ScienceAsia 27 (2001) : 67-71

On the Specific Heat of the Cubic Quasicrystals

Cuilian Li[a], Youyan Liu[b] and Wichit Sritrakool[c]

[a] Department of Physics, South China University of Technology, Guangzhou 510640, China.

[b] Department of Physics, South China University of Technology, Guangzhou 510640, China and International Center for Material Physics, Academia Sinica, Shenyang 110015, China.

[c] Department of Physics, Faculty of Science, Chulalongkorn University, Bangkok 10330, Thailand.

Received 9 Mar 2000
Accepted 11 Aug 2000

ABSTRACT Based on the linear elasticity theory of the cubic quasicrystals, we have derived the equations of wave propagating in the cubic quasicrystals and the analytical expression of the phase velocity of wave propagation. Moreover, we extend the Debye hypothesis of continuous elastic medium to study the specific heat of the cubic quasicrystals, for which we obtain an analytic expression of the specific heat as well as an approach to calculate the Debye temperature Θ_D.

KEYWORDS: specific heat, elasticity wave, quasicrystal.

INTRODUCTION

Since the discovery of the icosahedral quasicrystal in Al-Mn alloys, the quasicrystals with noncrystallographic symmetry, such as decagonal, dodecagonal and octagonal phases have been extensively studied.[1-4] For resent years in the process of the rapid solidified $V_6Ni_{16}Si_7$ alloy, Feng *et al*[5-6] discovered a kind of quasicrystal with cubic symmetry, which has been a new subject in the field of quasicrystals. Wang *et al*[7] have discussed the projection description of the cubic quasicrystals and Yang *et al*[8] have studied their linear elasticity theory. There are still many physical properties of the cubic quasicrystals have not been studied yet. For example, one of the important physical properties, the specific heat of cubic quasicrystals has not been studied. It is well-known that for the general quasicrystals it is impossible to obtain an analytical solution of lattice vibration properties. Therefore it is impossible to get an analytic result for the physical properties related to the quasicrystal-lattice dynamics. Due to the special structure of the cubic quasicrystals, we can obtain some analytical results on its lattice dynamics. In the present article we will report our study on the specific heat of cubic quasicrystals. We have first derived the equation of wave propagation in the cubic quasicrystals and then obtained the specific heat expression of the cubic quasicrystals. It is well-known that the calculation of the specific heat for both of the crystals and quasicrystals has to base on the knowledge of their lattice vibration modes. In order to simplify the calculation, Debye[9] assumed that the lattice wave of the solid is an elastic wave of continuous medium. Based on this hypothesis he successfully obtained the specific heat formulas and explained the experimental phenomenon that the specific heat of crystals decrease by T^3 at low temperature. In this paper, following the Debye hypothesis we will extend the continuous medium model to the cubic quasicrystals, in which the contributions of the phonons, phasons and their couplings on the specific heat are considered in the six-dimensional space but the wave propagaation still exists in the physical spaee.[5-8] By this generalized Debye hypothesis we first derive the wave equations to obtain the wave velocity expression, then we derive the analytical expression of specific heat for the cubic quasicrystals and provide a set of formulas to calculate the Debye temperature θ_D. This paper is organized as follows: In Section II based on the linear elasticity theory we derive the wave propagation equation and phase velocities for the cubic quasicrystals. In Section III, based on the results of Section II, we derive the formulas to calculate the specific heat of the cubic quasicrystals. The Section IV is a brief conclusion. Because up to now there is no related experiment dates reported yet, therefore in this article we only present the theoretical results.

LINEAR ELASTICITY THEORY AND WAVE PROPAGATION EQUATION OF THE CUBIC QUASICRYSTALS

According to the result of Wang *et al*[7], the cubic quasicrystals can be obtained by projecting a six-dimensional periodic structure onto a three-dimensional physical subspace. Letting $\vec{\xi}$ be a displacement vector in the six-dimensional space, u and w be the components of $\vec{\xi}$ in the parallel subspace (*ie*, physical subspace V_E) and perpendicular subspace (ie, complementary subspace V_I), respectively, then we have

$$\vec{\xi} = \mathrm{u} + \mathrm{w}. \tag{1}$$

For the cubic quasicrystals which possess the crystallographic point-group symmetry, physical-property tensors in V_E and V_I can be transformed under the same irreducible representation. Therefore, they will induce the same elastic behavior in that two subspaces. If u_1, u_2, u_3 stand for the displacement components of the phonon field u, and w_1, w_2, w_3 for the displacement components of the phason field w along main-axis x_1, x_2, x_3, respectively, then we have

$$\begin{aligned} u_i &= u_i\,(x_1, x_2, x_3;\, t)\ (i = 1, 2, 3); \\ w_i &= w_i\,(x_1, x_2, x_3;\, t)\ (i = 1, 2, 3). \end{aligned} \tag{2}$$

According to the linear elasticity theory of the cubic quasicrystals developed by Yang *et al*[8], the stress-strain relations become

$$\begin{aligned}
T_{11} &= C_{11}E_{11} + C_{12}E_{22} + C_{12}E_{33} + R_1F_{11} + R_2F_{22} + R_2F_{33} \\
T_{22} &= C_{12}E_{11} + C_{11}E_{22} + C_{12}E_{33} + R_2F_{11} + R_1F_{22} + R_2F_{33} \\
T_{33} &= C_{12}E_{11} + C_{12}E_{22} + C_{11}E_{33} + R_2F_{11} + R_2F_{22} + R_1F_{33} \\
T_{23} &= 2C_{44}E_{23} + 2R_3F_{23} = T_{32} \\
T_{31} &= 2C_{44}E_{31} + 2R_3F_{31} = T_{13} \\
T_{21} &= 2C_{44}E_{12} + 2R_3F_{12} = T_{12} \\
H_{11} &= R_1E_{11} + R_2E_{22} + R_2E_{33} + K_{11}F_{11} + K_{12}F_{22} + K_{12}F_{33} \\
H_{22} &= R_2E_{11} + R_1E_{22} + R_2E_{33} + K_{12}F_{11} + K_{11}F_{22} + K_{12}F_{33} \\
H_{33} &= R_2E_{11} + R_2E_{22} + R_1E_{33} + K_{12}F_{12} + K_{12}F_{22} + K_{11}F_{33} \\
H_{23} &= 2R_3E_{23} + 2K_{44}F_{23} = H_{32} \\
H_{31} &= 2R_3E_{31} + 2K_{44}F_{31} = H_{13} \\
H_{12} &= 2R_3E_{12} + 2K_{44}F_{12} = H_{21}
\end{aligned} \tag{3}$$

where E_{ij} are the strain components associated with phonon field u, F_{ij} the strain components associated with phason field w and

$$E_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right), \quad F_{ij} = \frac{1}{2}\left(\frac{\partial w_i}{\partial x_j} + \frac{\partial w_j}{\partial x_i}\right); \tag{4}$$

T_{ij} are the stress components similar to those in conventional crystals, H_{ij} the stress components due to the existence of the phason field, C_{ij} the elastic constants of the phonon field, K_{ij} the elastic constants of the phason field, and R_i, the phonon-phason coupling elastic constants. The corresponding equations of mass-point vibration are

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \frac{\partial T_{11}}{\partial x_1} + \frac{\partial T_{12}}{\partial x_2} + \frac{\partial T_{13}}{\partial x_3} \\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \frac{\partial T_{21}}{\partial x_1} + \frac{\partial T_{22}}{\partial x_2} + \frac{\partial T_{23}}{\partial x_3} \\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \frac{\partial T_{31}}{\partial x_1} + \frac{\partial T_{32}}{\partial x_2} + \frac{\partial T_{33}}{\partial x_3} \\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \frac{\partial H_{11}}{\partial x_1} + \frac{\partial H_{12}}{\partial x_2} + \frac{\partial H_{13}}{\partial x_3} \\
\rho\frac{\partial^2 w_2}{\partial t^2} &= \frac{\partial H_{21}}{\partial x_1} + \frac{\partial H_{22}}{\partial x_2} + \frac{\partial H_{23}}{\partial x_3} \\
\rho\frac{\partial^2 w_3}{\partial t^2} &= \frac{\partial H_{31}}{\partial x_1} + \frac{\partial H_{32}}{\partial x_2} + \frac{\partial H_{33}}{\partial x_3}
\end{aligned} \tag{5}$$

where ρ is the mass density of the quasicrystals. Because a cubic quasicrystal is an anisotropic crystal with nine independent elastic constants, the propagation of vibration varies with the polarization direction. In the following we first discuss the wave propagation in the direction $\wp$ of the physical space. Let *1, m, n* stand for the direction-cosines of $\wp$, we can rewrite the Eq (4) as follows:

$$\begin{aligned}
&E_{11} = l\frac{\partial u_1}{\partial \wp}, E_{22} = m\frac{\partial u_2}{\partial \wp}, E_{33} = n\frac{\partial u_3}{\partial \wp}, E_{23} = \frac{1}{2}\left(m\frac{\partial u_2}{\partial \wp} + n\frac{\partial u_3}{\partial \wp}\right), \\
&E_{13} = \frac{1}{2}\left(n\frac{\partial u_1}{\partial \wp} + l\frac{\partial u_3}{\partial \wp}\right), E_{23} = \frac{1}{2}\left(l\frac{\partial u_2}{\partial \wp} + m\frac{\partial u_1}{\partial \wp}\right), \\
&F_{11} = l\frac{\partial w_1}{\partial \wp}, F_{22} = m\frac{\partial w_2}{\partial \wp}, F_{33} = n\frac{\partial w_3}{\partial \wp}, F_{23} = \frac{1}{2}\left(m\frac{\partial w_2}{\partial \wp} + n\frac{\partial w_3}{\partial \wp}\right), \\
&F_{13} = \frac{1}{2}\left(n\frac{\partial w_1}{\partial \wp} + l\frac{\partial w_3}{\partial \wp}\right), F_{21} = \frac{1}{2}\left(l\frac{\partial w_2}{\partial \wp} + m\frac{\partial w_1}{\partial \wp}\right).
\end{aligned} \tag{6}$$

Substituting Eq (6) into Eq (3), then into Eq (5) again, we can obtain

$$\begin{aligned}
\rho\frac{\partial^2 u_1}{\partial t^2} &= \Gamma_{11}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{12}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{13}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{14}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{15}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{16}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 u_2}{\partial t^2} &= \Gamma_{21}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{22}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{23}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{24}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{25}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{26}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 u_3}{\partial t^2} &= \Gamma_{31}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{32}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{33}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{34}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{35}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{36}\frac{\partial^2 w_3}{\partial \wp^2} \\
\rho\frac{\partial^2 w_1}{\partial t^2} &= \Gamma_{41}\frac{\partial^2 u_1}{\partial \wp^2} + \Gamma_{42}\frac{\partial^2 u_2}{\partial \wp^2} + \Gamma_{43}\frac{\partial^2 u_3}{\partial \wp^2} + \Gamma_{44}\frac{\partial^2 w_1}{\partial \wp^2} + \Gamma_{45}\frac{\partial^2 w_2}{\partial \wp^2} + \Gamma_{46}\frac{\partial^2 w_3}{\partial \wp^2}
\end{aligned} \tag{7}$$

$$\rho\frac{\partial^2 w_2}{\partial t^2}=\Gamma_{51}\frac{\partial^2 u_1}{\partial\wp^2}+\Gamma_{52}\frac{\partial^2 u_2}{\partial\wp^2}+\Gamma_{53}\frac{\partial^2 u_3}{\partial\wp^2}+\Gamma_{54}\frac{\partial^2 w_1}{\partial\wp^2}+\Gamma_{55}\frac{\partial^2 w_2}{\partial\wp^2}+\Gamma_{56}\frac{\partial^2 w_3}{\partial\wp^2}$$

$$\rho\frac{\partial^2 w_3}{\partial t^2}=\Gamma_{61}\frac{\partial^2 u_1}{\partial\wp^2}+\Gamma_{62}\frac{\partial^2 u_2}{\partial\wp^2}+\Gamma_{63}\frac{\partial^2 u_3}{\partial\wp^2}+\Gamma_{64}\frac{\partial^2 w_1}{\partial\wp^2}+\Gamma_{65}\frac{\partial^2 w_2}{\partial\wp^2}+\Gamma_{66}\frac{\partial^2 w_3}{\partial\wp^2},$$

where

$$\begin{cases}\Gamma_{11}=C_{11}l^2+C_{44}(m^2+n^2)\\ \Gamma_{12}=C_{12}lm+C_{44}lm\\ \Gamma_{13}=C_{12}\,ln+C_{44}\,ln\\ \Gamma_{14}=R_1l^2+R_3(m^2+n^2)\\ \Gamma_{15}=R_2lm+R_3lm\\ \Gamma_{16}=R_2\,ln+R_3\,ln,\end{cases}\quad\begin{cases}\Gamma_{21}=C_{12}lm+C_{44}lm\\ \Gamma_{22}=C_{11}m^2+C_{44}(l^2+n^2)\\ \Gamma_{23}=C_{12}mn+C_{44}mn\\ \Gamma_{24}=R_2lm+R_3lm\\ \Gamma_{25}=R_1m^2+R_3(l^2+n^2)\\ \Gamma_{26}=R_2mn+R_3mn,\end{cases}\quad(8)$$

$$\begin{cases}\Gamma_{31}=C_{12}\,ln+C_{44}\,ln\\ \Gamma_{32}=C_{12}mn+C_{44}mn\\ \Gamma_{33}=C_{12}n^2+C_{44}(l^2+m^2)\\ \Gamma_{34}=R_2\,ln+R_3\,ln\\ \Gamma_{35}=R_2mn+R_3mn\\ \Gamma_{36}=R_1n^2+R_3(l^2+m^2),\end{cases}\quad\begin{cases}\Gamma_{41}=R_1l^2+R_3(m^2+n^2)\\ \Gamma_{42}=R_2lm+R_3lm\\ \Gamma_{43}=R_2\,ln+R_3\,ln\\ \Gamma_{44}=K_{11}l^2+K_{44}(m^2+n^2)\\ \Gamma_{45}=K_{12}lm+K_{44}lm\\ \Gamma_{46}=R_{12}mn+R_{44}mn,\end{cases}\quad(9)$$

$$\begin{cases}\Gamma_{51}=R_2lm+R_3lm\\ \Gamma_{52}=R_1m^2+R_3(l^2+n^2)\\ \Gamma_{53}=R_2mn+R_3mn\\ \Gamma_{54}=K_{12}lm+K_{44}lm\\ \Gamma_{55}=K_{11}m^2+K_{44}(l^2+n^2)\\ \Gamma_{56}=K_{12}mn+K_{44}mn\end{cases}\quad\begin{cases}\Gamma_{61}=R_2\,ln+R_3\,ln\\ \Gamma_{62}=R_2mn+R_3mn\\ \Gamma_{63}=R_1n^2+R_3(l^2+m^2)\\ \Gamma_{64}=K_{12}\,ln+K_{44}\,ln\\ \Gamma_{65}=K_{12}mn+K_{44}mn\\ \Gamma_{66}=K_{11}n^2+K_{44}(l^2+m^2).\end{cases}\quad(10)$$

Let $\vec{\xi}$ stand for elastic displacement vector related to the wave propagation along $\wp$ direction, and *p*, *q*, *r*, *p*', *q*', *r*' for its direction-cosines in the six-dimensional space, then

$$u_1=p\xi,\,u_2=q\xi,\,u_3=r\xi,\,w_1=p'\xi,\,w_2=q\xi,\,w_3=r\xi,$$
$$\xi=pu_1+qu_2+ru_3+p'w_1+q'w_2+r'w_3,\quad(11)$$

where ξ is the length of $\vec{\xi}$. Substituting Eq (11) into Eq (7), we obtain the following wave equation

$$p\frac{\partial^2\xi}{\partial t^2}=C^*\frac{\partial^2\xi}{\partial\wp^2},\quad(12)$$

which implies that the phase velocity $v=\sqrt{C^*/p}$, C^* is the effective elasticity coefficient, and satisfies the following equations:

$$\begin{aligned}&p\Gamma_{11}+q\Gamma_{12}+r\Gamma_{13}+p'\Gamma_{14}+q'\Gamma_{15}+r'_{16}\Gamma_{16}=pC^*\\&p\Gamma_{21}+q\Gamma_{22}+r\Gamma_{23}+p'\Gamma_{24}+q'\Gamma_{25}+r'_{26}\Gamma_{26}=qC^*\\&p\Gamma_{31}+q\Gamma_{32}+r\Gamma_{33}+p'\Gamma_{34}+q'\Gamma_{35}+r'_{36}\Gamma_{36}=rC^*\\&p\Gamma_{41}+q\Gamma_{42}+r\Gamma_{43}+p'\Gamma_{44}+q'\Gamma_{45}+r'_{46}\Gamma_{46}=p'C^*\\&p\Gamma_{51}+q\Gamma_{52}+r\Gamma_{53}+p'\Gamma_{54}+q'\Gamma_{55}+r'_{56}\Gamma_{56}=q'C^*\\&p\Gamma_{61}+q\Gamma_{62}+r\Gamma_{63}+p'\Gamma_{64}+q'\Gamma_{65}+r'_{66}\Gamma_{66}=r'C^*.\end{aligned}\quad(13)$$

Providing that the Eq (13) has a solution, then we have

$$\begin{vmatrix}\Gamma_{11}-C^*\Gamma_{12} & \Gamma_{13} & \Gamma_{14} & \Gamma_{15} & \Gamma_{16}\\ \Gamma_{21} & \Gamma_{22}-C^* & \Gamma_{23} & \Gamma_{24} & \Gamma_{25} & \Gamma_{26}\\ \Gamma_{31}-C^*\Gamma_{32} & \Gamma_{33}-C^* & \Gamma_{34} & \Gamma_{35} & \Gamma_{36}\\ \Gamma_{41} & \Gamma_{42} & \Gamma_{43} & \Gamma_{44}-C^* & \Gamma_{45} & \Gamma_{46}\\ \Gamma_{51} & \Gamma_{52} & \Gamma_{53} & \Gamma_{54} & \Gamma_{55}-C^* & \Gamma_{56}\\ \Gamma_{61} & \Gamma_{62} & \Gamma_{63} & \Gamma_{64} & \Gamma_{65} & \Gamma_{66}-C^*\end{vmatrix}=0.\quad(14)$$

Above Eq (14) is a secular-equation of effective elastic constants *C**. In principal, combining Eqs (8-10) we can solve the Eq (14) to obtain *C** and then calculate the phase-velocities of wave propagation along any direction. It is however very difficult to analytically solve the Eq (14) for all propagation direction. To simplify the calculation and obtain a possible analytical solution, we consider the wave propagating along the (100) direction of cubic quasicrystals in physical subspace. In this special cace Eq (l4) reduces to

$$\begin{vmatrix}C_{11}-C^* & 0 & 0 & R_1 & 0 & 0\\ 0 & C_{44}-C^* & 0 & 0 & R_3 & 0\\ 0 & 0 & C_{44}-C^* & 0 & 0 & R_3\\ R_1 & 0 & 0 & K_{11}-C^* & 0 & 0\\ 0 & R_3 & 0 & 0 & K_{44}-C^* & 0\\ 0 & 0 & R_3 & 0 & 0 & K_{44}-C^*\end{vmatrix}=0.\quad(15)$$

The solutions of above equation are, respectively,

$$C_1^* = C_4^* = \frac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C11-K11)^2+4R_1^2}}, \quad (16)$$

$$C_2^* = C_3^* = C_5^* = C_6^* = \frac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C44-K44)^2+4R_3^2}},$$

then the six velocities, $v_i(i = 1, \ldots 6)$, of wave propagating along the (100) direction of the cubic quasicrystals in physical-subspace have the following expressions:

$$v_1 = v_4 = \sqrt{\frac{\frac{1}{2}(C_{11} + K_{11}) + \frac{2R_1^2}{\sqrt{(C11-K11)^2+4R_1^2}}}{\rho}}$$

$$v_2 = v_3 = v_5 = v_6 = \sqrt{\frac{\frac{1}{2}(C_{44} + K_{44}) + \frac{2R_3^2}{\sqrt{(C44-K44)^2+4R_3^2}}}{\rho}}. \quad (17)$$

From above formulas we can see that Eq. (17) contains only four parameters C_{11}, K_{11}, R_1 and R_3. If we consider other propagation direction, says, to calculate the phase velocities of wave propagating along the (111) direction, then from Eq. (14) we will see that the velocity expression would involve nine independent elastic constants of the cubic quasicrystals. Obtaining an analytic solution is therefore very difficult. For these more general cases ones can only expect to have a numerical solution.

Specific Heat of thc Cubic Quasicrystals

After obtaining the above velocity expressions we now can evaluate the specific heat of the cubic quasicrystals by extending the Debye hypothesis to the studied systems. Debye[9] considered the crystals as a continuous elastic medium to propagate the waves of elastic vibration. Under this hypothesis he calculated the specific heat of ideal crystals, which was in good agreement with the experimental results at low temperature. We will now try to extend the Debye hypotheses to the cubic quasicrystals, i.e., we also consider the cubic quasicrystal as a continuous elastic medium. Noting that the phason do not form new degrees of freedom, the total number of freedom degrees remains three times the number of atoms contained in the cubic quasicrystal. Therefore, there are 3N independent harmonic vibration modes, where N is the number of atoms in the cubic quasicrystal. Denoting ω for the atom vibration circle-frequency and $g(\omega)$ for the frequency distribution function, then $g(\omega)d\omega$ is the number of the harmonic vibration modes between ω and $\omega + d\omega$, and we have

$$\int_0^\infty g(\omega)d\omega = 3N. \quad (18)$$

For the cubic quasicrystals containing phonon as well as phason by the Debye hypothesis we have

$$g(\omega)d\omega = B\omega^2 d\omega, \quad (19)$$

where

$$B = \frac{V}{2\pi^2}\left(\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3} + \frac{1}{v_4^3} + \frac{1}{v_5^3} + \frac{1}{v_6^3}\right), \quad (20)$$

and V represents the volume of the cubic quasicrystals, $v_i(i = 1, \ldots, 6)$ are defined by Eq (17).

Considering that the total number of freedom degrees should be finite, so there is a maximum frequency w_D, then Eq (18) can be rewritten as

$$\int_0^{\omega_D} g(\omega)d\omega = 3N. \quad (21)$$

Substituting Eq (19) into the above formula and because the phase velocities v_i, $i = 1,2, \ldots 6$ are independent of the frequency, so we easily obtain

$$\omega_D^3 = 9N/B. \quad (22)$$

If we introduce an effective average energy , then the total energy reads

$$E = E_0 + \sum_\omega \bar{\varepsilon}(\omega) = E_0 + \int_0^{\omega_D} \bar{\varepsilon}(\omega) g(\omega) d\omega, \quad (23)$$

where E_o is a constant and

$$\bar{\varepsilon} = \frac{\hbar\omega}{e^{\hbar\omega/kT} - 1}, \quad (24)$$

where k is the Boltzmann constant, T is the absolute temperature, respectively. According to the definition of specific heat,

$$C_V = \left(\frac{\partial E}{\partial T}\right)_V, \quad (25)$$

Using Eqs (22-24) we obtain

$$C_V = B\int_0^{\omega_D} (\frac{\hbar\omega}{kT})^2 \frac{e^{\hbar\omega/kT} k\omega^2 d\omega}{(e^{\hbar\omega/kT}-1)^2}, \qquad (26)$$

where B is given by Eq. (20). If we introduce two new parameters x and y as following:

$$y = \frac{\hbar\omega}{kT}, \quad x = \frac{\hbar\omega_D}{kT} = \frac{\Theta_D}{T}, \qquad (27)$$

where Θ_D is the generalized Debye characteristic temperature for the cubic quasicrystals, and evaluated as

$$\Theta_D = \hbar\omega_D / k = \frac{\hbar}{k}(\frac{9N}{B})^{1/3} = \frac{\hbar}{k}(\frac{18N\pi^2}{B})^{1/3}\frac{1}{\chi^{1/3}} \qquad (28)$$

with

$$\chi = (\frac{1}{v_1^3} + \frac{1}{v_2^3} + \frac{1}{v_3^3} + \frac{1}{v_4^3} + \frac{1}{v_5^3} + \frac{1}{v_6^3}), \qquad (29)$$

then the Eq. (26) can be rewritten as

$$C_V = Bk\int_0^x (kT/\hbar)^3 \frac{y^4 e^y}{(e^y-1)^2} dy$$

$$= \frac{9Nk}{x^3}\int_0^x \frac{y^4 e^y}{(e^y-1)^2} dy. \qquad (30)$$

Above Eq (30) is an analytic expression of specific heat for tbe cubic quasicrystals. It is also one of the main analytic results which we expect to obtain.

Conclusion

In this paper, we first obtained the wave propagation equation of the cubic quasicrystals. Based on this equation, we derived the formulas of wave velocities propagating in the cubic quasicrystals. By extending the Debye's continuous medium hypothesis for ideal crystals to the cubic quasicrystals, we obtained the analytic expresion of specific heat for the cubic quasicrystals and provided an approach to calculate the Debye temperature Θ_D. Formally the present specific heat and Debye temperature expressions for cubic quasicrystals are almost same as that of the ideal crystals, but the Θ_D contains the contributions of the phonons, the phasons, and the coupling between phonons and phasons. Thus, the present theoretical results on the specific heat of the cubic quasicrystals are an meaningful extension of the Debye theory for ideal crystals, and also only because the special geometric structure of the cubic quasicrystals we can obtain these interesting analytical results, for other kinds of quasicrystals we generally can not obtain such impact analytical solution. Ones can only expect a numerical result, but it is a heavy and tedious work.

Acknowledgements

This work (Li and Liu) was supported by the National Natural Science Foundation of China, Grant No.19874021, and W. Sritrakool was supported by the Thailand Research Fund.

References

1. Shechtman D S, Blech I, Gratias D and Cahn JW, (1984) *Phys Rev Iett* 53, 1951.
2. Bendersky L (1985) *Phys Rev Lett* 55, 1461.
3. Ishimasa T, Nissen H -U & Fukano Y (1985) *Phys Rev Lett* 55, 511.
4. Wang N, Chen H, and Kno KH, (1987) *Phys Rev Lett* 59, 1010.
5. Feng YC, Zhou DS, Li DX, Dong C, Van Tendeloo G & Kuo, KH (1987) *Philos Mag Lett* 55, 221.
6. Feng YC, Lu G, Ye HQ, Ruo KH, Withers RL & Van Tendeloo, G (1990) *J Phys Condens Matter* 2, 9749.
7. Wang RH & Qin CS (1994) *Acta Crystal* A 50, 366.
8. Yang WG, Wang RH, Ding DH & Hu CZ (1993) *Phys Rev B* 48, 6999.
9. Debye P (1912) *Ann d Phys* 39, 789.
10. Janot C (1993) Quasicrystals, Clarendon press (Oxford).