Thermodynamic properties of $Cu_3Au$ alloy

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Abstract. Based on the general expression of the Helmholtz free energy of alloys with $Ll_2$ structure obtained in previous works, we calculate the equations of the long-range order (LRO) parameter, and order-disorder transition (ODT) temperature in the $Cu_3Au$ alloy, and obtained thermodynamic quantities of $Cu_3Au$ alloy as simple functions of temperature and LRO-parameter, at pressures $P = 0$. Numerical results of the linear thermal expansion coefficient, isochoric and isobaric heat capacities, isothermal and adiabatic bulk modulus, are in good agreement with experiments.

1. Introduction
The techniques for a first principle has been used in the study of thermodynamic properties of metals and alloys. This type of first principle calculation involves the use of a pseudopotential model to describe the electron-ion interaction, and the variational principles based on the Gibbs-Bogoliubov inequality to determine the Helmholtz free energy of the system. The method has been applied successfully in the thermodynamic properties of liquid alloys [1] and of solid alloys [2,3]. The general solution model and the CALPHAD approach also used in the study of thermodynamic properties of phase diagram of alloys [4,5,6]. For the last three decades, the statistical moment method (SMM) has been used extensively in the study of thermodynamic properties of metals [7,8], and alloys [9,10].

Some of the thermodynamic properties of $Cu_3Au$ alloy have been studied using the Morse potential and free energy obtained by Bragg-Williams approximations [11], and using the SMM [9,10]. The results, however, obtained in these studies are still not straightforward, and the numerical results obtained by numerical programs are quite complex. So it is difficult to verify and apply.

In the current article, based on the general expression of Helmholtz free energy of alloys with $Ll_2$ structure obtained in previous work [12,20], we calculate the equations of the long-range order (LRO) parameter, and order-disorder parameter transition (ODT) temperature in the $Cu_3Au$ alloy, and obtained thermodynamic quantities of $Cu_3Au$ alloy as simple functions of temperature and LRO-parameter, at pressure $P = 0$. Numerical results of the linear thermal expansion coefficient, isochoric and isobaric heat capacities, isothermal and adiabatic bulk modulus, are in good agreement with experiments.

2. Theory
Using the general formulas calculated the free energy of the alloys in [9,10,24], we calculate the free energy expression of alloys with $Ll_2$ structure are given explicitly in terms of the effective
pair potentials and second-and fourth-ordered vibrational constant as [12,20](expressions of (1) to (6)):

$$\psi_{AB} = 3N \left[ C_A \left( \frac{u_{0A}}{6} + \psi_{0A} \right) + C_B \left( \frac{u_{0B}}{6} + \psi_{0B} \right) \right] +$$

\[ 3N \left[ \frac{\theta (k_B - k_A)^2}{k_A k_B} - \frac{2\omega}{6} \right] P_{AB} + \\
3N \left( C_A \frac{\gamma_{2A} - \gamma_{1A}}{k_A^2} + C_B \frac{\gamma_{2B} - \gamma_{1B}}{k_B^2} \right) \theta^2 - TS_{conf} \]  

(1)

with

$$k_\alpha = \frac{1}{2} \sum_i \left( \frac{\partial^2 \varphi_{\alpha i}}{\partial u_{ix}^2} \right)_{eq} \ , \ \gamma_{1\alpha} = \frac{1}{48} \sum_i \left( \frac{\partial^4 \varphi_{\alpha i}}{\partial u_{ix}^4} \right)_{eq} \ , \ \gamma_{2\alpha} = \frac{1}{8} \sum_i \left( \frac{\partial^4 \varphi_{\alpha i}}{\partial u_{ix}^2 \partial u_{iy}^2} \right)_{eq} \]  

(2)

In the above Eq. (2), the summations on \( i \) run over the neighbor sites of \( \alpha \) atoms in metal \( \alpha (\alpha = A, B); u_{0\alpha} \) in Eq. (1) denotes the effective pair interaction of \( \alpha \) atoms with other atoms in metal \( \alpha \) and \( \psi_{0\alpha} \) the Helmholtz free energy in the harmonic approximation of the atom \( \alpha \) in metal \( \alpha \):

$$u_{0\alpha} = \sum_i \varphi_{\alpha i} (r_{\alpha i}); \ \psi_{0\alpha} = 3N\theta \left[ x_\alpha + \ln(1 - e^{-2x_\alpha}) \right] \]  

(3)

where

$$x_\alpha = \frac{\hbar \omega_\alpha}{2\theta} , \ \text{and} \ \omega_\alpha = \sqrt{\frac{k_\alpha}{m^*}} , \ m^* = C_A m_A + C_B m_B \]  

(4)

with \( \alpha \), \( m_\alpha \) is the atomic mass \( \alpha \).

In the above Eq. (1), \( \omega \) and \( P_{AB} \) are order energy and probability of two atoms \( A \) and \( B \) next to each other, respectively; \( S_C \) is the configuration entropy; \( C_A, C_B \) are the concentrations of the \( A \) and \( B \) atoms, respectively; \( \theta = kT \), \( k \) is the Boltzmann constant, \( T \) is the absolute temperature, \( z \) is the coordination number.

$$S_C = -kN \sum_{\alpha \beta} \nu_\beta P_\alpha^\beta \ln P_\alpha^\beta = \frac{kN}{4} \left[ 3 \left( C_A + \frac{\eta}{4} \right) \ln \left( C_A + \frac{\eta}{4} \right) + \left( C_A - \frac{3\eta}{4} \right) \ln \left( C_A - \frac{3\eta}{4} \right) \right] +$$

\[ \frac{kN}{4} \left[ 3 \left( C_B - \frac{\eta}{4} \right) \ln \left( C_B - \frac{\eta}{4} \right) + \left( C_B + \frac{3\eta}{4} \right) \ln \left( C_B + \frac{3\eta}{4} \right) \right] \]  

(5)

where \( \nu_\beta, P_\alpha^\beta \) are the concentration of sub-lattice \( \beta \) and the probability of finding \( \alpha \) atom in the sub-lattice \( \beta \) \( (\alpha = A, B; \beta = a, b) \), respectively; \( \eta \) is the long-range order parameter (LRO parameter) in alloy.

$$P_{AB} = C_A C_B + \frac{1}{16} \eta^2 + \varepsilon_{AB} \]  

(6)

where \( \varepsilon_{AB} \) is the correlation parameter.

Using the expressions of (1) to (6), in this section we obtain new generalized results for the equations of the long-range order (LRO) parameter and the expressions of heat capacity, in simple analytical forms (expressions of (8) to (16)).

The \( LRO \) parameter \( \eta \) for binary order alloys calculated from equilibrium condition:

$$\left( \frac{\partial \psi_{AB}}{\partial \eta} \right)_{T,V,C_\alpha} = 0 \]  

(7)
Replace $\psi_{AB}$ in (7) by expression (1), we obtain the equation of order parameter $\eta$ with following form:

$$\frac{1}{2} \left( k_B - k_A \right)^2 - \frac{4\omega}{kT} = -\frac{1}{\eta} \ln \left( \frac{C_A + \eta}{4} \right) \left( \frac{C_B + \frac{3\eta}{4}}{4} \right)$$

(8)

where $\frac{\omega}{k}$ calculated from the equilibrium condition of the alloy at the order-disorder phase transition temperature.

Isochoric heat capacities, $C_V$ of alloys determined from the following formula:

$$C_V = \left( \frac{\partial E_{AB}}{\partial T} \right)_V = k \left( \frac{\partial E_{AB}}{\partial \theta} \right)_V$$

(9)

where, $\theta = kT$, $k$ is the Boltzmann constant; $T$ is the absolute temperature; $E_{AB}$ is the alloy’s energy, determined by Helmholtz free energy, $\psi_{AB}$, by the formula:

$$E_{AB} = \psi_{AB} - \theta \left( \frac{\partial \psi_{AB}}{\partial \theta} \right)_V$$

(10)

Substituting $\psi_{AB}$ by expression (1) into (10), we obtain the expression of $E_{AB}$ takes the following form:

$$E_{AB} = 3N \left[ C_A \frac{u_{0A}}{6} + C_B \frac{u_{0B}}{6} - 2\omega P_{AB} + \left( C_A X_A + C_B X_B \right) \theta \right]$$

$$- 3N \left( C_A \frac{\gamma_{2A} - \gamma_{1A}}{k_A^2} + C_B \frac{\gamma_{2B} - \gamma_{1B}}{k_B^2} \right) \theta^2$$

(11)

where $X_\alpha = x_\alpha \text{cth} x_\alpha$.

Substituting $E_{AB}$ in (9) by expression (11), we obtain the expression for the isochoric heat capacities, $C_V$, of 1 mol of alloys:

$$C_V = 3R \left[ C_A Y_A^2 + C_B Y_B^2 - 2 \left( C_A \frac{\gamma_{2A} - \gamma_{1A}}{k_A^2} + C_B \frac{\gamma_{2B} - \gamma_{1B}}{k_B^2} \right) \theta \right]$$

$$- \frac{3}{8} R\omega \left( \frac{\partial \eta^2}{\partial \theta} \right)_V = C^1_V + C^2_V$$

(12)

where

$$Y_\alpha = \frac{x_\alpha}{\text{sh} x_\alpha},$$

$$C^1_V = 3R \left[ C_A Y_A^2 + C_B Y_B^2 - 2 \left( C_A \frac{\gamma_{2A} - \gamma_{1A}}{k_A^2} + C_B \frac{\gamma_{2B} - \gamma_{1B}}{k_B^2} \right) \theta \right].$$

(13)

$$C^2_V = \frac{3}{8} R\omega \left( \frac{\partial \eta^2}{\partial \theta} \right)_V$$

(14)

From (8), we can calculate:

$$\left( \frac{\partial \eta^2}{\partial \theta} \right)_V = \frac{8\omega}{\theta^2} \eta^2 \left[ \frac{1}{\eta} \ln \left( \frac{C_A + \eta}{4} \right) \left( \frac{C_B + \frac{3\eta}{4}}{4} \right) - \frac{3C_A}{4} \frac{1}{C_A - \frac{1}{2} C_A \eta} \frac{3}{16} \eta^2 - \frac{3C_B}{4} \frac{1}{C_B + \frac{1}{2} C_B \eta} \frac{3}{16} \eta^2 \right]^{-1}$$

(15)
From (14) and (15), we obtain the expression for $C_V^2$:

$$C_V^2 = -3R \left( \frac{\omega}{k} \right)^2 \frac{\eta^2}{T^2} \left[ \frac{1}{\eta} \left( \frac{C_A + \frac{\eta}{4}}{C_A - \frac{3\eta}{4}} \right) \left( \frac{C_B + \frac{3\eta}{4}}{C_B - \frac{\eta}{4}} \right) - \frac{3C_A}{C^2_A - \frac{3}{16} C_A \eta - \frac{3}{16} \eta^2} - \frac{3C_B}{C^2_B + \frac{1}{2} C_B \eta - \frac{3}{16} \eta^2} \right]^{-1}$$

(16)

where $\omega$ calculated from the equilibrium condition of the phase transition in alloy.

Isobaric heat capacity of the alloys, has the following form:

$$C_P = C_V + \frac{9Rv\alpha^2_T}{k\beta_T}$$

(17)

where $\beta_T$ is the isothermal compression coefficient, having the following form:

$$\beta_T = -\frac{1}{V_0} \left( \frac{\partial V}{\partial P} \right)_T = \frac{3 \left( \frac{a}{a_0} \right)^3}{2P + \frac{a^2}{v} \Delta(P,T)}$$

(18)

with $\Delta(P,T) = \frac{1}{3N} \left( \frac{\partial^2 \varphi_{AB}}{\partial a^2} \right)_T$

Adiabatic compression coefficient, $\beta_S$, calculated from the formula:

$$\beta_S = \frac{C_V}{C_P} \beta_T$$

(19)

Isothermal and adiabatic bulk moduli:

$$K_T = \frac{1}{\beta_T} = \left( 2P + \frac{a^2}{v} \Delta(P,T) \right) \left[ 3 \left( \frac{a}{a_0} \right)^3 \right]^{-1}$$

(20)

$$K_S = \frac{1}{\beta_S} = \frac{C_P}{C_V} K_T$$

(21)

From (17), (18) and (20), we calculate the isobaric heat capacity:

$$C_P = C_V + \frac{4.5\sqrt{2} RT a^3}{k} K_T \alpha_T^2 = C_V + \frac{1.5\sqrt{2} RT a^3_0}{k_B} \left( 2P + \frac{a^2}{v} \Delta(P,T) \right) \alpha_T^2$$

(22)

3. Results and discussion

Using the general results obtained in section 2, we calculate lattice spacing, LRO-parameter and ODT-temperature for $Cu_3Au$ alloy. In discussing the thermodynamic properties of metals and alloys, the Lennard-Jones potential has been very successful. It has also been used to calculate mechanical properties of a wide variety of metals and alloys, including lattice defects [13,14,15] In view of this, we will use the Lennard-Jones potential $\varphi_{AB}$ for the $A - B$ atom pair in the alloys determined by pair of $A - A$ and $B - B$ atoms and order energy $\omega$ as:

$$\varphi_{AB}(r) = \frac{[\varphi_{AA}(r) + \varphi_{BB}(r)]}{2} - \omega.$$

Here, $A$ and $B$ represent $Cu$ and $Au$ atoms in the $Cu_3Au$ alloy. The Lennard-Jones potential $\varphi_{\alpha\alpha}$ for interaction between atoms $\alpha$ as:

$$\varphi(r) = \frac{D}{n-m} \left[ \frac{m}{r_0^n} - n \left( \frac{r}{r_0} \right)^m \right]$$

(23)

where $D, r_0, n$ and $m$ are the parameters of potential and have concrete values depending on each metal. For metals $Cu, Au$, values of potential parameters are given in Table 1.
Using the expressions of the parameters \( \gamma_{1a}, \gamma_{2a}, \gamma_\alpha \) calculated for the fcc lattice in [22,23] are based on the derivative formulas given by [17] and using the new results obtained in section 2 (expressions of (8) to (16)), in this section, we obtain new expressions of the isochoric and isobaric heat capacities, isothermal and adiabaric bulk modulus for \( Cu_3Au \) alloy (expressions of (24) to (29) and (32) to (37)).

Isochoric heat capacities, \( C_V \):

\[
C_V = C_V^1 + C_V^2
\]

(24)

\[
C_V^1 = 6.4 \left( 1 - 2.76.10^{-9} T a^9 \right) \left[ \frac{5.87}{(1 - 0.021a^{3.5})^2} \right] + 0.12 a^{1.5} \frac{1 - 0.001a^5}{(1 - 0.002a^3)^2}
\]

(25)

\[
C_V^2 = -3R \left( \frac{\omega}{k} \right)^2 \eta^2 \left[ \frac{1}{\eta} \frac{ln (1 + 3\eta)(3 + \eta)}{3(1 - \eta)^2} - \frac{3}{3 - 2\eta - \eta^2} - \frac{3}{1 + 2\eta - 3\eta^2} \right]^{-1}
\]

(26)

where \( \frac{\omega}{k} \) calculated from the equilibrium condition of the phase transition of the first type for ordered \( Cu_3Au \) alloy, satisfies the following two equation [20]:

\[
\frac{\omega}{k} = T_C \left[ \frac{1}{4\eta_0} ln \left( \frac{3 + \eta_0}{3(1 - \eta_0)^2} \right) + \left( 1.625.10^{-3} \frac{1 - 0.02a^{3.5}}{1 - 0.002a^3} + \frac{0.6}{a^{1.5}} \frac{1 - 0.002a^5}{1 - 0.02a^{3.5}} \right)_{T = T_0} - \frac{1}{4} \right]
\]

(27)

where \( T_C \) is the order-disorder transition temperature (ODT temperature) in the \( Cu_3Au \) alloy; \( \eta_0 \) is the LRO parameter at temperature of \( T_C \).

\[
3\frac{\eta_0}{8} ln \left( \frac{3 + \eta_0}{3(1 - \eta_0)^2} \right) - \frac{3}{4} \Delta (a, T_C) + 3ln3 - 4ln4 - \left( \frac{3}{4} - \frac{3\eta_0}{4} \right) ln \left( \frac{3}{4} - \frac{3\eta_0}{4} \right)
\]

\[
-3 \left( \frac{3}{4} + \frac{\eta_0}{4} \right) ln \left( \frac{3}{4} + \frac{\eta_0}{4} \right) - \left( \frac{1}{4} + \frac{3\eta_0}{4} \right) ln \left( \frac{1}{4} + \frac{3\eta_0}{4} \right) - 3 \left( \frac{1}{4} - \frac{\eta_0}{4} \right) ln \left( \frac{1}{4} - \frac{\eta_0}{4} \right) = 0
\]

(28)

where

\[
\Delta (a, T_C) = \left( \frac{2}{RT} \right) \left[ \psi_{Cu}(a) - \psi_{Cu}(a') \right] + \left( \frac{2}{3RT} \right) \left[ \psi_{Au}(a) - \psi_{Au}(a') \right]
\]

(29)

At pressure \( P = 0 \), we obtain the expressions \( a(0, T) \) and \( \alpha_T(0, T) \) takes the following form [12] (expressions of (30) to (31)):

\[
a(0, T) = 2.6358 \left( 1 + 1.474.10^{-5} T + 6.230.10^{-12} T^3 \right)
\]

(30)

\[
\alpha_T(0, T) = 1.474.10^{-5} \left( 1 + 12.68.10^{-7} T^2 \right)
\]

(31)

These expressions have been shown to match well with experimental results ranging from 300K to ODT- temperature, \( T_C \), and have also compared with the results calculated by other authors.
At pressure $P = 0$, the experimental of ODT-temperature, $T_C = 665K$, replacing this value to (30), (29), (28), (27), we calculated $\Delta(a, T_C) = 0.095\eta_0^2$, $\eta_0 = 0.69$, $\frac{\omega}{K} = 896K$. These results are consistent with the experimental data [19].

Substituting this value of $\frac{\omega}{K}$ into (26), we calculate:

$$C_V^2 = -5.99 \left(\frac{896}{T}\right)^2 \eta^2 \left[\frac{1}{\eta} \ln \left(\frac{1 + 3\eta}{3(1 - \eta)^2}\right) - 3 \left(\frac{1}{3 - 2\eta - \eta^2} + \frac{1}{1 + 2\eta - 3\eta^2}\right)\right]^{-1} \tag{32}$$

where LRO-parameter, $\eta$, calculated from (8), take the form:

$$\frac{1}{4\eta} \ln \left(\frac{3 + \eta}{3(1 - \eta)^2}\right) + 1.625.10^{-3} a^{1.5} \left(\frac{1}{1 - 0.02a^{3.5}} + \frac{0.6}{1 - 0.02a^{3.5}}\right) - \frac{1}{4} - \frac{896}{T} = 0 \tag{33}$$

Isobaric heat capacity of Cu$_3$Au alloy takes the following form

$$C_P = C_V + 30.56T\eta_0^3 \left(2P + \frac{141.4}{a}\Delta(P, T)\right) \alpha_T^2 \tag{34}$$

where

$$\Delta(P, T) = \frac{1}{3N} \left(\frac{\partial^2 \psi_{AB}}{\partial a^2}\right)_T = 10^6 a^{-11} \left[4.605(1 - 0.026a^{3.5}) + 28.5a^{-1.5}(1 - 0.003a^{5})\right] + 10P a^{-2}$$

$$\left[0.068 \frac{1}{1 - 0.02a^{3.5}} + 0.029 \frac{1}{1 - 0.002a^{5}} - 0.062 \left(\frac{1 - 0.015a^{3.5}}{1 - 0.02a^{3.5}}\right)^2 - 0.027 \left(\frac{1 - 0.001a^{5}}{1 - 0.0024a^{5}}\right)^2\right] \tag{35}$$

Isothermal and adiabatic bulk moduli, $K_T$ and $K_S$, of Cu$_3$Au alloy:

$$K_T = 0.25 \left(\frac{\eta_0}{a}\right)^3 \left(2P + \frac{141.4}{a}\Delta(P, T)\right) \tag{36}$$

$$K_S = \frac{1}{\beta_S} = \frac{C_P}{C_V} K_T \tag{37}$$

The numerical results of the lattice spacing, linear thermal expansion coefficient, LRO-parameter, isochoric and isobaric heat capacities, iso thermal and adiabatic bulk modulus of the Cu$_3$Au alloy at pressure $P = 0$ are include in Table 2, and shown in Figures 1 and 2. We also include in the Table and these figures experimental data for comparison. In numerical calculations, the lattice spacing, $a$, linear thermal expansion coefficient, $\alpha_T$, are calculated from the expressions (30) and (31), respectively, are results obtained in [12]; the LRO-parameter, $\eta$, is calculated from the equation (33); $C_V$ is calculated by the expression (24), (25) and (26); $C_P$ is calculated by the expressions (34); $K_T$ and $K_S$ are calculated from the expression (36) and (37), respectively.

The values of the thermodynamic quantities given in Table 2 are calculated directly from these expressions, very simple and do not need the assistance of any computational software.
Table 2. Values of thermodynamic quantities of the $Cu_3Au$ alloy at different temperature and pressure $P = 0$.

| $T(K)$  | 300  | 400  | 500  | 550  | 600  | 650  | 665-700 |
|---------|------|------|------|------|------|------|---------|
| $a(A_0)$ $[12]$ | 2.6479 | 2.6524 | 2.6573 | 2.6599 | 2.6627 | 2.6656 | 2.6665  |
| $\alpha T.10^5(K^{-1})[12]$ | 1.642 | 1.773 | 1.941 | 2.039 | 2.147 | 2.264 | 2.30    |
| $\eta$ | 0.9937 | 0.9695 | 0.9138 | 0.8690 | 0.8077 | 0.7215 | 0.6880  |
| $C_V(cal/molK)$ | 5.74 | 5.86 | 6.26 | 6.69 | 7.59 | 11.11 | 17.06   |
| $C_P(cal/molK)$ | 6.00 | 6.26 | 6.84 | 7.37 | 8.40 | 12.06 | 17.06   |
| Exp.$[18]$ | 6.0 | 6.1 | 6.2 | 6.8 | 8.4 | 11.8 | 7.6     |
| $K_T(kbar)$ | 1459 | 1400 | 1337 | 1303 | 1268 | 1232 | 1221    |
| $K_S(kbar)$ | 1527 | 1495 | 1460 | 1437 | 1404 | 1338 | 1297    |

Figure 1 is a curve depicting the dependence of the isobaric heat capacity $C_P$ on the temperature in the order domain of $Cu_3Au$ alloy. This curve spikes at temperatures very close to the transition temperature $T_C$. Table 1 also shows that at temperature very close to the transition temperature $T_C$, the LRO-parameter $\eta$ decreases rapidly with temperature. The cause of this phenomenon can be explained as follows: Due to the heat supplied to the alloy so that its temperature increased by 1K, partly to increase the temperature of the system, huge portions are used to bring the system to a much higher state of chaos (is a state with much higher energy). This part called the heat capacities of configuration. In the temperature range from $300K$ to transition temperature $T_C$, the isochoric heat capacities $C_V$, is increasing with temperature and high value is due to the heat capacity of configuration. The jump of heat capacity at the transition temperature is equivalent to the jump of the configuration heat capacity. In the temperature range from $300K$ to the transition temperature $T_C$, our theoretical curve fits well the experimental curve with smaller errors at 2%, except for the curve portion in the temperature range from $400K$ to $550K$ there are large differences, but the errors are less than 9%. The reason for the large differences in this temperature range ($400K$ to $550K$) is due to LRO-parameters calculated by theory is reduced more than the experimental data. In the temperature range from $650K$ to transition temperature $T_C$, curve sharply increase from 12.06 to 17.06 cal./molK, while the temperature only changed 15K, and reaches a maximum value of 17.06 cal./molK at the transition temperature $T_C = 665K$. In this temperature range, there is no experimental data, but the results are consistent with the extrapolated data of the experimental curve. We also calculate the jump in isochoric heat capacities at a transition temperature of $5R$, meanwhile some theoretical studies calculate the jump of the configuration heat capacity at the transition temperature of this alloy, giving a value of $2.5R$ [19], there is a big difference compared to the experiment. Figure 2 shows the dependence of the isothermal and adiabatic bulk modules, $K_T$ and $K_S$, on temperature of $Cu_3Au$ alloy. We found that the bulk modulus lines of the $Cu_3Au$ alloy alternated between the bulk modulus line for pure Au and Cu metal. All the upper bulk modulus lines are close to the straight line, except for the adiabatic modules curve $K_S$ of $Cu_3Au$ alloy, this line is only close to the straight line in the temperature of 300 to 550K. With temperatures from $550K$ to ODT-temperature, the adiabatic modules curve of $Cu_3Au$ alloy sharply decreased, this is due to a sharp increasen in the $C_V$ and $C_P$ capacities near the transition temperature.

Thus the results obtained in this paper on thermodynamic quantities of the $Cu_3Au$ alloy, at pressure $P = 0$, are simple functions of temperature and LRO-parameter. Numerical results of the linear thermal expansion coefficient, isochoric and isobaric heat capacities, isothermal and
4. Conclusion
By using SMM, we obtained thermodynamic quantities of Cu₃Au alloys as simple function of temperature and LRO-parameter, in the order domain of this alloy, from room temperature to transition temperature $T_C$, at pressure $P = 0$. Numerical results of the linear thermal expansion coefficient, isochoric and isobaric heat capacities, isothermal and adiabatic bulk modulus, are in good agreement with experiments. The results of calculating the isobaric heat capacities $C_P$, at temperature very close to the transition temperature $T_C$, great fit with experimental data.

The results obtained in this paper are new and has not been published, can be used in study of LRO-parameter and the thermodynamic properties of Cu₃Au alloy, and can be extended to other alloys with an $Ll_2$ structure.
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