PHYSICS AND CHEMISTRY
OF SOLID STATE
V.21, No.2 (2020) pp. 260-265

DOI: 10.15330/pcss.21.2.260-265

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ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 21, № 2 (2020) С. 260-265

UDK 680.18:669.71

ISSN 1729-4428

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Heat Capacity of Decagonal and Icosahedral Quasicrystalline Phases at High Temperatures

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The paper deals with the patterns of quasicrystalline decagonal $Al_{69}Co_{21}Ni_{10}$ and icosahedral $Al_{63}Cu_{25}Fe_{12}$ phases from the standpoint of the model of anisotropic crystals. In the *xy* plane, the structure of quasicrystalline decagonal phase features the quasicrystalline pattern and the dispersive law is represented by a quadratic dependence. In contrast, the dispersive law is linear in the direction of *z* axis, because of crystalline pattern of the structure. The dispersive law for the icosahedral phase in all directions is represented by quadratic dependence, since the structure of this phase is isotropic one. After calculations it is found that heat capacity of quasicrystalline phases at high temperatures exceeds the level of $3R$, i.e. the Dulong-Petit law is not complied with. Therefore, with the use of the model described in this paper we explain the previously established phenomenon of excessive heat capacity of quasicrystalline phases at high temperatures. It is also found that the heat capacity of the decagonal phase $Al_{69}Co_{21}Ni_{10}$ remains the excessive one to higher temperatures, compared to the icosahedral phase $Al_{63}Cu_{25}Fe_{12}$. According to the Gruneisen law, it indicates the greater stability of the decagonal phase at high temperatures.

Key words: quasicrystals, decagonal phase, icosahedral phase, dispersive law, anisotropy, isotropy, temperature heat capacity dependence, excessive heat capacity, the Dulong-Petit law.

Received 25 March 2020; Accepted 15 June 2020.

Introduction

The unique structure of quasicrystals determines their unusual physical and chemical properties. Quasicrystals have low coefficients of friction and surface tension, as well as high hardness, durability and corrosion resistance. Owing to these properties, quasicrystals find their practical use in the form of films, coatings and components of the composite materials. In the course of manufacturing of the composite materials with quasicrystalline fillers, the question arises with regard to stability of quasicrystalline phases to the temperature action of the molten binder. In the systems of Al–Cu–Fe and Al–Ni–Co the icosahedral $Al_{63}Cu_{25}Fe_{12}$ and decagonal $Al_{69}Co_{21}Ni_{10}$ quasicrystalline phases, respectively [1, 2], are found. These phases are formed from the melt at the normal cooling rates and kept after long-term heat treatment, i.e. they belong to equilibrium ones. However, the quasicrystalline decagonal phases are destroyed at higher temperatures [3, 4] than the icosahedral phases.

At present time, the attention of researchers is attracted by so called excessive heat capacity of quasicrystalline phases in the high temperature range [1, 5]. The excessive heat capacity is manifested in the system heat capacity excess of the $3R$ value in the Debye model and deviation from the Dulong-Petit law at the temperatures above 300 K. The heat capacity follows the Gruneisen law and depends on the coefficient of linear expansion. Thus, it can be said that the heat capacity reflects the quasicrystalline phases' stability to the temperature action. The first studies of this phenomenon of excessive heat capacity were conducted in the papers [6, 7]. O.F. Prekul et al. [1, 5] have found that the heat capacity of icosahedral phases $Al_{63}Cu_{25}Fe_{12}$ starting from the temperature of nearly 300 K rose continuously, reaching a maximum at about 1300 K and then dropped slowly. However, the phenomenon of excessing heat capacity has not been adequately explained yet.

In order to explain the phenomenon of the excessive heat capacity of quasicrystalline phases, as well as the fact of stability of decagonal phases at higher temperatures, this paper deals with the heat capacity of phases from the standpoint of the model of anisotropic crystals [8].

I. Model representation of the structure of crystalline phase

Pursuant to the Gruneisen law [8], if there are no significant variations in the pressure, it can be assumed that the coefficient of thermal expansion of the crystal lattice is linearly dependent on the heat capacity. As the coefficient of thermal expansion of the lattice grows the plasticity of the structure and, accordingly, its resistance to fracture. Therefore, heat capacity is an energy characteristic of the phase stability.

Free energy of the body F according to [8] is:

$$F = \frac{VT}{2\pi^2 u^3}\int_0^\infty \omega^2 \ln\left(1 - e^{-\frac{\hbar\omega}{T}}\right) d\omega, \qquad (1)$$

where V – body volume, T – temperature, u – group velocity, $\hbar$ – Plank’s constant. Because of the isotropic structure of the crystalline phase, only one direction of polarization is considered in (1). The dispersion relation has a linear dependence:

$$\omega = uk, \qquad (2)$$

where k – wave vector. Using the Debye formalism [8], we replace the upper integration limit in (1) with $y = \frac{\hbar\omega_D}{T}$, where ω_D – Debye frequency, and substitute (2) in (1); after that we obtain:

$$F = \frac{VTT^3}{2\pi^2 u^3 \hbar^3}\int_0^y \ln\left(1 - \exp(-x)\right) x^2 dx, \qquad (3)$$

where $x = \frac{\hbar uk}{T}$. After integrating by parts, we obtain:

$$F = \ln\left(1 - \exp(-x)\right)\frac{x^3}{3}\Bigg|_0^y - \int_0^y \frac{x^3}{3}\frac{1}{1 - \exp(-x)} dx \qquad (4)$$

We expand the function $\exp(-x)$ y (4) to the second term and after integration obtain the expression

$$F = \frac{Vk_D^3}{2\pi^2 3}\left(T\ln(\hbar uk) - T\ln T - \frac{T}{3}\right), \qquad (5)$$

where k_D – Debye wave vector. Hence, entropy of the body:

$$S = -\frac{\partial F}{\partial T} = \frac{Vk_D^3}{2\pi^2 3}\left(-\ln(\hbar uk) + \ln T + 1 + \frac{1}{3}\right). \qquad (6)$$

Internal energy of the body E and heat capacity C, accordingly, take the form of $E = F + TS = \frac{Vk_D^3}{2\pi^2 3}T$,

$$C = \frac{\partial E}{\partial T} = \frac{Vk_D^3}{2\pi^2 3}. \qquad (7)$$

It can be seen from expression (7) that the heat capacity of the crystalline phase is equal to the Debye sphere $3R = \frac{Vk_D^3}{2\pi^2 3}$. This corresponds to the fact that the heat capacity of the crystalline phase at high temperatures is equal to $3R$, i.e. the Dulong-Petit law is complied with.

II. Representation of the structure of quasicrystalline decagonal phase from the standpoint of the model of anisotropic crystals

Structure of the quasicrystalline decagonal phase $Al_{69}Co_{21}Ni_{10}$ of the Al–Co–Ni alloy is anisotropic one, i.e. it features the quasicrystalline pattern in the xy plane and crystalline pattern in the direction of the z axis [9]. We’ll describe the pattern of the structure of quasicrystalline decagonal phase with the use of the model of highly anisotropic crystals [8]. The decagonal phase can be considered as a layered structure with the interaction between its layers. The structure features the oscillations in the layers themselves and of the layers relative to each other. Oscillations in the bends of the layers are found as well. We assume that anisotropy of the quasicrystalline decagonal phase is manifested in the difference of the dispersive laws in the xy plane and in the z direction. In the xy plane for the quasicrystalline pattern [10] the dispersive law is represented by the quadratic dependence $\gamma\chi^2$ ($\chi^2 = k_x^2 + k_y^2$), where γ - group velocity in the plane, and in the z direction for the crystalline pattern it has the linear dependence $\approx uk_z$. The sum frequency of sound waves can be expressed as follows, according to [8]:

$$\omega^2 = u^2 k_z^2 + \gamma^2\chi^4. \qquad (8)$$

Taking into account the contribution from sound oscillations, free energy of quasicrystalline decagonal phase is determined by formula [8]:

$$F = \frac{8VT}{(2\pi)^3}\int_0^{\hbar uk_{\max}/T} dk_z \int_0^{\hbar\gamma\chi_{\max}^2/T} \ln\left(1 - \exp\left(-\frac{\hbar}{T}\sqrt{u^2k_z^2 + \gamma^2\chi^4}\right)\right) 2\pi\chi d\chi. \qquad (9)$$

In (9) the upper integration limits are replaced using the Debye formalism for the model of anisotropic crystals. Then formula (9) will be true for the case of high temperatures as well, as in the Debye model [8]. For the internal integral, we obtain the following expression:

$$\frac{\pi T}{\gamma\hbar}\int_0^x \ln\left(1-e^{-z}\right)dz = \frac{\pi T}{\gamma\hbar}\left[x\ln\left(1-e^{-x}\right)-3\int_0^x \frac{zdz}{e^z-1}\right], \tag{10}$$

where $z=\frac{\hbar}{T}\sqrt{a+\gamma^2\chi^4}$, a – parameter $\sim u^2k_z^2$, $x=\frac{\hbar}{T}\sqrt{a+\gamma^2\chi_{\max}^4}$ – integration limit. Coefficient 3 in (10) takes into account small oscillations of the lattice nodes lying in the integration plane in three directions. After expansion in the series e^z to the third term, and in e^x to the second term, we obtain the expression:

$$\frac{\pi T}{\gamma\hbar}\left[x\ln x-6\ln\left(1+\frac{x}{2}\right)\right]. \tag{11}$$

For the further integration in the direction of wave vector k_z, we additionally expand the function $\ln\left(1+\frac{x}{2}\right)$ to the sixth term. Then the internal integral of expression (9) will take the form:

$$\frac{\pi T}{\gamma\hbar}\left(x\ln x-6\left[\frac{x}{2}-\frac{x^2}{8}+\frac{x^3}{24}-\frac{x^4}{64}+\frac{x^5}{160}-\frac{x^6}{384}\right]\right) \tag{12}$$

Next, we make an additional replacement of the variable $x=\frac{\hbar}{T}\sqrt{u^2k_z^2+b}$, where $b=\gamma^2\chi_{\max}^4$ – parameter, $y=\frac{\hbar}{T}\sqrt{u^2k_{z\max}^2+b}$.

Then, taking into account the coefficient preceding the double integral in (9), we obtain:

$$F=\frac{VT^3}{\pi^2\gamma u\hbar^2}\left[\int_0^y x\ln x dx-6\int_0^y\left(\frac{x}{2}-\frac{x^2}{8}+\frac{x^3}{24}-\frac{x^4}{64}+\frac{x^5}{160}-\frac{x^6}{384}\right)dx\right]. \tag{13}$$

After integration, free energy takes the form of:

$$F=\frac{VL^2}{2\pi^2\gamma u}\left[T\ln\hbar L-T\ln T-\frac{7}{2}T+\frac{1}{2}\hbar L-\frac{1}{8}\frac{\hbar^2L^2}{T}+\frac{3}{80}\frac{\hbar^3L^3}{T^2}-\frac{3}{240}\frac{\hbar^4L^4}{T^3}+\frac{3}{672}\frac{\hbar^5L^5}{T^4}\right], \tag{14}$$

where $L=\sqrt{u^2k_{z\max}^2+\gamma^2\chi_{\max}^4}$. After simple calculations of the entropy $S=-\frac{\partial F}{\partial T}$ and the internal energy of the system $E=F+TS$, we obtain for the heat capacity the expression below:

$$C=\frac{\partial E}{\partial T}=\frac{VL^2}{2\pi^2\gamma u}\left[1+\frac{1}{4}\frac{\hbar^2L^2}{T^2}-\frac{9}{40}\frac{\hbar^3L^3}{T^3}+\frac{3}{20}\frac{\hbar^4L^4}{T^4}-\frac{5}{56}\frac{\hbar^5L^5}{T^5}\right]. \tag{15}$$

The expression $\hbar L=\hbar\sqrt{u^2k_{z\max}^2+\gamma^2\chi_{\max}^4}$ in its content is similar to the Debye temperature ~ $\theta=\hbar\omega_D$, since $uk_{z\max}$ and $\gamma\chi_{\max}^2$, in fact, are the components of the expression for the maximal frequency of the oscillating system generalized by space. Factor $\frac{VL^2}{2\pi^2\gamma u}$ is similar in its content to the Debye sphere $\frac{V}{(2\pi)^3}\frac{4}{3}\pi k_D^3\approx 3R$. Indeed, we assume that velocity of sound γ in the *xy* plane is equal to velocity of sound *u* in the *z* direction, and has some value *u*. Then the factor is equal to $\frac{V}{2\pi^2}\frac{u^2\left(k_{z\max}^2+\chi_{\max}^4\right)}{u^2}$. Vector χ^2 in the *xy* plane is determined by the sum of squares of vectors k_x i k_y: $\chi^2 = k_x^2+k_y^2$. Further, we'll add the vector directed along the axis *z* $k_{z\max}$ to vector χ^2 formed by vectors k_x and k_y in the plane. Hence we have the wave vector *K* in the space *xyz*, which is equal to $K^2 = k_{z\max}^2 + (\chi_{\max}^2)^2$. Then the factor in the expression for heat capacity becomes equal to $\frac{V}{2\pi^2}K^2$. Quasicrystalline decagonal phases have the ordered structure, but not the periodic one. Their atomic structure is characterized by the presence of highly symmetrical Mackay clusters [11]. It causes the shift of vectors $k_{z\max}$ and $\chi_{\max}^2$. Therefore K^2 should be considered as a certain variable, and it is necessary to integrate the factor which will be equal to $\frac{V}{2\pi^2}\int_0^k K^2dK=\frac{V}{2\pi^2}\frac{k^3}{3}$. If we assume $k=k_D$, the factor in the expression for heat capacity matches the generally valid 3*R*. In this case (15) can be represented in the form of:

$$C = 3R\left[1 + \frac{1}{4}\frac{\theta^2}{T^2} - \frac{9}{40}\frac{\theta^3}{T^3} + \frac{3}{20}\frac{\theta^4}{T^4} - \frac{5}{56}\frac{\theta^5}{T^5}\right]. \tag{16}$$

III. Model representation of the structure of quasicrystalline icosahedral phase

Structure of quasicrystalline icosahedral phase $Al_{63}Cu_{25}Fe_{12}$ of the Al–Cu–Fe has a quasicrystalline pattern in all directions. Therefore, the dispersive law will have the quadratic dependence both in the *xy* plane and in the direction of *z* axis. According to [8], sum frequency of the sound waves will be expressed as:

$$\omega^2 = u^2 k_z^4 + \gamma^2 \chi^4 . \tag{17}$$

Since the pattern of the icosahedral phase is an isotropic one, and only one direction of polarization is considered, expression (9) should be divided by 3. Besides, in (9) the integration limit will change:

$$F = \frac{8VT}{3(2\pi)^3} \int\limits_0^{\hbar u k_{\max}^2/T} dk_z \int\limits_0^{\hbar\gamma\chi_{\max}^2/T} \ln\left(1 - \exp\left(-\frac{\hbar}{T}\sqrt{u^2 k_z^4 + \gamma^2\chi^4}\right)\right) 2\pi\chi d\chi . \tag{18}$$

We integrate over $d\chi$ in the internal integral as in the previous case for the decagonal phase, and obtain:

$$F = \frac{VT^2}{3\pi^2\gamma\hbar}\int\limits_0^y \left(x\ln x - 6\ln\left(1 + \frac{x}{2}\right)\right) dk , \tag{19}$$

where $x = \frac{\hbar}{T}\sqrt{u^2 k_z^4 + b}$, where $b = \gamma^2 \chi_{\max}^4$ – parameter, $y = \frac{\hbar}{T}\sqrt{u^2 k_{z\max}^4 + b}$ – integration limit. We multiply the numerator and denominator under the integral by k^2, and then allow *k* within the differential sign. We obtain:

$$F = \frac{VT^2 k}{6\pi^2\gamma\hbar}\int\limits_0^y \left(x\ln x - 6\ln\left(1 + \frac{x}{2}\right)\right)\frac{1}{x} dx , \tag{20}$$

where *k* is factored outside the integral sign as a value which varies only slightly. After expansion of the $\ln\left(1 + \frac{x}{2}\right)$ to the sixth term and integration, free energy will take the form:

$$F = \frac{VLk}{6\pi^2\gamma}\left(T\ln\hbar L - T\ln T - 4T + \frac{3}{4}\hbar L - \frac{1}{12}\frac{(\hbar L)^2}{T} + \frac{3}{128}\frac{(\hbar L)^3}{T^2} - \frac{3}{400}\frac{(\hbar L)^4}{T^3} + \frac{1}{384}\frac{(\hbar L)^5}{T^4}\right), \tag{21}$$

where $L = \sqrt{u^2 k_{z\max}^4 + \gamma^2 \chi_{\max}^4}$. After calculation of the entropy and internal energy we obtain for the heat capacity of the icosahedral phase:

$$C = \frac{\partial E}{\partial T} = 3R\left[1 + \frac{1}{6}\frac{\theta^2}{T^2} - \frac{9}{64}\frac{\theta^3}{T^3} + \frac{9}{100}\frac{\theta^4}{T^4} - \frac{5}{96}\frac{\theta^5}{T^5}\right], \tag{22}$$

where expression $\hbar L = \hbar\sqrt{u^2 k_{z\max}^4 + \gamma^2 \chi_{\max}^4}$ in its content is similar to the Debye temperature. The factor $\frac{VLk}{6\pi^2\gamma}$ is similar in the content to the Debye sphere 3*R*. Indeed, we assume that velocity of sound γ in the *xy* plane is equal to velocity of sound *u* in the *z* direction, and has some *u*. Then the factor is equal to $\frac{Vk}{6\pi^2}\frac{u\left(k_{z\max}^4 + \chi_{\max}^4\right)^{1/2}}{u}$. Further, we'll add the vector directed along the axis *z* $k_{z\max}^2$ to vector χ^2, which is formed by vectors k_x and k_y in the plane. Hence we have the wave vector *K* in the space *xyz*, which is equal to $K^4 = k_{z\max}^4 + \chi_{\max}^4$. If we assume that $k = K = k_D$, the factor will be equal to $\frac{Vk_D^3}{6\pi^2} = 3R$.

IV. Analysis of results

From expressions (16) and (22) it is evident that heat capacity of the decagonal and icosahedral quasicrystalline phases at high temperatures will exceed the Dulong-Petit value 3*R* as distinct from crystalline phases. This result is confirmed by studies of the phenomenon of excessive heat capacity of quasicrystalline phases at high temperatures in the works [1, 5, 6, 7]. Consequently, according to the Gruneisen law, quasicrystalline phases have higher resistance to the temperature action, than crystalline ones. The Debye temperature according to [1, 12] for the icosahedral phase $Al_{63}Cu_{25}Fe_{12}$ of the Al–Cu–Fe alloy is 510 K, and for the decagonal phase $Al_{69}Co_{21}Ni_{10}$ of the Al–Co–Ni

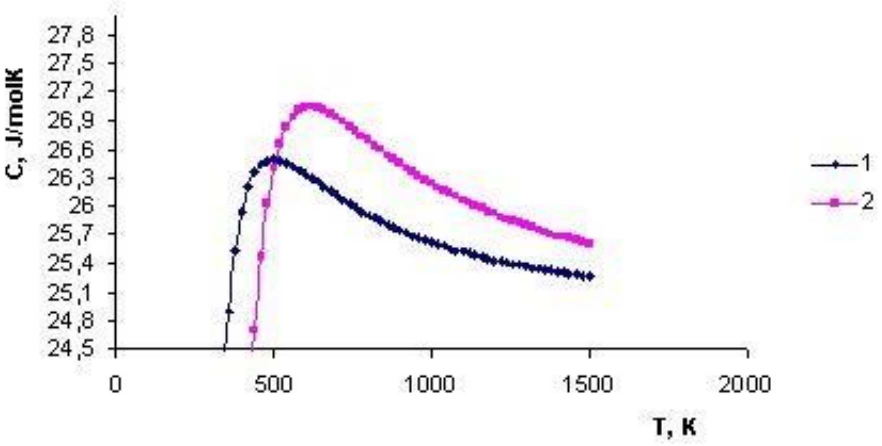

Fig.1. Temperature dependence of heat capacity of quasicrystalline phase: 1 – icosahedral phase $Al_{63}Cu_{25}Fe_{12}$ of the Al–Cu–Fe alloy; 2 – decagonal phase $Al_{69}Co_{21}Ni_{10}$ of the Al–Co–Ni alloy.

alloy – 602 К. The temperature dependence for these quasicrystalline phases is shown in Fig. 1.

The figure shows that heat capacity of quasicrystalline phases exceeds the level of 3*R*, with the maximums at 500 К – 26.5 J/mol·K for the icosahedral phase and at 620 К – 27.0 J/mol·K for the decagonal phase. Further the heat capacity begins to decrease, but remains elevated to the temperatures of ~1120 K for the icosahedral phase and ~1500 K for the decagonal phase. Accordingly, the decagonal quasicrystalline $Al_{69}Co_{21}Ni_{10}$ phase remains stable to higher temperatures, than the icosahedral phase of $Al_{63}Cu_{25}Fe_{12}$. This result is consistent with the literature data. Therefore, composite materials with the decagonal quasicrystalline fillers can be manufactured at higher temperatures, compared to icosahedral quasicrystals. Therefore, the usage of decagonal quasicrystals is more promising one [13, 14].

In contrast to the results given in this paper, in the works [1, 5] the heat capacity of quasicrystalline phases increases continuously to 1300 K. It can be connected with the fact that the authors measured the heat capacity of the pure quasicrystalline phase. Bat in real structure in the state of high temperatures it will be possibly to create defects of the quasicrystalline phase, as described in [15] or, possibly, quasicrystalline phase is transformed into crystalline approximants, which are implemented at high temperatures [16, 17, 18]. Therefore, due to reduction of the amount of quasicrystalline phase the heat capacity of the structure begins to decrease.

Conclusions

1. Structure of the quasicrystalline phase can be considered in the anisotropic crystals' model representation, according to which the dispersive law for the crystalline pattern is represented as a linear one, and for the quasicrystalline pattern – as a quadratic one. As a result, we obtained the expressions for the heat capacity of quasicrystalline phases at high temperatures, which exceeds the heat capacity of the crystalline phase 3*R*. Therefore, with the use of the model of anisotropic crystals we can explain the phenomenon of excessive heat capacity of quasicrystalline phases at high temperatures.
2. According to the results of calculations of the temperature heat capacity dependence of quasicrystalline phases, it is seen that the heat capacity of the decagonal phase $Al_{69}Co_{21}Ni_{10}$ of the Al–Co–Ni alloy has a higher maximum and remains excessive. That is, it exceeds the Dulong-Petit value up to higher temperatures, than the icosahedral phase $Al_{63}Cu_{25}Fe_{12}$ of the Al–Cu–Fe alloy. Pursuant to the Gruneisen law, it means that the decagonal phase is more stable at higher temperatures, than the icosahedral phase.

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Теплоємність декагональних та ікосаедричних квазікристалічних фаз при високих температурах

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В роботі розраховано теплоємність квазікристалічних декагональних $Al_{69}Co_{21}Ni_{10}$ та ікосаедричних $Al_{63}Cu_{25}Fe_{12}$ квазікристалічних фаз сплавів Al–Co–Ni і Al–Cu–Fe відповідно. Згідно з законом Грюнейзена теплоємність є енергетичною характеристикою, яка відображає стійкість фаз до руйнування. Для розрахунків теплоємності структуру квазікристалічних фаз розглянуто в уявленні моделі анізотропних кристалів. У результаті отримано, що теплоємність квазікристалічних фаз при високих температурах є надлишковою, тобто перевищує рівень Дюлонга-Пті. Таким чином квазікристалічні фази при високих температурах є більш стабільними, ніж кристалічна фаза. Для декагональної квазікристалічної фази теплоємність більше $3R$ в інтервалі температур ~ 480 - 1500 К, а для ікосаедричної квазікристалічної фази – в інтервалі температур ~ 380 – 1120 К. З цього випливає, що декагональні фази залишаються стійкими при високих температурах, за яких ікосаедричні фази руйнуються.

Ключові слова: квазікристали, декагональна фаза, ікосаедрична фаза, дисперсійний закон, анізотропія, ізотропія, температурна залежність теплоємності, надлишкова теплоємність, закон Дюлонга-Пті.