Baric and dimensional changes of niobium properties

S P Kramynin\textsuperscript{1,3} and E N Akhmedov\textsuperscript{2}
\textsuperscript{1}Amirkhanov Institute of Physics, Dagestan Scientific Center of Russian Academy of Sciences, 367015, M. Yaragskogo St., 94, Makhachkala, Dagestan Republic, Russian Federation
\textsuperscript{2}Institute of Geothermal Research, Dagestan Scientific Center of Russian Academy of Sciences, 367030, Imama Shamiya St., 39a, Makhachkala, Dagestan Republic, Russian Federation
\textsuperscript{3}E-mail: kraminin@mail.ru

Abstract. We have calculated the baric dependencies of thermophysical properties and melting temperature as well as the thermal equation of state for niobium based on the pair interatomic Mi-Lenard-Jones potential and the crystal Einstein model for niobium (Nb). Baric dependencies computations made along two isotherms 300 K and 3000 K are in good agreement with the experimental data for niobium. We have obtained the charts of pressure dependencies for the following properties: Debye temperature, the first, second and third Gruneisen parameters, isothermal compression modulus, isochoric and isobaric heat capacity, volumetric coefficient of thermal expansion and the melting temperature. The article investigates size dependencies of both specified properties and the melting temperature of niobium using an RP-model of nanocrystal.

1. Introduction

The baric dependencies of niobium thermophysical properties have not been properly studied. The dependencies of volumetric coefficient of thermal expansion: $\alpha_p = (\partial \ln V / \partial T)_p$, heat capacity ($C_v$ and $C_p$) and melting temperature ($T_m$) on hydrostatic (comprehensive) pressure ($P$) along various isotherms at high pressures ($P>1000$ kbar = 100 GPa) are still not quite clear. Various (both computational and analytical) methods used to study the state equation of crystal at high pressure have lots of fitting constants that are deprived of physical meaning in their formalism. That is why it is very difficult to both unambiguously define those fitting constants by means of experimental data and predict their pressure dependence along specific isotherm. The results obtained by such methods are inconvenient for further applications. Pressure dependencies for $\alpha_p$ and ($C_v$, $C_p$) have been calculated in one article [1] only. There is almost no data available for pressure dependence of melting temperature $T_m(P)$ for niobium. Dependence $T_m(P)$ was calculated only by Fellinger \textit{et al.} [2] in a very narrow pressure range: from 0 to $P=2.5$ GPa. Moreover, there is no data available for pressure dependence of surface energy ($\sigma$) for niobium. In this article we calculate both the state equation and change of thermophysical properties for niobium in hydrostatic compression along two isotherms: for low (300 K) and high (3000 K) temperatures using a relatively simple method. Our calculations have shown good agreement with the experimental estimates available in the literature. Due to these results we have calculated baric dependencies of $T_m(P), T_m'(P)$ and $\sigma(P)$. Dimensional dependences for surface energy and melting temperature have been obtained using the RP – model and interatomic Mie-Lenard-Jones potential in the framework of a unified formalism.
2. Calculation method for nanocrystal lattice properties

It is necessary to determine both the interatomic interaction potential and the calculation method based on this potential to calculate the lattice properties of a nanocrystal of a simple one-component substance. To represent interatomic interaction we have chosen the Mie-Lenard-Jones potential [3, ch. 3]:

\[
(r) = \frac{D}{(b/a)} \left[ a \left( \frac{r}{r_0} \right)^b - b \left( \frac{r}{r_0} \right)^a \right],
\]

(1)

\(b > a > 1\) are parameters, \(D\) and \(r_0\) are the depth and the coordinate of the potential minimum. Then, using the approximation “nearest neighbours interaction only”, the Debye temperature as function of the first coordination number and the distance between the centers of nearest-neighbor atoms can be defined from [3, ch. 2; 4]:

\[
\Theta(k_n, c) = A_w(k_n, c) \xi \left[ -1 + \left( 1 + \frac{8D}{k_B A_w(k_n, c) \xi^2} \right)^{1/2} \right],
\]

(2)

where \(k_B\) is the Boltzmann constant, \(A_w\) is the function that arises due to the accounting of zero-point oscillation energy of atoms in crystal, \(k_n\) is the first coordination number, that depends both on the size and surface form of nanocrystal [3, ch. 6], \(c = (6k_p v/\pi)^{1/3}\) is the distance between centers of nearest-neighbor atoms, \(v = V/N\) – specific volume, \(V\) is the volume, \(N\) is the number of atoms in the nanocrystal:

\[
A_w(k_n, c) = K_R \frac{5k_n a b (b + 1)}{144(b - a)} \left( \frac{r_o}{c} \right)^{b+2},
\]

(3)

where \(K_R\) is defined in the first coordination number in the volume of nanocrystal:

\[
m is the atomic mass, \(\hat{\hbar}\) is reduced Planck constant, \(k_p\) is the structure packing factor, \(k_n(\infty)\) – first coordination number in the volume of nanocrystal.

If the approximation of “only nearest neighbors interaction” is applicable to the nanocrystal that has Gibbs geometric surface, then the dependence of the nanocrystal energy on the size and shape will be determined by the size and shape dependence of the average (on the nanocrystal) value of the first coordination number. In this case, using the Einstein model for the vibrational spectrum of a nanocrystal, for the specific (per atom) free Helmholtz energy of the nanocrystal, we can accept the expression: [3, 5]:

\[
f_H(k_n, c, T) = \left\{ \frac{k_n}{2} \right\} D \cdot U(R) + 3k_B \Theta_E(k_n, c) \left\{ \frac{1}{2} + \left( \frac{T}{\Theta_E(k_n, c)} \right) \ln \left[ 1 - \exp \left( -\frac{\Theta_E(k_n, c)}{T} \right) \right] \right\},
\]

(4)

where \(\Theta_E\) is the Einstein temperature, which is related to Debye temperature by the ratio [5, p. 116]: \(\Theta = (4/3)\Theta_E\), \(R = r_o/c\) is the linear density of the crystal. Potential energy function is defined from:

\[
U(R) = \frac{a R^b - b R^a}{b - a}.
\]

We assume that the dependence of the \(k_n\) on the size and shape of a nanocrystal with Gibbs surface does not depend on the density and temperature, but is determined only by the number of atoms in the nanocrystal \((N)\), its shape parameter \((f)\) and constants \(k_n(\infty)\) and \(k_p\). Then from (4) for the thermal equation of state \((P)\) and isothermal bulk modulus \((B_T)\) we get:

\[
P = \left( \frac{\partial f_H}{\partial v} \right)_T = \left( \frac{k_n}{6} D \cdot U'(R) + 3k_B \Theta_E \cdot \gamma \cdot E_w \left( \frac{\Theta_E}{T} \right) \right) \frac{1}{v},
\]

(5)
\[ B_T = -v \left( \frac{\partial P}{\partial V} \right)_T = P + \left[ \frac{k_B}{18} D \cdot U''(R) + 3k_B \Theta_E \cdot \gamma \cdot (\gamma - q) \cdot E_w \left( \frac{\Theta_E}{T} \right) - 3N \cdot k_B \cdot \gamma^2 \cdot T \cdot F_E \left( \frac{\Theta_E}{T} \right) \right] \left( \frac{1}{v} \right). \] 

The following functions are used here:

\[ F_E(y) = \frac{y^2 \exp(y)}{[\exp(y) - 1]^2}, \quad E_w(y) = 0.5 + \frac{1}{\exp(y) - 1}, \quad U'(R) = R \left[ \frac{\partial U(R)}{\partial R} \right] = \frac{ab(R^b - R^a)}{b - a}, \quad U''(R) = R \left[ \frac{\partial U'(R)}{\partial R} \right] = \frac{ab(bR^b - aR^a)}{b - a}. \]

The first \((\gamma)\), second \((q)\) and third \((z)\) Gruneisen parameters in accordance with (2) have the forms:

\[ \gamma = \left( \frac{\partial \ln \Theta}{\partial \ln \nu} \right)_T = \frac{b + 2}{6(1 + X_w)}, \quad q = \left( \frac{\partial \ln \gamma}{\partial \ln \nu} \right)_T = \frac{X_w(1 + 2X_w)}{(1 + X_w)}, \]

\[ \gamma = (1 + 4X_w) - 2q = \frac{(1 + 3X_w)}{6}, \quad \frac{X_w}{1 + X_w} = \frac{\gamma}{1 + X_w}. \]

where \(X_w = \frac{1}{3} \frac{C_v}{\gamma} \Theta / \Theta \) defines contribution of quantum effects.

Since the Debye temperature (2) does not depend on the temperature at isochoric heating, the isochoric and isobaric heat capacity can be defined as [5, p. 125]:

\[ C_v = 3N \cdot k_B \cdot F_E \left( \frac{\Theta_E}{T} \right), \]

where isobaric thermal coefficient of volume expansion can be calculated from the Gruneisen equation [5, p. 121]:

\[ \alpha_p = \frac{C_v}{V \cdot B_T} = \frac{\gamma \cdot C_v}{N \cdot B_T \cdot \pi r^3 / (6k_p)} \left( \frac{v_n}{v} \right), \quad v_0 = \frac{\pi r^3}{6k_p}. \]

Expressions (2)–(10) allow us to calculate the dependence of both the state equation and lattice properties on the normalized volume \(v/v_0 = (cr_n)^3 = R^{-3}\) and temperature \(T\) for the unicomponent nanocrystal with given structure (i.e. with given values \(k_o(\infty)\) and \(k_p\)), if we know all the four parameters of the interatomic potential (1) and functional dependence of the first coordination number on the size and form of nanocrystal, i.e. function \(k_o(N, f)\).

Note that if we assume \(N \to \infty\), \(V \to \infty\) and \(v = V/N = \text{const}\), \(k_o(N, f) = k_o(\infty)\), then the formalism (2)-(10) allows calculating both the equation of state and pressure dependences of the macrocrystal’s thermodynamic properties. This method was successfully applied when studying the thermodynamic properties of iron, diamond, silicon, germanium [6] and molybdenum [7] at high \(P\cdot T\) conditions. Comparing experimental data with our calculations for all these substances showed good results.

3. RP-model of nanocrystal

We use RP-model of nanocrystal to define function \(k_o(N, f)\). The essence of the RP-model is as follows. Let us assume that nanocrystal with Gibbs free surface has the form of a rectangular parallelepiped with a square base, faceted with (100) faces. Value \(f = N_p/N_{po}\) – is a form parameter, that is defined by the ratio of atoms number on the lateral edge \(N_{po}\) to the number of atoms on the edge of the base \(N_{po}\). For a rod-shaped form, \(f > 1\); for a cube, \(f = 1\); for a plate shaped nanocrystal, \(f < 1\). The number of atoms in a nanocrystal, which equals to: \(N = fN_{po}/\alpha\), varies in the range: \(2^3/\alpha \leq N \leq \infty\), where \(\alpha = \pi/\alpha(6k_p)\) is a structure parameter.

Limitation of the system by the surface will break the bonds at the boundary. Therefore, if the
“only nearest neighbors” interaction approximation is used, then instead of the first coordination number \(k_0(\infty)\) we must take \(k_0(N, f)\) – the average (over the nanocrystal) value of the first coordination number, which will depend on both \(N\) and \(f\) [3, 8].

The structure of the system (characterized by the packing factor \(k_0\)) is assumed to be the same: \(k_0 = \text{const.}\)

In the RP-model the dependence of the normalized average value of the first coordination number on the size \((N)\) and shape \((f)\) of the nanocrystal has the form [3, 8]:

\[
k_n^\ast = \frac{k_n(N, f)}{k_n(\infty)} = 1 - Z_s(f) \left( \frac{\alpha^2}{N} \right)^{1/3},
\]

(11)

where \(k_n(\infty) = k_n(N = \infty)\) – macrocrystal coordination number,

\[
Z_s(f) = \frac{1 + 2f}{3f^{2/3}}.
\]

(12)

The function of form \(Z_s(f)\) reaches a minimum of unity at \(f = 1\), i.e. in the shape of a cube. For plate \((f=1)\) or rod-shaped \((f=1)\) forms, the value of \(Z_s(f)\) is greater than one. Therefore, the function \(k_n(f)^\ast\) from (11) for any value of \(N\) has a maximum at \(f = 1\), i.e. for the most energetically optimal (the cubic) shape of a rectangular parallelepiped.

The volume and area of surface for the RP-model are:

\[
V = N_m f c^3 = N \alpha c^3, \quad \Sigma = 6 c^2 \alpha_s (N \alpha)^{2/3} Z_s(f),
\]

where \(\alpha_s\) is the coefficient taking into account the packing density of atoms on the face (i.e., in the surface layer) of the nanocrystal: \(\alpha_s = \alpha_s^{2/3}\). It is easy to see that the volume \(V\) of the nanocrystal does not depend on the shape of the system, i.e. on the volume of \(f\).

In the RP-model, \(\sigma(N, f)\) — the specific (per unit area) surface energy of the \((100)\) face of the nanocrystal, its isochoric and isobaric temperature derivatives and for the surface pressure \((P_s)\) the following expressions were obtained [3, ch. 6; 8]:

\[
\sigma(N, f) = - \frac{k_n(\infty) D R^2}{12 \alpha^{2/3} r_0} L_E(N, f),
\]

(13)

\[
L_E(N, f) = U(R) + 3H_w(N, T),
\]

(14)

\[
H_w(N, T) = \frac{6 \gamma(N, f)}{(b + 2)} \left( \frac{k_B \Theta_E(N, f)}{D k_n(N, f)} \right) E_w \left( \frac{\Theta_E}{T} \right), \quad t_y(y) = 1 - \frac{2y \exp(y)}{[\exp(2y) - 1]}.
\]

(15)

Thus, the function \(k_n(N, f)\) obtained in the RP-model with the formalism of (2) - (15) allows us to calculate the dependence of all lattice and surface properties on the size and shape of the nanocrystal at given temperatures and specific volume.

4. Niobium interatomic potential parameters

Niobium crystal \((m(Nb) = 92.906 \text{ a.m.u.})\) has a body-centered cubic (bcc) structure with the following values: \(k_0=8, k_p=0.6802\). It is difficult to study niobium thermodynamic properties under high \(P-T\) conditions because Nb is one of the hardest crystals. Therefore, there are no published experimental results for the baric dependencies of the thermal expansion coefficient and the melting temperature. Initially, the Mie-Lenard-Jones potential parameters for niobium were defined by the method described in [3, ch. 3; 9] from a closed set of four equations. These parameters are:

\[
r_0 = 2.8648 \times 10^{-10} \text{ m}, \quad D / k_B = 21706.44 \text{ K}, \quad a = 1.88, \quad b = 5.81.
\]

(16)

This set includes the following four experimentally determined quantities at \(T=0\) K and \(P=0\) GPa: \(\Theta_0\) is the Debye temperature, and \(\gamma_0\) is the first Gruneisen parameter, \(V_0\) is the molar volume, \(L_0\) is the specific atomization energy. The method [3, ch. 3; 9] was used to compute the set of parameters (16). Values \(\gamma_0\) and \(\Theta_0\) are defined from the experiment with inaccuracies, as it was noticed in [6]. Thereby,
we have optimized $a$, $b$ and $D$ using both isotherm $T=300$ K of the thermal state equation $P(V/V_0,300$ K) and $\alpha_P(P, T)$, measured under normal conditions, i.e., when $P=0$ GPa and $T=300$ K. Values used for the optimization of the potential parameters for niobium are: $[10, p. 173]: \alpha_P(0,300$ K) = 21.3$ \times 10^{-6}$ K $^{-1}$. Dependencies $P(V/V_0,300$ K) have been taken from [1, 11-13]. They are shown in Figure 1.

Thus, we have obtained optimized parameters of potential (1) for the bcc Nb:

$\mathbf{r}_0 = 2.8648 \times 10^{-10}$ m, $D/D_k = 30200$ K, $a = 2.3$, $b = 6.2$ (17)

Note that both self-diffusion of atoms and vacancies are not accounted because their effect in compression of the niobium crystal becomes insignificant [14]. Here, as in work [14], the contribution to the thermodynamic parameters of the electronic subsystem is also not accounted because the Mie-Lenard-Jones potential describes the pair interaction of electrically neutral atoms.

5. State equation and baric dependences of niobium properties

We have computed both state equation and baric dependencies of different bcc Nb properties, using formalism (1)-(10) and interatomic potential parameters (17).

Figure 1 shows isotherms of the state equation for bcc Nb. Solid and dashed curves represent our calculations made for 300 K and 3000 K, respectively. Open circles – experimental data from [11]. Stars represent theoretical calculation results [1], triangles – theoretical calculation [12], squares - theoretical calculation [13]. Our calculation results agree well with the data from other sources, both experimental and theoretical [1, 11-13], as shown in Figure 1.

Figure 1. State equation isotherms for niobium.

We can get pressure dependence of any property $X(P)$ along specific isotherm by calculating $P(V)$ and $X(V)$ along this isotherm.

We have calculated the pressure dependences of the Debye temperature $\Theta(P)$, the first $\gamma(P)$, the second $q(P)$ and the third $z(P)$ Gruneisen parameters. Our calculations have shown that the Debye temperature increases, and $\gamma(P)$ decreases with increasing pressure, $q(P)$ and $z(P)$ monotonously increase with increasing pressure. Note that there is no data on the pressure dependence for $q(P)$ and $z(P)$ in the literature, and in most works it is unreasonably believed that $q$ value does not depend on $V/V_0$, i.e. it is accepted that $q = \text{const}$ and $z = 0$ [15, 16]. As it follows from our results, this assumption is not quite correct. Figure 2 shows baric dependencies of isothermal bulk modulus $B_T(P) = -(\partial P/\partial \ln V)_T$ along 300 K and 3000 K isotherms for Nb. Solid and dashed curves – our computed values of $B_T(P)$ at 300 K and 3000 K; dotted and dash-dotted curves – computed values from [1] at 298K and 3000 K; symbols – data from [17-20]. Estimates for isothermal bulk modulus for $P=0$ and $T=300$K are in the interval: $B_T(0)/[\text{GPa}] = 144.2$ [17] + 161 [18] + 166 [19] + 174 [20].
Figure 3 shows isotherms of baric dependencies of niobium thermal expansion coefficient $\alpha_p(P)$ ($10^6$ K$^{-1}$) on the pressure. Solid and dashed curves – our computed values of $\alpha_p(P)$ at 300 K and 3000 K; open and upside triangles – computed values from [1] at 298K and 3000 K; circle – experimental value at 300 K from [10]. Computations of baric dependencies of $\alpha_p$ and pressure derivative $-\alpha'_p(P) = (\partial \alpha_p / \partial P)_{T}$ ($10^6$ (K-GPa)) have shown that when $P \rightarrow \infty$, function $\alpha_p$ tends to zero and $\alpha'_p(P)$ tends to zero too from the negative range of values.

Figure 3

Figure 4. Baric dependences for $\sigma$ – specific (per area unit) surface energy of face (100).

Figure 4 represents baric dependencies for $\sigma(100)$ - specific (per area unit) surface energy along 300 K and 3000 K isotherms by means of solid and dashed curves, respectively. Function $\sigma(P)$ increases and reaches maximum value at $P_{\text{max}}$ and then it decreases dramatically, reaching zero at $\sigma(P_0) = 0$, it gets negative values with further increase of pressure.

$$\sigma(100)_{\text{max}} = 4.447 \text{ J/m}^2 \text{ at } P = 76.5123 \text{ GPa for 300 K,}$$
$$\sigma(100)_{\text{max}} = 4.288 \text{ J/m}^2 \text{ at } P = 84.9383 \text{ GPa for 3000 K,}$$
$$P_0 = 752.3 \text{ GPa for 300 K,}$$
$$P_0 = 725.0 \text{ GPa for 3000 K.}$$

The same behavior of $\sigma(P)$ is observed for iron [14, 21], diamond [22], silicon [6], germanium [6] and molybdenum [7]. The structure of niobium crystal will decay into domains, increasing the area of the inter-domain surface, when $\sigma$ reaches the negative values region.

The published values for niobium $\sigma(100)$ at $P = 0$ and $T = 298$ K are in the interval: $\sigma(100)/[ \text{ J/m}^2] = 1.93–2.79$ [2], 2.00–2.99 [3], 2.66–2.99 [23], 1.968–2.715 [24]. Our data fits well with these estimates, as shown in Figure 4.

6. Baric dependencies of niobium melting temperature

We can get estimates for melting temperature baric dependence by using the obtained state equation for niobium. Thus, we have calculated the dependence of the melting temperature ($T_m$) on the relative volume ($V/V_0$), using the Lindemann relation [3, 25] that has the form:

$$T_m(P) = T_m(0) \left( \frac{V(P)}{V(P = 0)} \right)^{2/3} \left[ \Theta \left( \frac{V(P)}{V_0} \right) / \Theta \left( \frac{V(P = 0)}{V_0} \right) \right],$$

where $T_m(0)$ and $V(P = 0)$ are melting temperature and volume at $P = 0$. We have computed dependencies for $T_m(P)$, using $T_m(0) = 2742$ K [2] and obtained baric dependencies of Debye temperature and volume for niobium, shown in Figure 5 as solid curve. Unfortunately, as noted by the authors of [2], there is no experimental data for the pressure dependence of melting temperature of niobium in the literature. Therefore, we compared the results of our calculations only with the calculations obtained by the molecular dynamics method in [2].
Solid curve in Figure 5 represents our calculation results for $T_m(P)$ of macrocrystal, curve with circles – our calculations for nanocrystal composed of $N = 83$ atoms with cubic form ($f = 1$). Squares – calculations from [2], dashed curve - quadratic polynomial fit (20).

Baric dependencies for $dT_m/dP$. Dashed curve – calculations for nanocrystal ($N = 83$ and $f = 1$), solid curve – for macrocrystal, symbols – numerical differentiation of polynomial (20).

7. Size dependencies of niobium properties

Two isothermal pressure dependencies on the normalized volume $(v/v_o)$ for niobium calculated using the potential (1) and expressions (5) are shown in Figure 7. Curves (1, 3) – isotherms of 300 K, (2, 4) – isotherms of 3000 K. Solid curves – calculation results for macrocrystal, dashed ones – isomorph-isomeric (i.e., at constant $f$ and $N$ values) dependencies for a cubic nanocrystal composed of $N = 83$ atoms ($N_{iso} = 4$ and $f = 1$). A decrease in the pressure rising during the transition from macro to nanocrystal indicates a decrease in the bulk modulus with decreasing size.

Isothermal $P(v/v_o)$ dependencies for nanocrystal and macrocrystal intersect at a certain value of the relative volume $(v/v_o)_0$, as shown in Figure 7. Thus, at $(v/v_o)_0$ the surface pressure becomes zero: $P_{sd}(v/v_o)_0 = P$(Macro)$-P$(N=83, $f=1$) = 0. At $v/v_o < (v/v_o)_0$ the surface pressure compresses the nanocrystal ($P_{sd} > 0$), at $v/v_o > (v/v_o)_0$ the surface pressure stretches nanocrystal: $P_{sd} < 0$. 
Figure 7. Isothermal pressure dependencies on the normalized volume \( (v/v_o) \) for macro and nanocrystal \( (N = 83 \text{ and } f = 1) \).

Figure 8. Isotherms of thermal expansion coefficient baric dependencies \( \alpha_p(P) \) for macro and nanocrystal \( (N = 83 \text{ and } f = 1) \).

The pressure in the nanocrystal passes through zero when the value of \( v/v_o \) is greater than that for the macrocrystal, as shown in Figure 7, i.e. with isobaric decrease of the number of atoms the nanocrystal becomes more stretched by the negative surface pressure than the macrocrystal. That is why it is incorrect to assume that with isobaric decrease of the number of atoms the density of the nanocrystal is maintained constant. In this case, the farther from the point of “zero surface pressure” the pressure of the isobar is, the more the nanocrystal density will change with an isothermal-isomorphic decrease of the number of atoms in it.

Figure 8 shows the comparison of the baric dependencies of niobium volumetric thermal expansion coefficient \( \alpha_p(P) \) for macro (curves 1, 2) and nanocrystal (curves 3, 4) with \( N = 83 \text{ and } f = 1 \). The dependencies of \( \alpha_p(P) \) for the nanocrystal lie higher than for the macrocrystal.

Figure 9. Baric dependencies of bulk modulus \( B_T(P) \) for macro and nanocrystal \( (N = 83 \text{ and } f = 1) \).

Figure 10. Baric dependencies of \( \sigma \) – specific (per area unit) surface energy of face (100) for macro and nanocrystal \( (N = 83 \text{ and } f = 1) \).

Figure 9 shows comparison of the baric dependencies of niobium bulk modulus \( B_T(P) \) for macro (curves 1, 2) and nanocrystals (curves 3, 4) with \( N = 83 \text{ and } f = 1 \). The dependencies of \( B_T(P) \) for the nanocrystal lie lower than for the macrocrystal, as seen from Figure 9. Comparison of the baric dependencies of the \( \sigma(P) \) of niobium for macro (curves 1, 2) and nanocrystal (curves 3, 4) along two isotherms of \( T = 300 \text{ K} \) and \( T = 3000 \text{ K} \) with \( N = 83 \text{ and } f = 1 \) is shown in Figure 10. Isotherms of \( T = \)
300 K for nano and macrocrystal intersect at $P=62.9450$ GPa and $\sigma=4.4404$ J/m$^2$, as can be seen in Figure 10.

8. Conclusion
We have determined parameters of the pair interatomic Mi-Lenard-Jones potential for bcc-Nb. Baric dependencies of the thermophysical properties and melting temperature as well as the thermal equation of state for niobium were obtained based on the pair interatomic Mi-Lenard-Jones potential and the crystal Einstein model. Baric dependencies computations made along two isotherms 300 K and 3000 K, are in good agreement with the experimental data. We have obtained charts of the pressure dependencies for the following properties: Debye temperature, the first, second and third Gruneisen parameters, isothermal bulk modulus, isochoric and isobaric heat capacity, volumetric coefficient of thermal expansion and melting temperature. Dimensional dependencies of both specified properties and melting temperature of niobium are studied using the RP-model of nanocrystal.

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