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 \( \alpha_p = \gamma v / B_T \), 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): \( \alpha_p = [\partial \ln (v)/\partial T]_\rho \) is the thermal expansion coefficient; \( \rho = N m/V \) – density; \( B_T = -V (\partial P/\partial V)_T \) is the bulk modulus, \( C_r \) and \( C_p = C_v (1 + \gamma \alpha_p) \) are the isochoric and isobaric heat capacities. The Debye temperature \( \Theta \) and Grüneisen parameter \( \gamma \) 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: \( \varphi(r) = [D(b - a)](a(r_a/r)^b - b(r_a/r)^a) \). Here \( D \) and \( r_a \) are different for varied isotopes; \( b \) and \( a \) are the constants: \( b > a \). For the relative isoelse displacement of a potential minimum \( r_o \) and the bulk modulus of crystals we used the values [1]:

**for lithium**

\[
\begin{align*}
\Delta_C &= 1 - r_o(\nu(7Li))/r_o(\nu(6Li)) = 9.56 \times 10^{-4}, \\
\Delta_B &= B_T/\nu(7Li)/B_T(\nu(6Li)) = 1 = 2 \times 10^{-2},
\end{align*}
\]

**for diamond**

\[
\begin{align*}
\Delta_C &= 1 - r_o(\nu(^{13}\text{C}))/r_o(\nu(^{12}\text{C})) = 1.5 \times 10^{-4}, \\
\Delta_B &= B_T/\nu(13C)/B_T(12C) = 1 = 1.5 \times 10^{-3}.
\end{align*}
\]

Here, the function with asterisk \( F(X) \) defines the reduced value: \( F^* = F(\nu(1M))/F(\nu(4M)) \).

Then the displacement of depth of the interatomic interaction well be determined from a ratio [1]: \( D^* = D(\nu(1M))/D(\nu(4M)) = (1 + \Delta_B)(1 - \Delta_C)^3 \), and one obtains:

**for lithium**

\[
D^* = D(\nu(7Li))/D(\nu(6Li)) = (1 + 2 \times 10^{-2})(1 - 9.56 \times 10^{-4})^3 = 1.01708,
\]

**for diamond**

\[
D^* = D(\nu(^{13}\text{C}))/D(^{12}\text{C}) = (1 + 1.5 \times 10^{-3})(1 - 1.5 \times 10^{-4})^3 = 1.00105.
\]

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 \( (T/\Theta)^3 \) – at low \( (T/\Theta) << 1 \) temperatures, and \( (T/\Theta) \) – when \( T/\Theta > 1 \). Bulk modulus and density monotonously decrease at isobaric heating. For crystals from \(^{14}\)M and from \(^{12}\)M we obtained the inequality: \( C_v(^{14}\text{M}) > C_v(^{12}\text{M}) \); \( C_p(^{14}\text{M}) > C_p(^{12}\text{M}) \). At the same time it is received, that a difference between temperature dependences of various properties for a crystal from \(^{14}\)M and from \(^{12}\)M decreases with increasing temperature. For Li we found: \( B_T(\text{Li}) > B_T(\text{Li}) \); and the dependences \( \alpha_p(T) \) for crystals from \(^{14}\)Li and from \(^{12}\)Li crossed at a point: \( T_x = 303.7 \) K; \( \alpha_p(T_x) = 12.6 \times 10^{-5} \) 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: \( T_s = 626.7 \) K \& \( B_T(x) = 4492.5 \) kbar.

The change of a difference of properties isotope-different crystals of lithium and diamond with growth of pressure is investigated and we obtained:

\[
\begin{align*}
(\partial [D(\nu(1M))/D(\nu(4M))]/\partial P)_T > 0; \\
(\partial [\Theta(\nu(1M))/\Theta(\nu(4M))]/\partial P)_T > 0; \\
(\partial [B_T(\nu(7Li))/B_T(\nu(6Li))]/\partial P)_T > 0; \\
(\partial [B_T(^{13}\text{C}))/B_T(^{12}\text{C})]/\partial P)_T > 0; \\
(\partial [C_v(^{14}\text{M})]/C_v(^{12}\text{M})]/\partial P)_T > 0; \\
(\partial [C_p(^{14}\text{M})]/C_p(^{12}\text{M})]/\partial P)_T > 0.
\end{align*}
\]