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MELTING OF METALS COPPER, SILVER AND GOLD UNDER PRESSURE

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Abstract. *The dependence of the melting temperature of metals Cu, Ag and Au on pressure in the interval from 0 to 40 kbar is studied by the statistical moment method. This dependence has the form of near linearity and the calculated slopes of melting curve are 3.9 for Cu, 5.7 for Ag and 6 for Au. These results are in good agreement with the experimental data.*

I. INTRODUCTION

The melting of crystals is a popular phenomenon in nature and is generated at high temperature. Many research methods are developed in studying the melting process of crystal, where there are two different basic approaches. According to the first way of approach, the melting happens when the free energy of solid phase is equal to the one of liquid phase. With this way of approach, it is necessary to know the structure of both phases. However, the structure of liquid phase is very complex and usually is limited like pseudocrystal. The second way of approach for melting of crystal relates to the instability of solid phase. Many theories in this direction are applied such as the vibrational theory, the thermodynamic theory, the mechanical theory, etc. [1, 2]. Nevertheless, these theoretical results fully do not describe the melting curve of crystal. A study on the melting of crystal under pressure (the melting curve) has been attracted researchers attention and there are many methods applied in studying this problem [3, 4, 5].

In this paper, the dependence of melting temperature on pressure for metals Cu, Ag and Au is investigated by the statistical moment method. Our obtained simple equations rather well describe quantitatively the above mentioned dependence.

II. MELTING CURVE

Applying the Lindermann hypothesis, we find the equation for melting curve from the following condition:

$$\frac{\langle u^2 \rangle}{a^2} = \delta_L, \tag{1}$$

where $\langle u^2 \rangle$ and a are the mean square displacement and the lattice parameter at the melting temperature, respectively and δ_L is the Lindermann parameter. From the result obtained in [6], we have:

$$\langle u^2 \rangle = \frac{\theta_m}{k_0} + \frac{\gamma_0 \theta_m^2}{k_0^3} = \frac{\theta_m}{k_0}\left(1 + \frac{\gamma_0 \theta_m}{k_0^2}\right), \tag{2}$$

where $\theta_m = k_B T_m; k_0, \gamma_0$ are the coefficients depending on pressure [7]. Substituting (2) into (1), we obtain the following equation:

$$\frac{\theta_m}{k_0 a^2}\left(1 + \frac{\gamma_0 \theta_m}{k_0^2}\right) = \delta_L. \tag{3}$$

Using the Lennard-Jones potential (n-m) [9]:

$$\varphi(a) = \frac{D}{n-m}\left[m\left(\frac{r_0}{a}\right)^n - n\left(\frac{r_0}{a}\right)^m\right], \tag{4}$$

we find:

$$k_0 = \frac{DmnB_1}{(n-m)a_0^2}\left(\frac{r_0}{a_0}\right)^n\left[1 - \frac{B_2}{B_1}\left(\frac{a_0}{r_0}\right)^{(n-m)}\right], \tag{5}$$

$$\gamma_0 = \frac{DmnA_1}{(n-m)a_0^4}\left(\frac{r_0}{a_0}\right)^n\left[1 - \frac{A_2}{A_1}\left(\frac{a_0}{r_0}\right)^{(n-m)}\right], \tag{6}$$

where $B_1 = n-1; B_2 = m-1; A_1 = \frac{2}{3}n^3 + 3n^2 + \frac{25}{3}n + 10; A_2 = \frac{2}{3}m^3 + 3m^2 + \frac{25}{3}m + 10; r_0$ is the equilibrium distance between two atoms when they stand independently, $a_0 < r_0$. The lattice parameter a is determined from [6, 8]. Here, we approximately consider this parameter in the form:

$$a = a_0 + \theta\sqrt{\frac{\gamma_0}{k_0^3}}. \tag{7}$$

Substituting (5), (6) and (7) into (3), we obtain the following equation for the melting of crystal:

$$\theta_m^2\left[\frac{A_1}{AB_1^2}\left(\frac{2B_2}{B_1} - \frac{A_2}{A_1}\right) + \frac{1}{A}\sqrt{\frac{A_1}{B_1^3}}\left(\frac{A_2}{A_1} - \frac{3B_2}{B_1}\right)\right]y^{3n-m} + \theta_m^2\left[\frac{A_1}{AB_1^2} - \frac{2}{A}\sqrt{\frac{A_1}{B_1^3}}\right]y^{2n}$$
$$+ \theta_m y^n + AB_2\delta_L y^{n-m} - AB_1\delta_L = 0, \tag{8}$$

where $A = \frac{Dmn}{n-m}$ and $y = \frac{a_0}{r_0}$. The quantity y is determined from the equation of state for crystal at temperature $T = 0$ K and pressure p [6] as follows:

$$-p\delta a_0^2 = \frac{1}{6}\frac{\partial u(a_0)}{\partial a} + \frac{\hbar}{4}\frac{1}{\sqrt{Mk_0}}\frac{\partial k_0}{\partial a}, \tag{9}$$

where $u(a_0)$ is determined in [7], M is the mass of atom, δ is the coefficient depending on the structure of crystal. From (5), (6) and (9), we calculate the equation of state for crystal at temperature $T = 0$K and pressure p according to variables p and y.

III. EQUATIONS FOR MELTING CURVE OF METALS COPPER, SILVER AND GOLD UNDER PRESSURE

Values of potential parameters D, r_0, n and m for metals Cu, Ag and Au are taken from [9] and are summarized in Table 1.

Table 1. Parameters D, r_0, n and m for metals Cu, Ag and Au

Metals	$D/k_B(K)$	$r_0(\AA)$	n	m
Cu	3401,0	2,5487	9,0	5,5
Ag	3325,6	2,8760	9,5	5,5
Au	4683,0	2,8751	10,5	5,5

Substituting these values into (8) and (9), we find the equations for curve of melting of metals Cu, Ag and Au under pressure.

III.1. Equation for melting curve of Cu under pressure

This equation has the form:

$$2,12.10^{-4}T_m^2 y^{18}(1+0,84y^{3,5}) + T_m y^9 + 2246,4y^{3,5} - 4004 = 0, \tag{10}$$

where y is determined by the equation of state as follows:

$$0,0095py^{12} - 0,039y^{10,5} + 0,242y^7 + 9,973y^{3,5} - 9,83 = 0. \tag{11}$$

Solutions of Eqs. (10) and (11) at different pressures are given in Table 2

Table 2. Solutions of Eqs. (10) and (11) at different pressures

p(Kbar)	0	10	20	30	40	$\Delta T/\Delta p$
y	0,9901	0,9878	0,9855	0,9834	0,9814	
$T_m(K)$	1358,4	1398,5	1439,5	1478	1515,6	4,0

III.2. Equation for melting curve of Ag under pressure

This equation has the form:

$$2,3.10^{-4}T_m^2 y^{19}(1+0,85y^4) + T_m y^{9,5} + 1774,5y^4 - 3358 = 0, \tag{12}$$

where y is determined by the equation of state as follows:

$$0,0152py^{12,5} - 0,024y^{11,75} + 0,157y^{7,75} + 9,33y^4 - 0,256y^{3,75} - 8,85 = 0. \tag{13}$$

Solutions of Eqs. (12) and (13) at different pressures are given in Table 3

Table 3. Solutions of Eqs. (12) and (13) at different pressures

p(Kbar)	0	10	20	30	40	$\Delta T/\Delta p$
y	0,9901	0,9865	0,9832	0,9801	0,9772	
$T_m(K)$	1235,9	1295,9	1353,2	1409,3	1463,6	5,7

III.3. Equation for melting curve of Au under pressure

This equation has the form:

$$2,82.10^{-4}T_m^2y^{21}(1+0,55y^5)+T_my^{10,5}+1582,2y^5-3346,6=0, \tag{14}$$

where y is determined by the equation of state as follows:

$$0,0213py^{13,5}-0,019y^{14,25}+0,137y^{9,25}+11,62y^5-0,243y^{4,25}-10,96=0. \tag{15}$$

Solutions of Eqs. (14) and (15) at different pressures are given in Table 4

Table 4. Solutions of Eqs. (14) and (15) at different pressures

p(Kbar)	0	10	20	30	40	$\Delta T/\Delta p$
y	0,9905	0,9873	0,9842	0,9814	0,9788	
$T_m(K)$	1336,9	1398,6	1460,9	1519,4	1575,6	6,0

IV. DISSCUSION OF OBTAINED RESULTS

IV.1. Qualitative investigation

From Eqs. (11), (13) and (15) we derive the clear dependence of p on y. Functional investigation shows that when p increases, y decreases (with $y < 1$).

Eqs. (10), (12) and (14) are the equation of the second degree according to T_m with the coefficients depending to the parameter y. Positive solution T_m obtained from these equations depends on the parameter y and shows that when y decreases (i.e. p increases), T_m increases.

IV.2. Quantitative investigation

Results of investigating the pairs of equation (10) and (11), (12) and (13), (14) and (15) in the interval of pressure from 0 to 40 kbar are represented in Figure 1. The detailed results are given in numerical tables.

Three obtained melting curves approximately have the form of straight lines with different slopes. The calculated mean slopes of melting curves are 3.9 for Cu, 5.7 for Ag and 6.0 for Au. These results are in very good agreement with the experimental data [10].

In conclusion, our obtained results on the equations of melting curve for metals Cu, Ag and Au (the pairs of equation (10) and (11), (12) and (13), (14) and (15)) have simple analytic forms and rather well describe the melting of metals.

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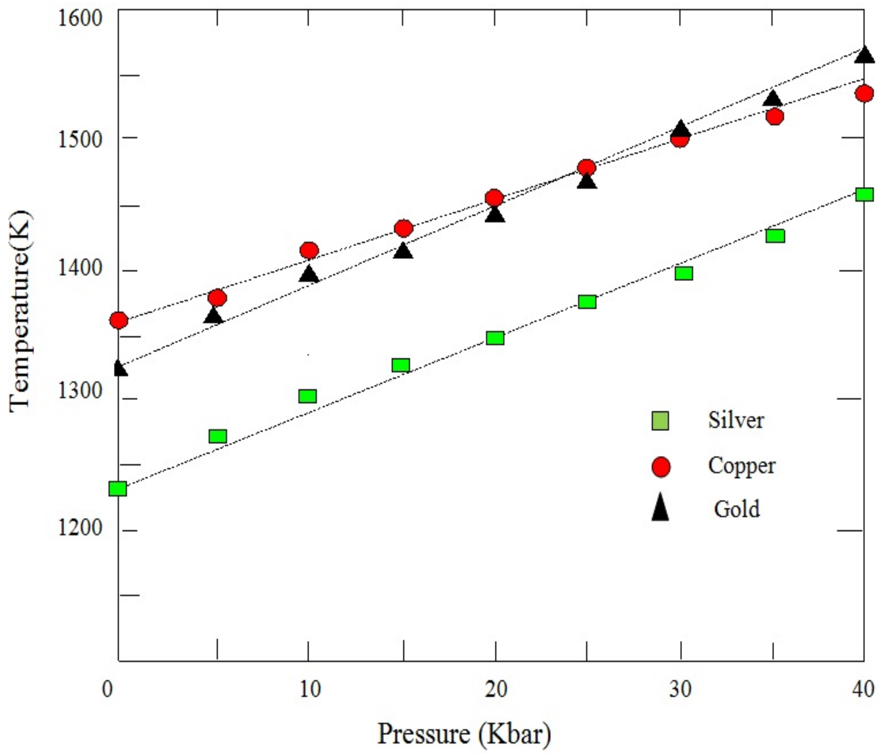

Fig. 1. The melting temperature of Cu, Ag and Au at various pressures

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