increase of T_c upon amorphization is also connected with the increase of the electron density of states on the Fermi surface. In this case T_c increases somewhat on account of the decrease of μ^* due to the weakening of the electron–electron interaction. As for the change of the mean square matrix element $\langle J^2\rangle$ of the electron-ion interaction, its contribution to the change of T_c is negative.

TABLE II.

Form of $\alpha^2(\omega)$	State	λ	$N(\varepsilon_F)$, state/ev·at	μ^*	$\langle\omega\rangle_\omega$, K	$\langle\omega^2\rangle_\omega^{1/2}$, K
const	Cryst.	0,43	0.48	0.083	214	278
	Amorph.	0,52	0.62	0,081	191	255
$M^{-1/2}$*	Cryst.	0,41	0,49	0.085	283	385
	Amorph.	0,48	0,64	0.083	258	359
$(\omega M)^{-1}$	Cryst.	0,44	0.48	0,082	195	289
	Amorph.	0,55	0.61	0.080	156	249
ω^{-1}	Cryst.	0,47	0,47	0,080	138	172
	Amorph.	0,63	0,58	0,078	109	144

*$M = M_{Zr}$ at $\omega < 60$ meV, $M = M_{Be}$ at $\omega > 60$ meV.

TABLE III.

Form of $\alpha^2(\omega)$	$\langle\omega\rangle_\omega$	$\langle\omega^2\rangle_\omega$	$N(\varepsilon_F)$	$\langle J^2\rangle$	μ^*
const	−11	37	127	−56	4
$M^{-1/2}$	−9	33	142	−70	4
$(\omega M)^{-1}$	−20	60	112	−57	5
ω^{-1}	−22	63	92	−36	4

As already noted, the spectral function $S(\omega)=\alpha^2(\omega)F(\omega)$ of the $Zr_{70}Be_{30}$ system investigated by us is a sum of two peaks with greatly differing characteristic frequencies. McMillan's formula does not describe T_c satisfactorily for such a system, since the formula was derived for the case of a phonon spectrum with two closely located peaks. More adequate for the problem analysis of the amorphization change of T_c by using the derivations of the paper by Dreksler and Zhernov.[19]

In that paper they developed a method of solving the Éliashberg equation with a nonstandard kernel $S(\omega)=\alpha^2F(\omega)$, when $S(\omega)$ is a sum of two peaks, $S_1(\omega)$ and $S^2(\omega)$, with substantially differing characteristic frequencies. The simple analytic formula obtained in the paper for T_c is valid for weak and intermediate coupling, and is similar in structure to the formulas previously proposed in Ref. 20 and 21. Unlike the latter, however, the parameters of this formula are functionals of the form of the phonon spectrum.

According to Ref. 19, the equation for T_c is

$$T_c=1.135\omega_1\exp\left[\tilde{\nu}_1+\frac{\tilde{\nu}_2-\tilde{\mu}}{(\tilde{\nu}_2-\tilde{\mu})\ln(\omega_2/\omega_1)}\right]^{-1}, \qquad (5)$$

where

$$\tilde{\nu}_{1,2}=\frac{\nu_{1,2}}{1+\nu_{1,2}\eta_{1,2}/2},\quad \nu_{1,2}=\frac{\lambda_{1,2}}{1+\lambda},\quad \lambda=\lambda_1+\lambda_2,$$

$$\tilde{\mu}=\frac{\mu^*}{1+\lambda},\quad \mu^*=\frac{\mu}{1+\mu\ln(\varepsilon_F/\omega_2)}.$$

In Eq. (5), ω_i and η_i are functionals of $\operatorname{Re}Z(\omega)$, where $Z(\omega)$ is the electron-mass renormalization parameter. In the case of $Zr_{70}Be_{30}$ one can use for ω_i and η_i the approximate equations

$$\lambda_i=2\int_0^\infty\frac{S_i(\omega)}{\omega}d\omega,$$

$$\ln\omega_i=\frac{1}{\lambda_i}\int_0^\infty\frac{\ln\omega S_i(\omega)}{\omega}d\omega,$$

$$\eta_i=\frac{1}{\lambda_i^2}\int_0^\infty\int_0^\infty\frac{S_i(\omega)}{\omega}\frac{S_i(\omega')}{\omega'}\ln\left(\frac{\omega'^2}{\omega^2}\right)\frac{\omega'^2}{\omega'^2-\omega^2}d\omega\,d\omega',$$

$$i=1,2, \qquad (6)$$

where the subscripts 1 and 2 correspond to integration over the first and second peaks. Since the contributions to the low- and high-frequency peaks come mainly from acoustic and optical vibrations, respectively, we shall use λ_{ac} and λ_{op} for λ_1 and λ_2.

All the parameters in (6) were calculated on the basis of the approximate phonon spectra of $Zr_{70}Be_{30}$ and four forms of $\alpha^2(\omega)$. An iteration procedure, just as in the case of calculations by McMillan's equation, determined the parameters in Eq. (5). They are listed in Table IV.

In the employed scheme it is possible to examine the role of optical phonons in the formation of T_c. If we eliminate from (5) the interaction of the electrons with the optical peak, i.e., put $\lambda_2=0$ and $\omega_2=\omega$, then Eq. (5) goes over into the expression for T_c obtained in Ref. 22 for the usual form of the function $F(\omega)$. This approximation was used to estimate the contribution of the acoustic vibrations to T_c. The contribution of the optical vibrations to T_c was determined as $T_{op}/T_c=(T_c-T_c^{ac})/T_c$ in percent. Table IV gives also the contribution of λ_{op}k to the electron-phonon interaction λ.

It should be noted that even small changes of λ, due to optical vibration and contained in the exponential, influence the changes of T_c substantially.

It can be seen from Table IV that the estimate of the contribution of the optical phonons to T_c depends strongly on the choice of the function $\alpha^2(\omega)$. Since the true form of $\alpha^2(\omega)$ is unknown, it is customary to use in the calculations $\alpha^2(\omega)=\text{const}$. This results in a noticeable contribution (~15–20%) of the optical phonons to T_c of the $Zr_{70}Be_{30}$ system. To determine the possible extent of the influence of various parts of the spectrum on T_c as a result of the form of

TABLE IV.

Form of $\alpha^2(\omega)$	State	λ	λ_{ac}	λ_{op}	$\frac{\lambda_{op}}{\lambda}$, %	$N(\varepsilon_F)$, $\frac{\text{state}}{\text{ev}\cdot\text{at}}$	μ^*	ω_1, K	ω_2, K	η_1	η_2	T_K^{ac}	$\frac{T_K^{op}}{T_K}$, %
const	Cryst.	0.48	0.45	0.03	6	0.47	0,094	156	850	1,15	1,01	1,46	19
	Amorph.	0.63	0.59	0.04	5	0.58	0.092	134	812	1,20	1.00	2.99	15
$M^{-1/2}$	Cryst.	0.47	0.39	0.07	16	0.47	0.094	156	850	1,15	1.01	0,79	56
	Amorph.	0,60	0.51	0.09	16	0.59	0,092	134	812	1,20	1.00	1.88	46
$(\omega M)^{-1}$	Cryst.	0.54	0,49	0,05	9	0.45	0.094	108	842	1,23	1,01	1.32	27
	Amorph.	0.80	0,74	0,06	7	0.52	0.093	80	810	1,29	1.00	2,93	16
ω^{-1}	Cryst.	0,55	0.54	0,01	1	0.45	0.094	108	842	1,23	1.01	1,84	−2
	Amorph.	0.83	0.82	0,01	0,7	0.51	0.093	80	810	1,29	1,00	3,56	−2

TABLE V.

Form of $\alpha^2(\omega)$	ω_1	η_1	λ_1^Φ	λ_2^Φ	$N(\varepsilon_F)$	μ^*
const	−15	−4	22	1	94	3
$(\omega M)^{-1}$	−22	−3	77	2	45	1

$\alpha^2(\omega)$, we have considered two limiting cases: $\alpha^2(\omega) \sim M^{-1/2}$, which enhances the high-frequency part of the spectrum and accordingly decreases the role of the optical phonons ($T_{\rm op}/T_c \sim 50\%$), and $\alpha^2(\omega) \sim 1/\omega$, which practically excludes the optical phonons and enhances the role of the low-frequency part of the spectrum ($T_{\rm op}/T_c \sim -2\%$). The approximation $\alpha^2(\omega) \sim 1\omega M$ is intermediate between the considered limiting cases when the role of the optical phonons is estimated, and its result is close to that obtained at $\alpha^2(\omega) = \text{const}$.

The extent of variation of T_c on account of the changes in the electron and phonon spectra upon amorphization was estimated on the basis of Ref. 19. To this end, λ_i was represented in the form

$$\lambda_i = N(\varepsilon_F)\lambda_i^{\rm ph},$$

where $\lambda_i^{\rm ph}$ is given by Eq. (6), and the analysis was carried out for the approximations $\alpha^2(\omega) = \text{const}$ and $\alpha^2(\omega) \sim 1/\omega M$. The calculated partial contributions to the change of T_c is given in percent in Table V.

Allowance for the change of all the phonon characteristics ω, η, and $\lambda_i^{\rm ph}$ permits us to conclude that at $\alpha^2(\omega) = \text{const}$ the phonons make a noticeable contribution to the change of T_c on amorphization, although the contribution of the electrons is also substantial. In the $\alpha^2(\omega) \sim 1/\omega M$ approximation the phonon contribution is found to predominate in the change of T_c.

We note that although the role of optical phonons in T_c of the $Zr_{70}Be_{30}$ system is substantial, it is not large in the change of T_c during amorphization, as follows from Tables IV and V.

CONCLUSIONS

The experimental investigations of the heat capacity, of the magnetic susceptibility, and of the critical temperature T_c of the alloy $Zr_{70}Be_{30}$ in the amorphous and metastable crystalline states has enabled us to track the restructuring of the electron and phonon spectra of this alloy upon amorphization. Analyses both on the basis of the McMillan equation and using the conclusions of Ref. 19 enabled us to determine the contributions of these restructurings to the change of T_c of the alloy.

Amorphization of $Zr_{70}Be_{30}$ softens both the low-frequency part of the spectrum and the spectrum as a whole (decrease of $\langle\omega^2\rangle_\omega$), in contrast to the alloys $Zr_{75}Rh_{25}$ and $Zr_{54}Cu_{46}$, where the spectrum as a whole become harder upon amorphization, notwithstanding the increase of the density of the vibrational states in the low-frequency region.

The density of the electronic states on the Fermi level increases considerably on amorphization, and the mean square matrix element $\langle J^2\rangle$ of the electron-ion interaction decreases noticeably.

The superconducting temperature T_c of the amorphous $Zr_{70}Be_{30}$ is almost double the value of T_c of the crystalline system and, unlike the alloy $Zr_{75}Rh_{25}$, the contribution of the phonon-spectrum restructuring is positive and accounts for a significant fraction (20–30%) of the change of T_c upon amorphization.

It can be proposed that the softening of the phonon spectrum as a whole and the ensuing positive contribution to the change of T_c on account of the restructuring of the phonon spectrum, which are observed in $Zr_{70}Be_{30}$ upon amorphization, are due to the unusual phonon spectrum of this alloy, whose acoustic- and optical-vibration energy regions are greatly separated.

The estimate based on the conclusions of Ref. 19 shows that in this system the interaction with the optical phonons contributes significantly to the establishment of the value of T_c.

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