

PAPER • OPEN ACCESS

Determination of Binding Energy For Cu and Cu₂O Based X-Ray Diffraction Spectrum

To cite this article: Heryanto *et al* 2018 *J. Phys.: Conf. Ser.* **979** 012055

View the [article online](#) for updates and enhancements.

You may also like

- [Experimental Determination of Depth Distribution Function of Carbon K-Rays](#)
Shigemi Furuno and Kazuhiko Izui
- [Repetitively pulsed X-ray laser operating on the 3p — 3s transition of the Ne-like argon in a capillary discharge](#)
Aleksandr V Vinogradov and J J Rocca
- [Multi-millijoule, deeply saturated x-ray laser at 21.2 nm for applications in plasma physics](#)
B Rus, T Mocek, A R Präg et al.



245th ECS Meeting • May 26-30, 2024 • San Francisco, CA

Don't miss your chance to present!

Connect with the leading electrochemical and solid-state science network!

Deadline Extended: December 15, 2023

Submit now!



Determination of Binding Energy For Cu and Cu₂O Based X-Ray Diffraction Spectrum

Heryanto, Bualkar Abdullah, Dahlang Tahir

Department of physics, Hasanuddin University, Makassar, 90245 Indonesia

E-mail: dtahir@fmipa.unhas.ac.id

Abstract. Binding Energy of Cu and Cu₂O was determined by using semi-empirical method based on X-ray diffraction (X-RD) spectra. Parameter Method 3 (PM3) single point method in hyperChem used to analysis Binding Energy of Cu and Cu₂O. Cu was annealing at temperature 600°C, 800°C for 30 minutes to get the oxide form. X-RD use to obtain lattice and distance between neighbor atoms formed in the samples as input parameter for empirical method by using Material Analysis Using Diffraction (MAUD). The Binding Energy for Cu is -87,69 kcal/mol at room temperature (RT). The binding energy for Cu₂O are -156.29 kcal/mol and -159.36 kcal/mol, at 600°C and 800°C respectively. The advantage of the method used in this study is not required the input parameter of ionic energy interaction, which is very difficult to determine based on X-RD data. This mean, the method in this study is effectively and efficiently for determining the binding energy of element metal and their oxides.

1. Introductions

Process of chemical bonds never break or form with spontaneously, but it require the role of energy. calculate the energy, it takes a study of the mechanical properties of the nanoscale system that now presents new theoretical and experimental challenges [1]. Relation of the crystal structure and the binding energy from the analyzed XRD data was reported by [2]. Processing computationally to define crystals that have lattice information and atomic spacing serve as one of the foundations in an attempt to estimate of binding energy a molecule. Negative value on the calculation of energy binding means the process of releasing energy, whereas if positive signifies the process experienced in the formation of molecules of the test material occurs the process of binding / receiving energy. The potential energy equations for molecules can be written [3].

$$Up = \left[\frac{Az^+z^-}{4\pi\epsilon_0 r} e^2 \right] + \left[\frac{B}{r^n} \right] \quad (1)$$

U_p is a potential energy (joule), A is constant's madelung, r distance between atoms (Å) and B is interaction of atomic repulsion as well as z^+ as cation and z^- as anion. The Coulomb (U_c) energy be obtained by the equation [4].

$$U_c = \frac{z^2 e^2}{4\pi\epsilon_0} \quad (2)$$



One of the factor determinants value of binding energy is influenced by distance between atoms in a molecule. The interaction between electrons determines the structure and properties of matter from molecules to solids [5]. Estimation of binding energy in this study does not require parameter input such as ionic interaction energy for simple models crystal. Calculation of binding energies metal with cubic structure using several mathematical approaches that facilitate [6]. Knowledge of binding energy of metal and their oxide is essential for search oxide material which suitable in the semiconductor and superconductor applications. In this work, we focus our attention for calculation of binding energy by using the size of lattice and the distance between atoms from the x-ray diffraction data. We used some applications free software MAUD, GaussView and HyperChem which facilitate the process of analysis and calculation in this study.

2. Material and Method

Copper CAT 2703 powder samples were given thermal treatment with variation of 30⁰C, 600⁰C and 800⁰C respectively in 30 minutes. the voltages input is 40kV and currents input is 30mA. Observation angle from are 20⁰ to 80⁰, appliance type of x-ray diffractions is Shimadzu X-RD 7000. MAUD applications are used to estimate lattice parameters in molecules. Estimation lattice parameters in MAUD applications using standards data [7, 8, 9, 10]. After adjustment of diffraction pattern with standard data has been completed in MAUD application, then determine distance between atoms using GaussView5.0 applications.

GaussView5.0 applications reads format CIF data. Determination distance between atoms based geometri and crystal system. After modeling is completed by using GaussView applications, the data is stored in protein data base (pdb) formats. HyperChem applications read and process pdb format. Semi-Empirical Method Parameter Method 3 (PM3) [11] use in this paper as a basic technique for optimizing element parameters by utilizing available data in HyperChem applications [12].

Single point calculations process the static properties of molecules that include potential energy, electrostatic potential, molecular orbital energy and orbital coefficients. Single point calculations are used to calculate the magnitude of the bonding energies based on the geometry of molecular structures that have been modeled based on X-RD data.

2.1 Result and Discussion

Data of diffraction shows the composition and lattice parameters, by thermal variations for Cu and Cu₂O.

Table 1. Lattice parameters and percentage of Cu and Cu₂O.

Compound	Lattice Parameter	Composition (%)
Cu (RT)	3,58	99
Cu_ref ^[7]	2,55	none
Cu_ref ^[16]	2,53	none
Cu ₂ O (600 ⁰ C)	4,24	46,5
Cu ₂ O_ref ^[13]	4,25	none
Cu ₂ O (800 ⁰ C)	4,25	22
Cu ₂ O_ref ^[14]	4,26	none

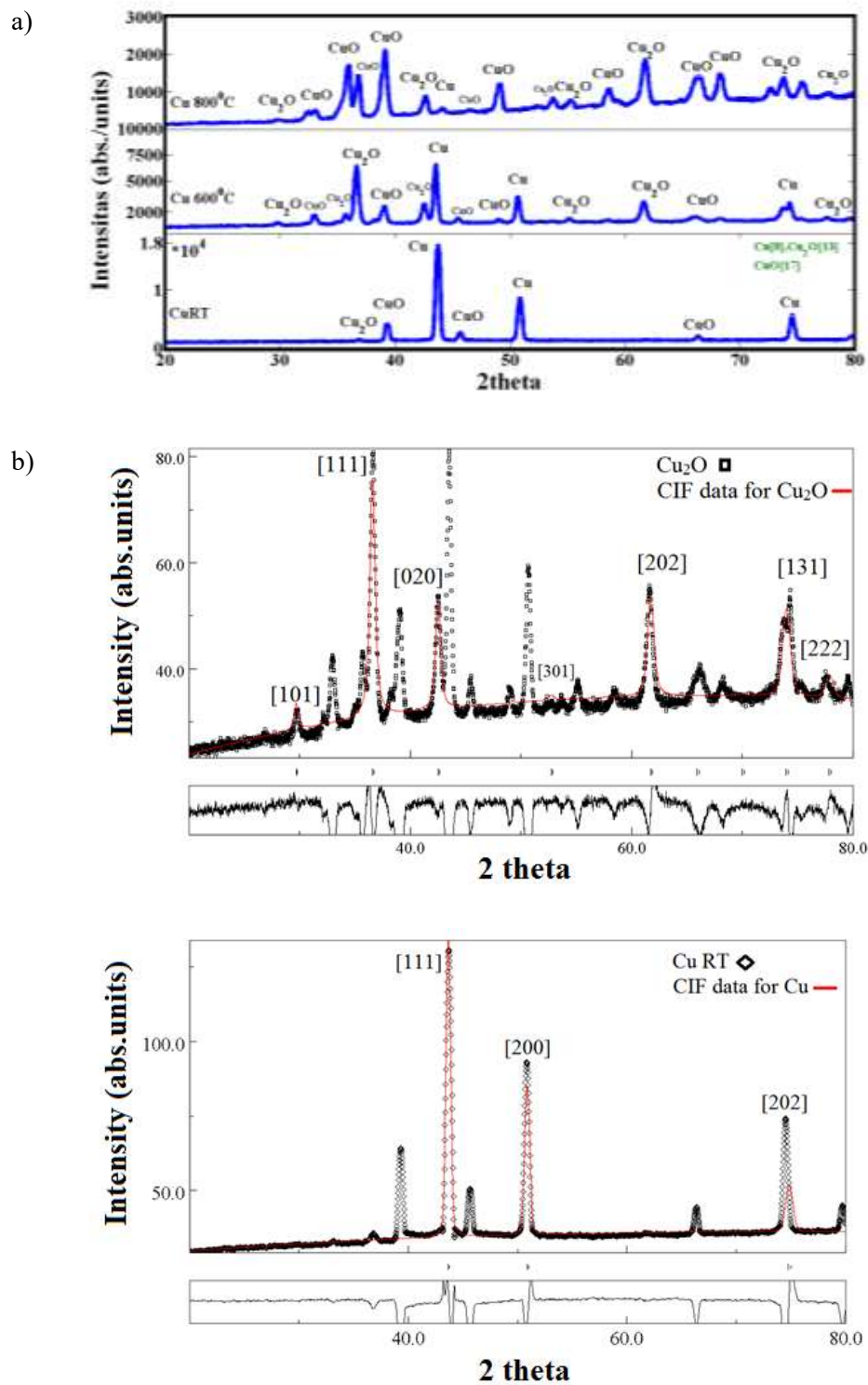


Figure 1. XRD data in this study (a) diffraction peak assignment as Cu [8] CuO [13] and Cu₂O [14] (b) compared with crystallography information file (CIF) data for Cu at RT [7] Cu₂O at 600⁰C and 800⁰C [9].

Table 1 shows the lattice parameter and composition of Cu as the effect of annealing Cu powder from (RT) to 800°C. We can see clearly from the table 1, Cu at room temperature is 99% and decrease to 46.5% and 22% for the temperature 600°C and 800°C, respectively. Lattice parameter shows slowly increase with increasing the annealing temperature. We applied MAUD for determining the lattice parameters by fitting the peak diffractions until good agreement. Figure 1 shows the composition amount of for Cu shows variations for different annealing temperature.

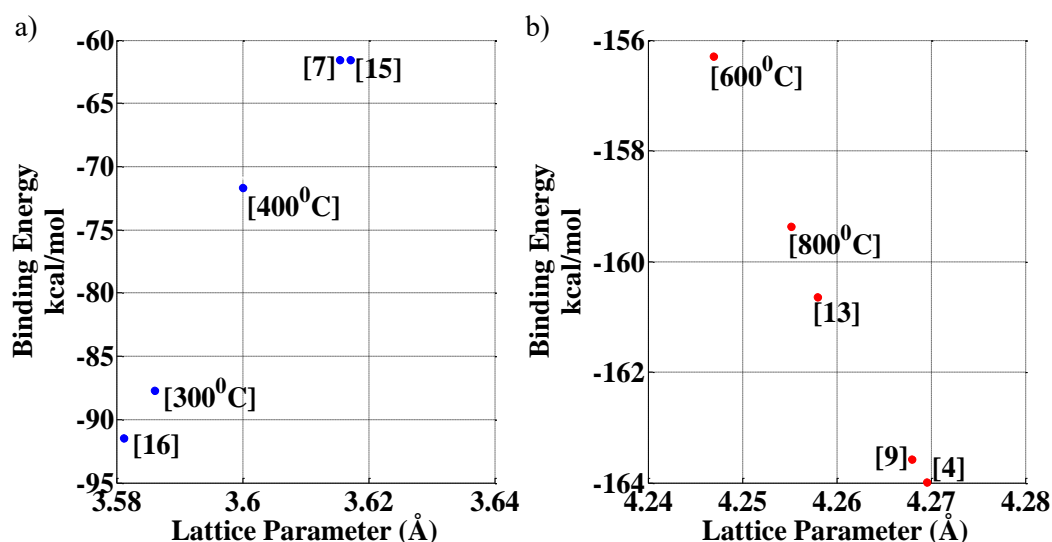


Figure 2. (a) The binding energy (kcal/mol) of Cu₂O variations in temperature with matching the database of [14], [15] dan [9]. (b) The binding energy (kcal/mol) of Cu variations in temperature with matching the database of [16], [17] dan [7].

Figure 2 Cu molecules gained energy (ΔE) from room temperature (RT) to 400°C during in the thermal treatment process is about 15,92 kcal / mol and thermal treatments on Cu₂O molecule releases energy about 3,07 kcal / mol. From this results, we obtained for the distance between atomic of Cu elements at RT is 2,536Å. Almost Similarly with the distance between atoms reported [7] is 2,55Å and [17] is 2,532Å. Binding energy of Cu molecules at RT is -87 kcal / mol and fairly agreement reported [7, [17]. The lattice parameter in this study for Cu₂O at 600°C and 800°C are 4,24 Å and 4,25 Å, respectively, and very good agreemnet with [14] about 4,25 Å and also reported [15, 17] about 4,26 Å. Binding energy of Cu₂O molecules at 600°C and 800°C are -156,2 kcal / mol and -159,3 kcal/mol, respectively and good agreement with binding energy reported [9, 15]. Analysis of binding energy for Cu and Cu₂O by using free software MAUD, GaussView and HyperChem in this study shows useful method for applications in determining the binding energy of metal and their oxide.

3. Conclusions

We annealing Cu at 600°C and 800°C to form Cu₂O and succesfull analysis the lattice parameter and the binding energy. The lattice parameter for Cu at room temperature is 3,58 Å increase about 4,24 Å at 600°C and 800°C. Cu composition at room RT is 99%, Cu₂O is 46,5% and 22% for 600°C and 800°C, respectively. Binding energy for Cu is -87,6 kcal/mol. The lattice parameter for Cu₂O at 600°C and 800°C are 4,24 Å and 4,25 Å, respectively. Binding energy for Cu₂O are -156,2 kcal/mol and -159,3 kcal/mol at 600°C and 800°C.

References

- [1] Autreto P A S, Legoas S B, Flores M Z S S, Galvao D S 2010 *America J. Chem. Phys.* **133** 124513
- [2] Lee H U, Lee S C, Won J, Byung-Chul S, Soehoe C, Kim Y, Park S Y, Hee-Sik K, Young-Chul L, Lee J 2015 *Scientific reports* **5** 8691
- [3] Johnson 2002 *Metals and chemical change* (Cambridge: Royal Society of Chemistry)
- [4] Ismunandar 1996 *Kimia anorganik* (Indonesia: Portal Pendidikan Gratis Indonesia) p 34
- [5] Aron J C, Mori-Sanchez P, Yang W 2008 *Sciencemag* **321**
- [6] Shimada K 1974 *J. Physics* **61** 325
- [7] Catherine F S, Dinah R P, Mohamed Z, Mark R J, Zoltán A G, Simon J C 2011 *J. American Chemical Society* **133** 2691-2705
- [8] Suh I K, Ohta H, Waseda Y 1988 *J. Materials Science* **23** 757-760
- [9] Kirfel A, Eichhorn K 1990 *Acta Crystallographica Section A* **46** 271-284
- [10] Volanti, Diogo P, Orlandi, Marcelo O, Andrés, Juan, Longo, Elson 2010 *CrystEngComm.* **12** 1696
- [11] James J P S 1988 Optimization of Parameters for Semiempirical Methods *J. Computational Chemistry* **10** 209-220
- [12] James J P S 1990 Optimization of Parameters for Semiempirical Methods. II
Extension of PM3 to Be, Mg, Zn, Ga, Ge, As, Se, Cd, In, Sn, Sb, Te, Hg, Tl, Pb, and Bi *J. Computational Chemistry* **12** 320-341
- [13] Niggli P 1922 *Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie* **57** 253-299
- [14] Yamaguti T 1938 *Proceedings of the Physico-Mathematical Society* **20** 230-241
- [15] Hafner S S, Nagel S 1983 *Physics and Chemistry of Minerals* **9** 19-22
- [16] Simon C, Oliver J R, Gareth R W 2006 *Chemical Communications*
- [17] Fortes A D, Emmanuelle S, Lemée-Cailleau, Marie-Hélène, Pickard, Christopher J, Needs R J 2009 *J. of the American Chemical Society* **131** 13508-13515