The Change of Thermoelastic Properties at a Variation of Isotope Composition of Lithium and Diamond

Mahach Magomedov [C, S]
Institute for Geothermal Research of Daghestan Scientific Centre RAS, Makhachkala, Daghestan, Russia

Proceeding from the Debye model of a crystal and the Grüneisen law ($\alpha_p = \gamma\, C_v / B_T\, V$), we calculated the temperature dependencies of thermoelastic properties for isotope-different crystals of lithium (from ^{7}Li or from ^{6}Li) and diamond (from ^{12}C or from ^{13}C): $\alpha_p = [\partial \ln(V)/\partial T]_P$ is the thermal expansion coefficient; $\rho = N\, m/V$ – density; $B_T = -V\,(\partial P/\partial V)_T$ is the bulk modulus, C_v and $C_p = C_v\,(1 + \gamma\, \alpha_p\, T)$ are the isochoric and isobaric heat capacities. The Debye temperture Θ and Grüneisen parameter γ were calculated by the parameters: the mass of atom, the first coordination number, the four parameters of interatomic potential, which has the Mie–Lennard-Jones form: $\varphi(r) = [D/(b-a)][a(r_o/r)^b - b(r_o/r)^a]$. Here D and r_o are different for varied isotopes; b and a are the constants: $b > a$. For the relative isotope displacement of a potential minimum r_o and the bulk modulus of crystals we used the values [1]:

for lithium

$\Delta_C = 1 - r_o^* = 1 - [r_o(^7\text{Li})/r_o(^6\text{Li})] = 9.56\times10^{-4}$,
$\Delta_B = B_{T=0}^* - 1 = [B_T(^7\text{Li}) / B_T(^6\text{Li})] - 1 = 2\times10^{-2}$,

for diamond

$\Delta_C = 1 - r_o^* = 1 - [r_o(^{13}\text{C})/r_o(^{12}\text{C})] = 1.5\times10^{-4}$;
$\Delta_B = B_{T=0}^* - 1 = [B_T(^{13}\text{C})/B_T(^{12}\text{C})] - 1 = 1.5\times10^{-3}$.

Here, the function with asterisk $F^*(X)$ defines the reduced value: $F^* = F(^{k+1}\text{M})/F(^k\text{M})$.

Then the displacement of depth of the interatomic interaction well be determined from a ratio [1]: $D^* = D(^{k+1}\text{M})/D(^k\text{M}) = (1 + \Delta_B)(1 - \Delta_C)^3$, and one obtains:

for lithium

$$D^* = D(^7\text{Li})/D(^6\text{Li}) = (1 + 2\times10^{-2})(1 - 9.56\times10^{-4})^3 = 1.01708,$$

for diamond

$$D^* = D(^{13}\text{C})/D(^{12}\text{C}) = (1 + 1.5\times10^{-3})(1 - 1.5\times10^{-4})^3 = 1.00105.$$

Using the potential parameters and expressions above we calculated temperature dependent thermoelastic properties from $T = 0$ K up to $T = 455$ K – for BCC-Li, and up to $T = 4000$ K – for diamond with step $\Delta T = 5$ K. Good agreement with experimental dependences of the specified parameters were obtained: $\alpha_p(T)$ and thermal capacity increase as $\sim (T/\Theta)^3$ – at low ($T/\Theta << 1$) temperatures, and $\sim (T/\Theta)$ – when $T/\Theta > 1$. Bulk modulus and density monotonously decrease at isobaric heating. For crystals from $^{k+1}$M and from ^{k}M we obtained the inequality: $C_v(^{k+1}\text{M}) > C_v(^k\text{M})$; $C_p(^{k+1}\text{M}) > C_p(^k\text{M})$. At the same time it is received, that a difference between temperature dependences of various properties for a crystal from $^{k+1}$M and from ^{k}M atoms decreases with increasing temperature. For Li we found: $B_T(^7\text{Li}) > B_T(^6\text{Li})$; and the dependences $\alpha_p(T)$ for crystals from ^{7}Li and from ^{6}Li crossed at a point: $T_x = 303.7$ K; $\alpha_p(T_x) = 12.6\times10^{-5}\,\text{K}^{-1}$. The crossings of dependences $\alpha_p(T)$ for isotope-different diamonds on all the investigated interval of temperatures it is not revealed: $\alpha_p(^{13}\text{C}) > \alpha_p(^{12}\text{C})$. However the crossing dependences $B_T(T)$ for diamonds from ^{12}C and from ^{13}C is revealed in a point: $T_x = 626.7$ K и $B_{Tx} = 4492.5$ kbar. The change of a difference of properties isotope-different crystals of lithium and diamond with growth of pressure is investigated and we obtained:

$(\partial [D(^{k+1}\text{M}) - D(^k\text{M})] / \partial P)_T > 0$; $(\partial [\Theta(^k\text{M}) - \Theta(^{k+1}\text{M})] / \partial P)_T > 0$;
$(\partial [B_T(^7\text{Li}) - B_T(^6\text{Li})] / \partial P)_T > 0$; $(\partial [B_T(^{13}\text{C}) - B_T(^{12}\text{C})] / \partial P)_{T<Tx} > 0$;
$(\partial [C_v(^{k+1}\text{M}) - C_v(^k\text{M})] / \partial P)_T > 0$; $(\partial [C_p(^{k+1}\text{M}) - C_p(^k\text{M})] / \partial P)_T > 0$.

[1] Magomedov M.N. // High Temperature. 2006. V. 44. N 6. P. 861 – 870.