CALCULATION OF TOTAL ENERGY USING THE EMBEDDED ATOM METHOD (EAM) / TIGHT BINDING SECOND MOMENT APPROXIMATION (TB-SMA)

(IMPLEMENTED USING MICROSOFT EXCEL PROGRAMMING)

BY

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BENIN CITY.

JANUARY, 2023

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A PROJECT SUBMITTED TO THE DEPARTMENT OF PHYSICS, FACULTY OF PHYSICAL SCIENCES, UNIVERSITY OF BENIN, BENIN CITY. IN PARTIAL FULFILMENT OF THE REQUIREMENT FOR THE AWARD OF BACHELOR OF SCIENCE (B.Sc.) DEGREE IN INDUSTRIAL PHYSICS

JANUARY, 2023

CERTIFICATION

This is to certify that this research was carried out by **Odia Osemwengie David**, in the Department of Physics, Faculty of Physical Sciences in the University of Benin.

_____ _____

PROF. E. AGHEMENLOH Date
(Project Supervisor)

_____ _____

PROF. OSAHON O. D. Date
(Head of Department)

_____ _____

External Examiner Date

DEDICATION

This project is dedicated to God Almighty for His ever-fulfilling protection, provision, strength and grace and to my family for their unmatching love, support and encouragement.

CERTIFICATION OF DISSERTATION ON PLAGIARISM

We the undersigned attest and declare that the dissertation of **Odia Osemwengie David** titled "Calculation of Total Energy Using the Embedded Atom Method (EAM) / Tight Binding Second Moment Approximation (TB-SMA) (Implemented Using Microsoft Excel Programming)" has successfully passed the anti-plagiarism test and doesn't violate any copyright regulations

ACKNOWLEDGEMENT

The completion of this work would not be possible if not for the kindness and mercy of God Almighty who gave me the strength and grace to complete this project work.

I greatly appreciate my project supervisor, Prof. E. Aghemenloh for his immense contribution, constructive corrections, suggestions and recommendations and also assistance with providing me with materials needed for the completion of my project work.

My greatest gratitude goes to my family, my mum, Mrs. Roseline Odia for her unwavering support, to my brother Joshua Odia for his encouragement and constant reminder that I can be street smart and still own a degree. I would also like to express my gratitude to my friends and course mate from the University of Benin., I love you all.

ABSTRACT

This study has used the recently established combination between EAM and the TB-SMA scheme to determine the n, p, q parameters values needed for the calculation of total energy of the three FCC metals which include Ag, Pd and Pt.

The EAM and TB-SMA was established to replace the old approach of determining parameters for calculating total energy because of its improved computational efficiency and accurate results.

The Microsoft excel programming language has been employed in this study to reproduce results with good accuracy as compared with previous studies using other programming software.

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CHAPTER ONE

INTRODUCTION

1.1 TOTAL ENERGY

The Total Energy of a material is the sum of its Kinetic Energy and Potential Energy. The total energy is used in solving the many body problems associated with the study of interest of interest to the material scientist, these are large or small systems including extended defects, surfaces, complex allows involving total or partial loss of periodicity.

1.2 BACKGROUND OF THE STUDY

There are various approaches to calculating the total energy of a system, due to the difficulty in calculation posed by these approaches, (2-3) Ab Initio method (1) and fast self-consistent calculational techniques may not be convenient due to the burden and time-consuming problems it possesses hence **the Semi Empirical Approach**, which have been found to provide fairly accurate results with considerably improved computational efficiency compared to other approaches. For instance, it is now widely recognized that semiempirical many-body potentials can reproduce with good accuracy the thermodynamic and structural properties of several metals, In the past few decades, these many-body potentials have been extensively used to solve various problems in material science, sometimes with the

help of molecular-dynamic computer simulation techniques by iterating multiple times.

The Semi Empirical Approach solves a problem determining a functional form for the cohesive force properties, based on some physical models and parameters. This functional form includes the TB parameters which are to be determined by fitting to experimental properties, once these properties have been determined, it is then applied in the functional form to calculate various other total energy properties such as defect energies etc.

A relatively simple scheme for relating the atomic and electronic structure of metals, without resorting to the complex treatment of first principles calculations, is the tight-binding (TB) theory of cohesion. The second moment approximation (SMA) of the TB theory expresses the cohesive energy of a metallic solid as a sum of two terms, hence the reason it's referred to as "Second Moment". For both energies, one coming from the band energy E_B (The attractive term) and the other term, energy E_R, being a repulsive contribution. In this TB-SMA scheme the interaction between two atoms depends on the interatomic distance and also on the local environment around each atom.

The entire TB-SMA scheme contains five model parameters, usually denoted as A, ε, p, q, and n. These parameters can be calculated by fitting them

into the experimental values/properties of the cohesive energy, the mono vacancy formation energy, and the independent elastic constants, and also by taking the equilibrium conditions into account. In several applications of the TB-SMA scheme, the model parameter **n** is often taken as $\frac{1}{2}$. With such a choice, Rodriguez et al. (1993) determined the values of the other four parameters for several metals, by fitting to the experimental cohesive energy E_C, the bulk modulus B_0, the elastic constant C_{44}, and also by taking the equilibrium condition into account. For several metals, the predicted values of the monovancy formation energy E_{1v}^F, as well as the other elastic constants (C_{11} and C_{12})disagreed with these experimental values.

In this project, we set out to assume the parameter n on an equal footing with the other four parameters, disregarding the theoretical justifications behind the choice of $n = \frac{1}{2}\ or\ n = \frac{2}{3}$. That is, the five parameters in the TB-SMA scheme have been determined by fitting to the experimental value of E_C, E_{1v}^F, B_0, C_{11} and C_{12}, and also taking the equilibrium conditions into account. Results shown in this research project that the value of the parameter n does not come out to be a constant for the three typical FCC metals (Ag, Pd and Pt), whose calculated parameters are explicitly represented. At the same time the new results lead to good agreement with experiment in the physical quantities whose values are predicted. This work

therefore provides an easy alternative approach for determining tight-binding potentials

1.3 AIM AND OBJECTIVES

The aim of this study is to determine the n, p, q parameters needed in calculation of the total energies of the three FCC metals (Ag, Pd and Pt).

The objectives of this work are to;

1. employ the EMA/TB-SMA Semi-empirical approach.
2. employ Microsoft excel programme in calculating the three basic equations gotten from the application of EAM and TB-SMA equations to determine the parameters n, p and q for the three FCC metals.
3. compare results of the experiment to the results gotten from previous experiment that were carried out by Cleri *et* al., to further confirm that in calculation for the total energy, the value of the parameter **n** isn't constant for all metals.

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CHAPTER TWO

LITERATURE REVIEW

The TB-SMA scheme is formally analogous to the embedded-atom method (EAM) scheme as pointed out by Cleri and Rosato [2]. 7 major equations are frequently used in EAM calculations and we will apply them to our TB-SMA scheme, which will be mainly solved over several iterations using the Microsoft excel programming. Below are the 7 major equations most applicable in the EAM.

$$U_0 = 6\Phi_1''(r_o) + F(\rho_e) \qquad (2.10)$$

Where U_o is the equilibrium energy per atom, Φ_1 is a repulsive pair potential, r_o is the equilibrium nearest neighbour distance, ρ_e is the equilibrium density and F is an embedding function with respect to the density.

$$0 = 6\Phi_1'(r_o) + F'(\rho_e)[\rho'(r_o)] \qquad (2.20)$$

where Φ_1' is the first derivative of Φ_1 with respect to radial distance r ($r = r_o$)

$$\frac{a}{2} aB_o = 6\Phi_1''(r_o) + F''(\rho_e)[\rho'(r_o)]^2 + F'(\rho_e)[\rho''(r_o)] \qquad (2.30)$$

where Φ_1'' is the second derivative of Φ_1 with respect to r ($r=r_o$), a is the equilibrium lattice constant, B_o is the bulk modulus, F' and F'' are

respectively the first and second derivatives of F with respect to the density, ρ′ and ρ′ ′ are the first two derivatives of ρ with respect to r_o

(All quantities are evaluated at $r = r_o$)

$$\frac{a}{4}C_{11} = \{\frac{\Phi_1^{'}(\mathrm{ro})}{2ro} + \frac{\Phi_1^{''}(\mathrm{ro})}{2}\} + \frac{aF'(\rho e)}{4\Omega o} W_{11} + \frac{aF''(\rho e)}{4\Omega o} V_{11}^2 \quad (2.40)$$

$$\frac{a}{4}C_{12} = \{-\frac{-5\Phi_1^{'}(\mathrm{ro})}{2ro} + \frac{\Phi_1^{''}(\mathrm{ro})}{4}\} + \frac{aF'(\rho e)}{4\Omega o} W_{12} + \frac{aF''(\rho e)}{4\Omega o} V_{11}^2 \quad (2.50)$$

where C_{11} and C_{12} are elastic constants, Ω_o is the volume per atom in the solid, V_{11}, W_{11} and W_{12} are EAM parameters

$$\frac{a}{4}C_{44} = \{\frac{-5\Phi_1^{'}(\mathrm{ro})}{2ro} + \frac{\Phi_1^{''}(\mathrm{ro})}{4}\} + \frac{aF'}{4\Omega o} W_{12} \quad (2.60)$$

$$E_{1v}^F = 12F\{\frac{11\rho e}{12}\} - 11F\{\rho_e\} - U_O \quad (2.70)$$

For FCC lattice, $r_0 = a/\sqrt{2}$ and $\Omega_o = a3/4$, and expression for V_{11}, W_{11} and W_{12} in terms of the derivatives of the density (Daw and Baskes, 1984) which can be written in the algebraic form:

$$V_{11} = r_o\rho'(r_o)/3 \quad (2.80)$$

$$W_{11} = \frac{a^2}{12}\{\rho''(r_o) + \frac{\rho'(r_o)}{r_o}\} \quad (2.90)$$

$$W_{24} = \frac{a^2}{24}\{\rho''(r_o) - \frac{5\rho'(r_o)}{r_o}\} \quad (2.10)$$

From the above equations, it's noticed that the Embedded Atom Method EAM has three basic functions, i.e., $\Phi_1(r)$, $F(\rho)$, and $\rho(r)$ which in turn produces the 8 EAM parameters; $\Phi_1(r_o)$, $\Phi_1'(r_o)$, $\Phi_1''(r_o)$, $F(\rho_e)$, $F'(\rho_e)$, $F''(\rho_e)$, $\rho'(r_o)$, and $\rho''(r_o)$. All other EAM parameters like V_{11}, W_{11} and W_{12} are all generated from these eight major parameters.

From the EAM functions it is obvious that the experimental input data required for the solution of the 7 EAM equations are the cohesive energy $E_c(= -U_o)$, the lattice constant a, the bulk modulus B_o, the three independent elastic constants (C_{11}, C_{12}, and C_{44}), and the monovacancy formation energy E_{1v}^F, once the 8 EAM parameters have been determined, then various other physical quantities of interest can be determined from our knowledge of the functions $\Phi_1(r)$, $F(\rho)$, and $\rho(r)$.

In correspondence with the Embedded Atom Method EAM scheme, the expression for cohesive energy U_o which is described in chapter 1 as the "sum of two terms" in the TB-SMA scheme is given as;

$$U_o = E_R + E_B \tag{2.11}$$

The functions E_R and E_B above are usually rewritten below as 2.12 and 2.13 respectively.

$$E_R = 6\Phi_1(r_{11}) = A\sum_j exp\,[-\rho(r_{ij}/r_o)-1]'' \tag{2.12}$$

$$E_B = F(\rho) = \zeta \sum_j exp\ [-2q(r_{ij}/r_o)-1]' \quad ' \qquad (2.13)$$

It is clearly shown that the density function $\rho(r)$ is;

$$\rho(r) = \sum exp[-2q(r_{ij}/r_o-1)] \qquad (2.14)$$

Equation 2.12 to 2.14 are the three basic functions for TB-SMA scheme.

The sum over j in Eqns. (2.12) to (2.14) is actually a sum over neighbours, r_{ij} being the distance between atom j and atom i (the reference atom). The TB-SMA expressions for the functions $\Phi_1(r)$, $F(\rho)$ and $\rho(r)$ as seen in the Eqns. (2.12) to (2.14) are governed by only 5 parameters [A, ρ, ε, q and n], instead of the 8 parameters

[Φ_1 (r_o), Φ_1' (r_o), $\Phi_1''(r_o)$, $F(\rho_e)$, $F'(\rho_e)$, $F''(\rho_e)$, $\rho'(r_o)$, and $\rho''(r_o)$] which are encountered in the EAM scheme. Hence, the 7 EAM equations can be immediately solved if we substitute the expression (2.12) to (2.14) and their derivatives for the functions $\Phi_1(r)$, $F(\rho)$, $\rho(r)$ and their derivatives, encountered there (Mehel et al., 1996). That is, the TB-SMA scheme developed here has a total of 5 parameters that must be determined from the 7 equations (2.1) to (2.7).

In several applications of the TB-SMA scheme the parameter n is specified a priori to be $\frac{1}{2}$ or $\frac{2}{3}$. In this case the four remaining free parameters of the TB-SMA scheme can be determined from the EAM equations either using Eqns. (2.1), (2.2),

(2.3) and (2.7) or Eqns. (2.1), (2.2), (2.3) and any one of (2.4) to (2.6). We pursue a different approach in this study. The parameter n and the four others are determined on an equal footing from Eqs. (2.1), (2.2), (2.3), (2.7) and the equation

CHAPTER THREE

METHODOLOGY.

The TB-SMA equation and EAM equations have been converted into a computer programming language. They have been made to be iterated over and over again until the system gives the accurate results for the parameters n, p and q values of any FCC metals. The Microsoft Excel programming language has been developed to make the calculations less difficult and faster as it uses less time to compute many values which cannot be done easily while solving manually, with the help of Microsoft Excel, the value for n, p and q parameters can easily be calculated in few minutes as the programming can be made to run thousands of iterations in matter of minutes which is highly impossible for anyone solving manually.

The finding of the n, p and q parameters are aided by three equations, and they are written below;

$$9\Omega_{0(}C_{12}\text{-}C_{44}) = \frac{n(n-1)\left(E_{1v}^{F}+Uo\right)}{[12[{}^{11}/_{12}]^{n}-11]} \text{ x}$$

$$r_o^2(\frac{-2q}{r_0})^2 \ [\frac{12+6\sqrt{2}\ e^{-2q(\sqrt{2}-1)}+24\sqrt{3}e^{-2q(\sqrt{3}-1)}+24e^{-2q}+24\sqrt{5}\ e^{-2q(\sqrt{5}-1)}}{12+6e^{-2q(\sqrt{2}-1)}+24e^{-2q(\sqrt{3}-1)}+12e^{-2q}+24e^{-2q(\sqrt{5}-1)}}] \quad (3.1)$$

$$(p)^2 \quad [\ \frac{12+6\sqrt{2}e^{-p(\sqrt{2}-1)}+24\sqrt{3}e^{-p(\sqrt{3}-1)}+24e^{-p}+24\sqrt{5}e^{-p(\sqrt{5}-1)}}{12+6e^{-p(\sqrt{2}-1)}+24e^{-p(\sqrt{3}-1)}+12e^{-p}+24e^{-p(\sqrt{5}-1)}}\ ] \ = \ \frac{n[12[{}^{11}/_{12}]^{n}-11]}{(n-1)} \ .$$

$$\frac{\left(E_{1v}^{F}+U_0\right)\{9\Omega o(C12-C44)\}}{\left[U_0\ \left\{12({}^{11}/_{12})^{n}-11\right\}-\left(E_{1v}^{F}+U_0\right)\right]^2} \quad (3.2)$$

The above equation was used to find the pairs n and p which satisfy the equation. The third equation is;

$$[\ \frac{9}{2}aB_0-\frac{9\Omega_0}{r_0^2}(C_{12}-C_{44})]r_0^2 = \ (p)^2\ [U_0 -$$

$$\frac{\left(E_{1v}^{F}+U_0\right)}{\left\{12({}^{11}/_{12})^{n}-11\right\}}][\frac{12+12e^{-p(\sqrt{2}-1)}+72e^{-p(\sqrt{3}-1)}+48e^{-p}+120e^{-2p(\sqrt{5}-1)}}{12+6e^{-p(\sqrt{2}-1)}+24e^{-p(\sqrt{3}-1)}+12e^{-p}+24e^{-p(\sqrt{5}-1)}}] +$$

$$\frac{n\left(E_{1v}^{F}+U_0\right)}{\left\{12({}^{11}/_{12})^{n}-11\right\}}\cdot\frac{(2q)^2}{1}[\frac{12+12e^{-2q(\sqrt{2}-1)}+72e^{-q(\sqrt{3}-1)}+48e^{-2q}+120e^{-2q(\sqrt{5}-1)}}{12+6e^{-2q(\sqrt{2}-1)}+24e^{-2q(\sqrt{3}-1)}+12e^{-2q}+24e^{-2q(\sqrt{5}-1)}}]$$

(3.3)

The above equation 3.1 was used to find the trio n, p and q that satisfy the equation.

The values of n and q must satisfy the whole of the first equation and n must also agree with second equation and n, p and q must converge to satisfy the third equation while other parameters are fitted into experimental data. The Tight Binding equations written above are computed into the Microsoft excel sheet, it is written in such a way that n and p will be found, then n and q is also found before we finally converge the n, p and q results to finally find the n that satisfies the FCC Metal of choice.

Now, in order to calculate using the excel sheet, all the equations were converted in excel format and inputted into the system and each of the n, p and q parameters have their programmed formulas. First for the p programme, we assumed a value for n, say 0.61265 for platinum (Pt) and the p value becomes 9.13E+00, the same procedure is repeated for q taking n to be 0.61265 and it converges to 3.37. The third programme is the n, p, q trio and when the values that converged for n and q are inputted into the triod programme with the same n value of 0.61265 the value for the trio becomes T_1=12.13324644., T_4=12.1324467 and T=7.9974E-04

Where T_1 is the constant of the FCC metal, T_4 is the value gotten with respect to n and T is the difference between T_1 and T_4, after trying for the initial assumption n = 0.61265, it's clear that it has not converged (when at least the first two digits after the decimal point in T tallies with that of T_1 which is the constant). This process is

continuously repeated until a value of n that will converge to give the right figure for the FCC metal in consideration is attained. The same process is repeated by trying different values of n until we get the same digits that confirms the convergence. The next stop is to start fine turning the n value as it also affects both the p and q values which are finally merged to give us the final result similar to say T_1=12.13324644., T_4=12.1324467 and T=7.9974E-04. In this project work, we solved to compute the n, p and q value of FCC metals Pt, Pd and Ag and we compute their parameters from their first to their fifth nearest neighbour. So, after computing to solve the first nearest neighbour of each FCC metal we did the same for others until every metal converges from the first to the fifth nearest neighbours of Pt, Pd and Ag respectively.

3.1 ALGORITHM FOR CALCULATIONS

Step 1: Find (n, p) pair which satisfies EQ 3.2

Step 2: Use the assumed n from step 1 to find the (n,q) pair which satisfy EQ 3.1

Step 3: Use the accepted (n,p) pair from step 1 in EQ 3.2 to find the (n, p, q) trio that satisfy EQ 3.3. If the q found here is equal to the q in step 2

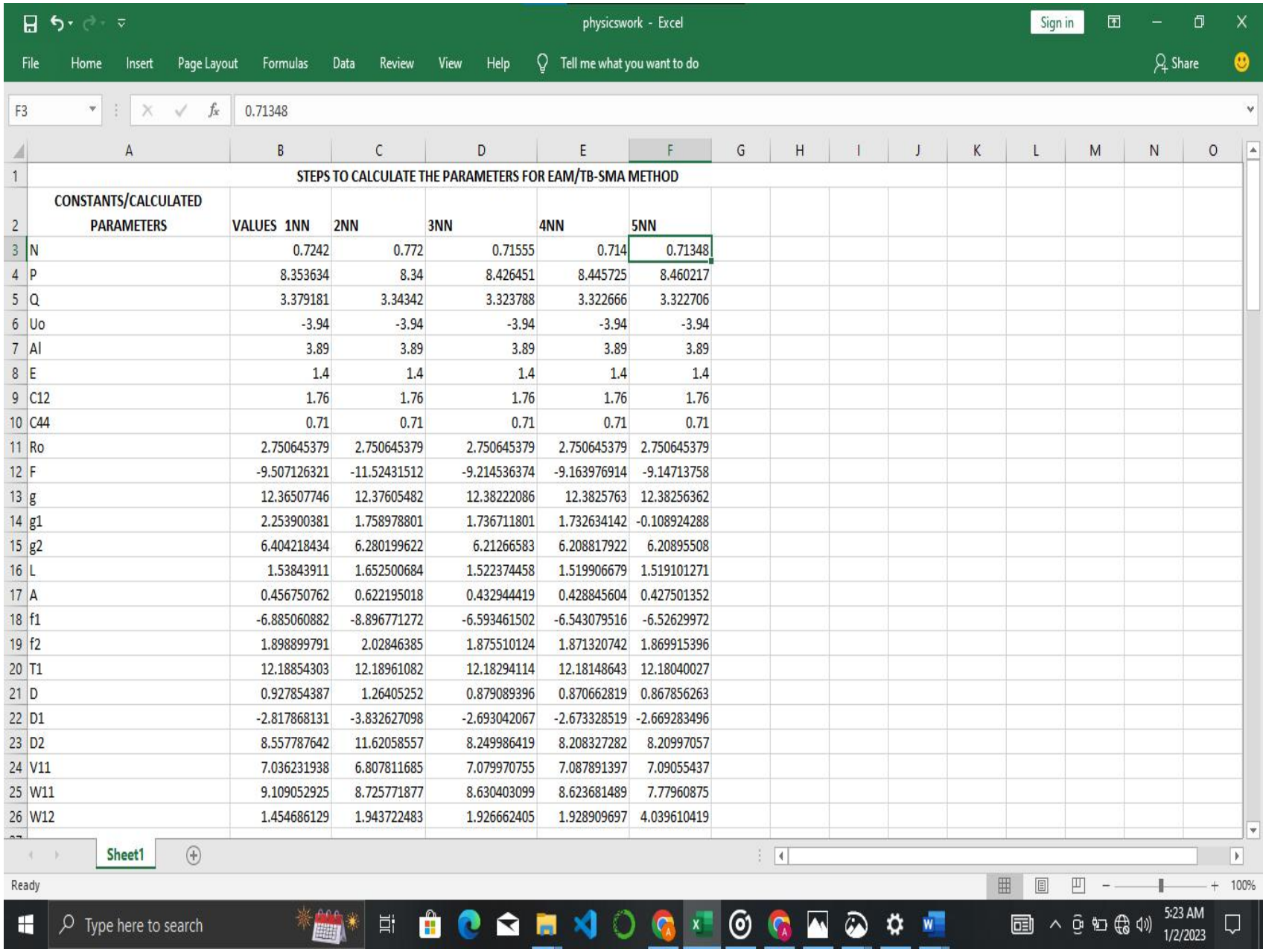
then we are okay, otherwise we go back to step 1 and take another (n, p) pair.

It should be noted that every entry made into the system to be calculated could still be subject to correction because sometimes when results are printed, such results may need verification. It is also important to make sure all parameters are stated correctly because if there is one mistake the whole work will give wrong results. A little shift in the value of n, p or q could affect the overall output.

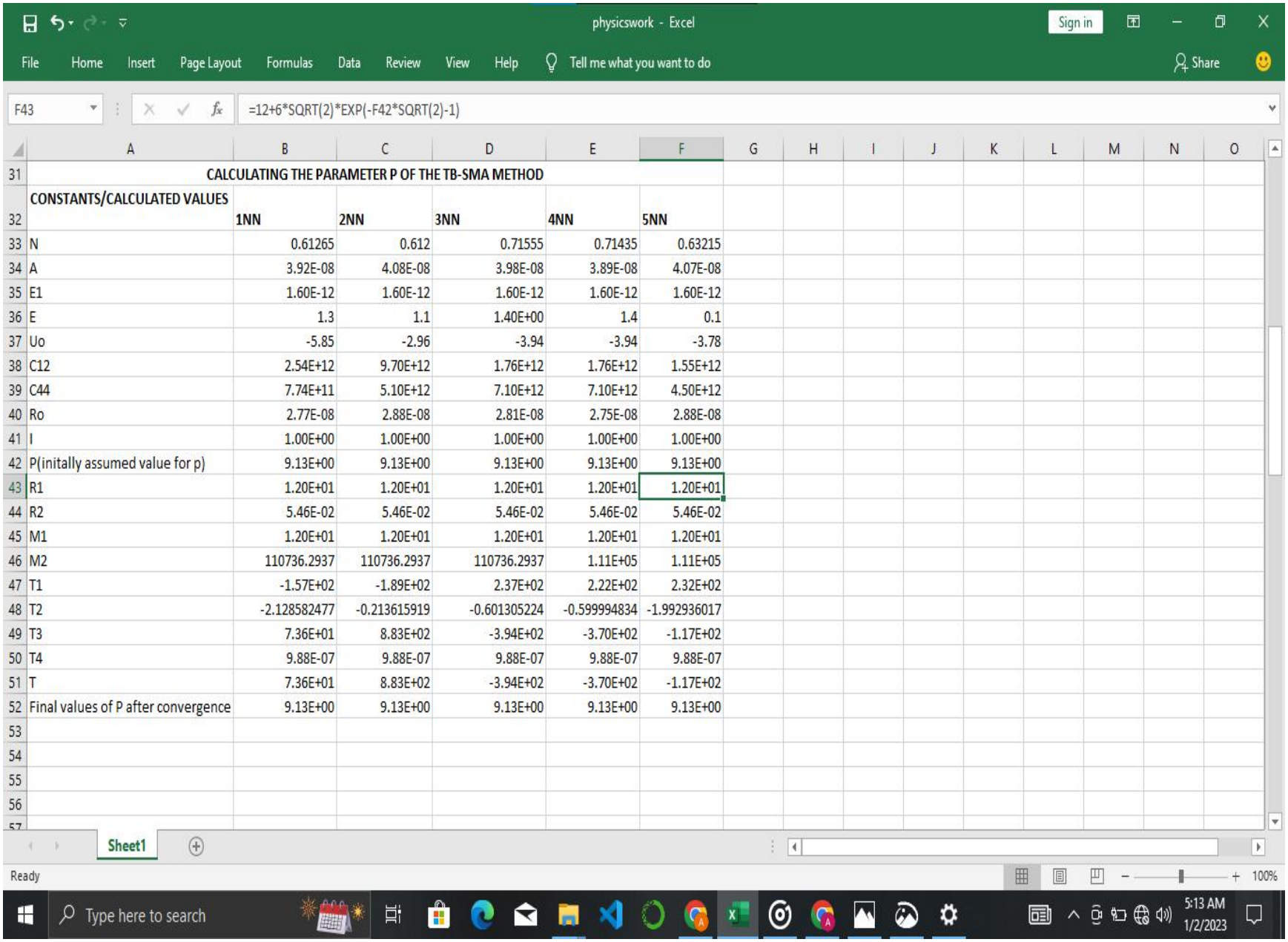
3.2 METHOD OF CALCULATIONS

Four tables were created in excel namely to show how the parameters were generated, how p was calculated for, how q was calculated for and lastly whether p and q are consistent with n of the TB-SMA method. Each parameter used can be obtained from [4] The others were calculated for. N in this instance was obtained.

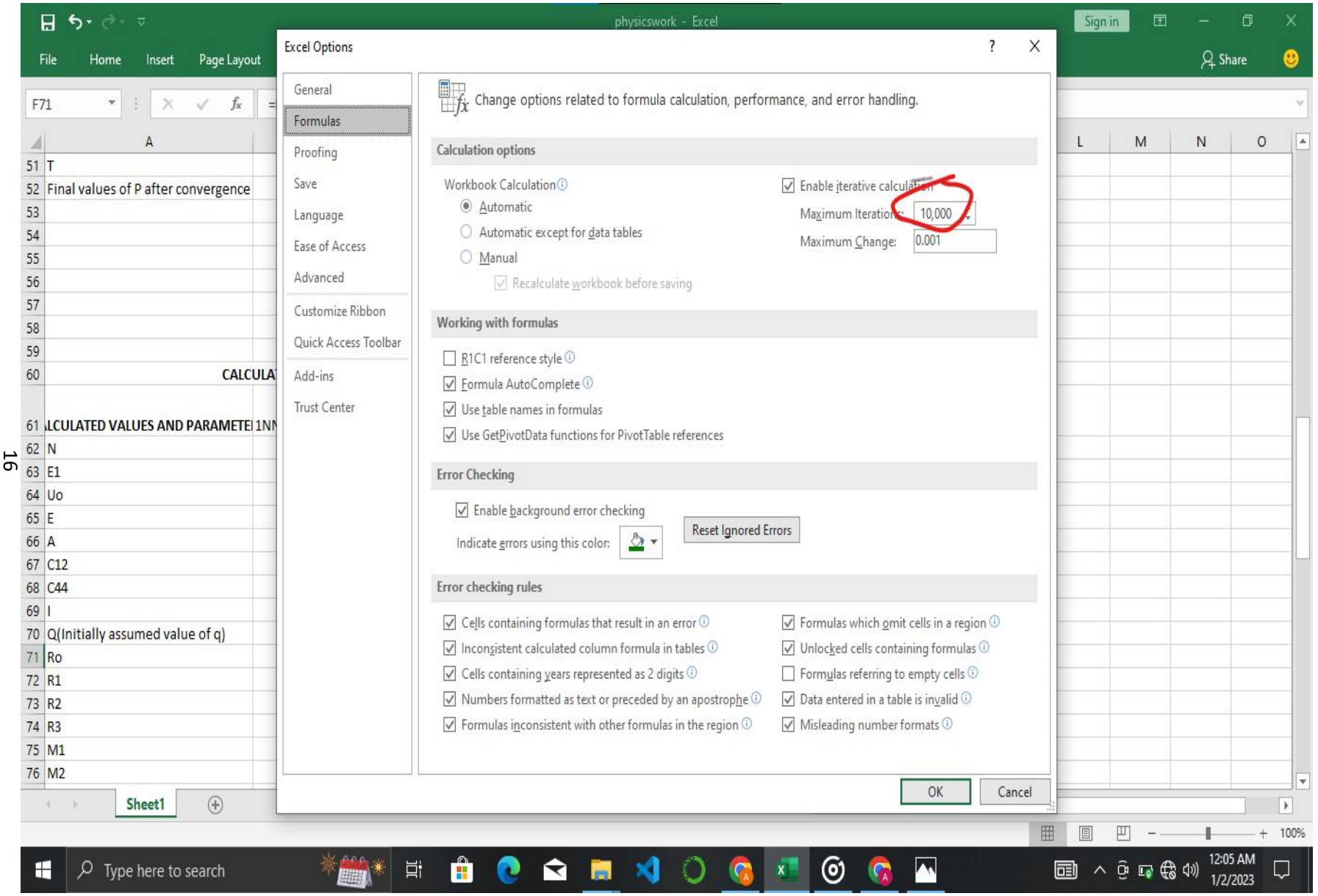
R1 on the other hand was calculated for as the formula can be seen in the formula bar. In the calculations of p and q parameter an assumed initial value of 0.6 was assumed and then iterated over each five instances until final average values of 9.13 and 3.78 were obtained respectively. the max iteration was set as 10,000 in excel.



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O
1	STEPS TO CALCULATE THE PARAMETERS FOR EAM/TB-SMA METHOD														
2	CONSTANTS/CALCULATED PARAMETERS	VALUES 1NN	2NN	3NN	4NN	5NN									
3	N	0.7242	0.772	0.71555	0.714	0.71348									
4	P	8.353634	8.34	8.426451	8.445725	8.460217									
5	Q	3.379181	3.34342	3.323788	3.322666	3.322706									
6	Uo	-3.94	-3.94	-3.94	-3.94	-3.94									
7	Al	3.89	3.89	3.89	3.89	3.89									
8	E	1.4	1.4	1.4	1.4	1.4									
9	C12	1.76	1.76	1.76	1.76	1.76									
10	C44	0.71	0.71	0.71	0.71	0.71									
11	Ro	2.750645379	2.750645379	2.750645379	2.750645379	2.750645379									
12	F	-9.507126321	-11.52431512	-9.214536374	-9.163976914	-9.14713758									
13	g	12.36507746	12.37605482	12.38222086	12.3825763	12.38256362									
14	g1	2.253900381	1.758978801	1.736711801	1.732634142	-0.108924288									
15	g2	6.404218434	6.280199622	6.21266583	6.208817922	6.20895508									
16	L	1.53843911	1.652500684	1.522374458	1.519906679	1.519101271									
17	A	0.456750762	0.622195018	0.432944419	0.428845604	0.427501352									
18	f1	-6.885060882	-8.896771272	-6.593461502	-6.543079516	-6.52629972									
19	f2	1.898899791	2.02846385	1.875510124	1.871320742	1.869915396									
20	T1	12.18854303	12.18961082	12.18294114	12.18148643	12.18040027									
21	D	0.927854387	1.26405252	0.879089396	0.870662819	0.867856263									
22	D1	-2.817868131	-3.832627098	-2.693042067	-2.673328519	-2.669283496									
23	D2	8.557787642	11.62058557	8.249986419	8.208327282	8.20997057									
24	V11	7.036231938	6.807811685	7.079970755	7.087891397	7.09055437									
25	W11	9.109052925	8.725771877	8.630403099	8.623681489	7.77960875									
26	W12	1.454686129	1.943722483	1.926662405	1.928909697	4.039610419									



	A	B	C	D	E	F
31	CALCULATING THE PARAMETER P OF THE TB-SMA METHOD					
32	CONSTANTS/CALCULATED VALUES	1NN	2NN	3NN	4NN	5NN
33	N	0.61265	0.612	0.71555	0.71435	0.63215
34	A	3.92E-08	4.08E-08	3.98E-08	3.89E-08	4.07E-08
35	E1	1.60E-12	1.60E-12	1.60E-12	1.60E-12	1.60E-12
36	E	1.3	1.1	1.40E+00	1.4	0.1
37	Uo	-5.85	-2.96	-3.94	-3.94	-3.78
38	C12	2.54E+12	9.70E+12	1.76E+12	1.76E+12	1.55E+12
39	C44	7.74E+11	5.10E+12	7.10E+12	7.10E+12	4.50E+12
40	Ro	2.77E-08	2.88E-08	2.81E-08	2.75E-08	2.88E-08
41	I	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
42	P(initally assumed value for p)	9.13E+00	9.13E+00	9.13E+00	9.13E+00	9.13E+00
43	R1	1.20E+01	1.20E+01	1.20E+01	1.20E+01	1.20E+01
44	R2	5.46E-02	5.46E-02	5.46E-02	5.46E-02	5.46E-02
45	M1	1.20E+01	1.20E+01	1.20E+01	1.20E+01	1.20E+01
46	M2	110736.2937	110736.2937	110736.2937	1.11E+05	1.11E+05
47	T1	-1.57E+02	-1.89E+02	2.37E+02	2.22E+02	2.32E+02
48	T2	-2.128582477	-0.213615919	-0.601305224	-0.599994834	-1.992936017
49	T3	7.36E+01	8.83E+02	-3.94E+02	-3.70E+02	-1.17E+02
50	T4	9.88E-07	9.88E-07	9.88E-07	9.88E-07	9.88E-07
51	T	7.36E+01	8.83E+02	-3.94E+02	-3.70E+02	-1.17E+02
52	Final values of P after convergence	9.13E+00	9.13E+00	9.13E+00	9.13E+00	9.13E+00
53						
54						
55						
56						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Formulas
Proofing
Save
Language
Ease of Access
Advanced
Customize Ribbon
Quick Access Toolbar
Add-ins
Trust Center
Change options related to formula calculation, performance, and error handling.
Calculation options
Workbook Calculation
Automatic
Automatic except for data tables
Manual
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51 T
52 Final values of P after convergence
60 CALCULA
61 LCULATED VALUES AND PARAMETE 1NN
62 N
63 E1
64 Uo
65 E
66 A
67 C12
68 C44
69 I
70 Q(Initially assumed value of q)
71 Ro
72 R1
73 R2
74 R3
75 M1
76 M2
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CHAPTER FOUR

RESULTS AND DISCUSSION

Table 4.1

Physical qty.	Palladium (Pd)	Platinum (Pt)	Silver (Ag)
E_C(eV)	3.94	5.85	2.96
E_{11}^F(eV)	1.40	1.50	1.10
a ($\boldsymbol{A}^0$)	3.89	3.92	4.08
B_0 (Mbar)	1.95	2.88	1.08
C_{11} (Mbar)	2.34	3.58	1.31
C_{12} (Mbar)	1.76	2.54	0.97
C_{44} (Mbar)	0.71	0.72	0.51
C_{12} - C_{44}	1.05	1.82	0.46

Table 4.1 above showing the various input parameters used in calculating the n, p and q values for 3 FCC metals (Pd, Pt and Ag) [1,6,12]

TABLE 4.2

NN	N	P	Q	NPQ PAIR/COMMENTS
1NN	0.7242	8.353634	3.379181	T1= 12.18854303 T4=12.1855601 T=2.98293E-03
2NN	0.772	8.34	3.34342	T1= 12.18854303 T4= 12.18961082 T=-1.106779E-03
3NN	0.71555	8.426451	3.323788	T1= 12.18854303 T4= 12.18294114 T=5.60189E-03
4NN	0.714	8.445725	3.322666	T1= 12.18854303 T4= 12.18148643 T=7.0566E-03
5NN	0.71348	8.460217	3.322706	T1= 12.18854303 T4= 12.18040027 T=8.14276E-03

The results of Palladium (Pd) showing n, p and q pairs from 1st nearest neighbour (NN) to the 5th nearest neighbour as shown in the table 4.2 above.

TABLE 4.3

NN	N	P	Q	NPQ PAIR/COMMENTS
1NN	0.6125	9.19167	3.967828	T1= 12.13324644 T4=12.1324467 T=7.9974E-04
2NN	0.6108011	9.187041	3.665783	T1= 12.13324644 T4= 12.13350217 T=-1.525879-04
3NN	0.60625	9.249125	3.657708	T1= 12.13324644 T4= 12.1301128 T=6.04248E-03
4NN	0.605	9.28048	3.65745	T1= 12.13324644 T4= 12.12843386 T=4.241943E-03
5NN	0.6502	9.267692	3.657754	T1= 12.13324644 T4= 12.12911597 T=6.713867E-04

The results of Platinum (Pd) showing n, p and q pairs from 1st nearest neighbour (NN) to the 5th nearest neighbour as shown in the table 4.3 above.

TABLE 4.4

NN	N	P	Q	NPQ PAIR/COMMENTS
1NN	0.622229	9.135677	3.036721	T1= 12.13637295 T4= 12.13356789 T= 2.80506E-03
2NN	0.61549	9.254628	3.004158	T1= 12.13637295 T4= 12.12981655 T=6.55604E-03
3NN	0.66571165	9.377615	2.962804	T1= 12.13637295 T4= 12.12336895 T=1.3004E-02
4NN	0.61012	9.399318	2.957618	T1= 12.13637295 T4= 12.12226487 T=1.1410808E-02
5NN	0.6894	9.42624	2.954794	T1= 12.13637295 T4= 12.12090901 T=1.546394E-02

The results of Silver (Ag) showing n, p and q pairs from 1st nearest neighbour (NN) to the 5th nearest neighbour as shown in the table 4.4 above.

SUMMARY OF RESULTS

Parameters	1st Nearest neigbour	1st – 2nd Nearest neigbour	1st – 3rd Nearest neigbour	1st – 4th Nearest neigbour	1st – 5th Nearest neigbour
n	0.7242	0.772	0.71555	0.714	0.71348
p	8.353634	8.34	8.426451	8.445725	8.460217
q	3.379181	3.34342	3.323788	3.322666	3.322706

Table 4.5: Summary of results for Palladium Pd

SUMMARY OF RESULTS FOR PALLADIUM PD

Metal	Reference	Parameter	P	Q
Pd	[2]	2/3	0.71555	0.714
	[7]	1/2	8.426451	8.445725
	This study	0.61265	8.460217	3.322706

	A	B	C	D	E	F
1	STEPS TO CALCULATE THE PARAMETERS FOR EAM/TB-SMA METHOD PALLADIUM					
2	CONSTANTS/CALCULATED PARAMETERS	VALUES 1NN	2NN	3NN	4NN	5NN
3	N	0.7242	0.772	0.71555	0.714	0.71348
4	P	8.353634	8.34	8.426451	8.445725	8.460217
5	Q	3.379181	3.34342	3.323788	3.322666	3.322706
6	Uo	-3.94	-3.94	-3.94	-3.94	-3.94
7	Al	3.89	3.89	3.89	3.89	3.89
8	E	1.4	1.4	1.4	1.4	1.4
9	C12	1.76	1.76	1.76	1.76	1.76
10	C44	0.71	0.71	0.71	0.71	0.71
11	Ro	2.750645379	2.750645379	2.750645379	2.750645379	2.750645379
12	F	-9.507126321	-11.52431512	-9.214536374	-9.163976914	-9.14713758
13	g	12.36507746	12.37605482	12.38222086	12.3825763	12.38256362
14	g1	2.253900381	1.758978801	1.736711801	1.732634142	-0.10892429
15	g2	6.404218434	6.280199622	6.21266583	6.208817922	6.20895508
16	L	1.53843911	1.652500684	1.522374458	1.519906679	1.519101271
17	A	0.456750762	0.622195018	0.432944419	0.428845604	0.427501352
18	f1	-6.885060882	-8.896771272	-6.593461502	-6.543079516	-6.52629972
19	f2	1.898899791	2.02846385	1.875510124	1.871320742	1.869915396
20	T1	12.18854303	12.18961082	12.18294114	12.18148643	12.18040027
21	D	0.927854387	1.26405252	0.879089396	0.870662819	0.867856263
22	D1	-2.817868131	-3.832627098	-2.693042067	-2.673328519	-2.6692835
23	D2	8.557787642	11.62058557	8.249986419	8.208327282	8.20997057
24	V11	7.036231938	6.807811685	7.079970755	7.087891397	7.09055437
25	W11	9.109052925	8.725771877	8.630403099	8.623681489	7.77960875
26	W12	1.454686129	1.943722483	1.926662405	1.928909697	4.039610419

	G	K	L	M	N	O	P
1		STEPS TO CALCULATE THE PARAMETERS FOR EAM/TB-SMA METHOD PLATINUM					
2		1NN	2NN	3NN	4NN	5NN	
3	N	0.6125	0.6108011	0.60625	0.605	0.6502	
4	P	9.19167	9.187041	9.249125	9.28048	9.267692	
5	Q	3.967828	3.665783	3.657708	3.65745	3.657754	
6	Uo	-3.94	-3.94	-3.94	-3.94	-3.94	
7	Al	3.92	3.92	3.92	3.92	3.92	
8	E	1.5	1.5	1.5	1.5	1.5	
9	C12	2.54	2.54	2.54	2.54	2.54	
10	C44	0.72	0.72	0.72	0.72	0.72	
11	Ro	2.771858582	2.771858582	2.771858582	2.771858582	2.771858582	
12	F	-6.468555186	-6.439840486	-6.36413919	-6.343652545	-7.177534882	
13	g	12.22418204	12.28791943	12.28985194	12.28991389	12.28984089	
14	g1	1.460765607	1.313013194	1.305014166	1.488286597	-0.090150228	
15	g2	8.50265513	7.331740353	7.301718557	7.30076044	7.301889391	
16	L	1.395999153	1.39129919	1.390599319	1.390472293	1.40459893	
17	Al	0.208398898	0.206027942	0.199844736	0.198183259	0.266922576	
18	f1	-3.961990051	-3.933461653	-3.858259384	-3.83790979	-4.66683318	
19	f2	1.535271145	1.530898948	1.519189632	1.515974367	1.632458246	
20	T1	12.13324644	12.13350217	12.1301128	12.12843386	12.12911597	
21	D	0.421425864	0.416640081	0.404023198	0.400608757	0.539589147	
22	D1	-1.397476588	-1.38091082	-1.348142754	-1.341281112	-1.80411297	
23	D2	4.634126616	4.57688729	4.498476557	4.490753105	6.032040541	
24	V11	7.608497721	7.619354783	7.648661914	7.65676873	7.378539687	
25	W11	11.5627726	9.995119061	9.952979788	10.03642043	9.308665481	

P	Q	R	S	T	U	V
	STEPS TO CALCULATE THE PARAMETERS FOR EAM/TB-SMA METHOD SILVER					
	1NN	2NN	3NN	4NN	5NN	
N	0.622229	0.61549	0.66571165	0.61012	0.6894	
P	9.135677	9.254628	9.377615	9.399318	9.42624	
Q	3.036721	3.004158	2.962804	2.957618	2.954794	
Uo	-3.94	-3.94	-3.94	-3.94	-3.94	
Al	4.08	4.08	4.08	4.08	4.08	
E	1.5	1.5	1.5	1.5	1.5	
C12	0.97	0.97	0.97	0.97	0.97	
C44	0.51	0.51	0.51	0.51	0.51	
Ro	2.884995667	2.884995667	2.884995667	2.884995667	2.884995667	
F	-6.63796902	-6.519708305	-7.515682248	-6.428398858	-8.097255961	
g	12.48483698	12.49809398	12.51545373	12.517673	12.5188855	
g1	1.023477436	1.182100806	0.975525169	1.258425767	-0.12526142	
g2	4.789908956	4.697317747	4.581091015	4.566622788	4.558754244	
L	1.379856745	1.377627437	1.397608149	1.375566894	1.417999562	
Al	0.222304393	0.212674964	0.294941304	0.205275077	0.342982194	
f1	-4.130336825	-4.012815264	-5.00327723	-3.922094711	-5.58224826	
f2	1.560321473	1.542967597	1.67253729	1.529146286	1.733846309	
T1	12.13637295	12.12981655	12.12336895	12.12226487	12.12090901	
D	0.449661503	0.429951384	0.595947041	0.414733143	0.692875994	
D1	-1.423905866	-1.37921875	-1.937112758	-1.351200884	-2.263856227	
D2	4.508964854	4.424324309	6.29654244	4.402213471	7.396770942	
V11	8.653419305	8.701946077	8.358086974	8.741184231	8.208985557	
W11	7.136683032	7.084511797	6.823953771	6.939911279	6.263674112	
W12	2.091977532	1.837078046	2.004783942	1.654679197	3.312526382	

	A	B	C	D	E	F
31	CALCULATING THE PARAMETER P OF THE TB-SMA METHOD					
32	CONSTANTS/CALCULATED VALUES	1NN	2NN	3NN	4NN	5NN
33	N	0.61265	0.612	0.71555	0.71435	0.63215
34	A	3.92E-08	4.08E-08	3.98E-08	3.89E-08	4.07E-08
35	E1	1.60E-12	1.60E-12	1.60E-12	1.60E-12	1.60E-12
36	E	1.3	1.1	1.40E+00	1.4	0.1
37	Uo	-5.85	-2.96	-3.94	-3.94	-3.78
38	C12	2.54E+12	9.70E+12	1.76E+12	1.76E+12	1.55E+12
39	C44	7.74E+11	5.10E+12	7.10E+12	7.10E+12	4.50E+12
40	Ro	2.77E-08	2.88E-08	2.81E-08	2.75E-08	2.88E-08
41	I	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
42	P(initally assumed value for p)	9.13E+00	9.13E+00	9.13E+00	9.13E+00	9.13E+00
43	R1	1.20E+01	1.20E+01	1.20E+01	1.20E+01	1.20E+01
44	R2	5.46E-02	5.46E-02	5.46E-02	5.46E-02	5.46E-02
45	M1	1.20E+01	1.20E+01	1.20E+01	1.20E+01	1.20E+01
46	M2	110736.2937	110736.2937	110736.2937	1.11E+05	1.11E+05
47	T1	-1.57E+02	-1.89E+02	2.37E+02	2.22E+02	2.32E+02
48	T2	-2.128582477	-0.213615919	-0.601305224	-0.599994834	-1.99293602
49	T3	7.36E+01	8.83E+02	-3.94E+02	-3.70E+02	-1.17E+02
50	T4	9.88E-07	9.88E-07	9.88E-07	9.88E-07	9.88E-07
51	T	7.36E+01	8.83E+02	-3.94E+02	-3.70E+02	-1.17E+02
52	Final values of P after convergence	9.13E+00	9.13E+00	9.13E+00	9.13E+00	9.13E+00

	A	B	C	D	E	F
60	CALCULATING THE PARAMETERS Q OF THE TB-SMA METHOD					
61	CALCULATED VALUES &	1NN	2NN	3NN	4NN	5NN
62	N	0.61255	0.612	0.71555	0.71435	0.71
63	E1	1.60E-12	1.60E-12	1.60E-12	1.60E-12	1.60219E-12
64	Uo	-5.85	-2.96	-3.94	-3.94	-3.94
65	E	1.3	1.1	1.40E+00	1.4	1.4
66	A	0.000000039	4.88E-08	3.98E-08	3.89E-08	0.000000039
67	C12	2.54E+12	9.70E+12	1.76E+12	1.76E+12	1.76E+12
68	C44	7.70E+12	5.10E+12	7.10E+12	7.10E+12	7.1E+12
69	I	1	1.00E+00	1.00E+00	1.00E+00	1
70	Q(Initially assumed value of q)	3.37	3.378	3.376	3.379	3.373
71	Ro	2.75772E-08	3.45068E-08	2.81428E-08	2.75065E-08	2.75772E-08
72	R1	12	18.08613381	18.08627664	18.08606249	18.08649133
73	R2		0.295710223	2.97E-01	0.29527759	0.297882915
74	R3		0.040608279			0.041046657
75	M1	12	12.36543482	12.36604079	12.36513221	12.36695164
76	M2		0.00172521	0.001735094	0.001720289	0.001750027
77	M3					0.005739055
78	T1	-429.8451432	750.7335055	-472.7798675	-441.4266635	-444.839741
79	T2	2.863143129	1.169348692	1.875510124	1.872266683	1.860512
80	T3	5.97339E+16	3.83E+16	5.75611E+16	6.03625E+16	5.98403E+16
81	T4	1	1.462636299	1.462576175	1.462666325	1.462485814
82	T5	1.71027E+17	9.58929E+16	2.30933E+17	2.41783E+17	2.38127E+17
83	T	-1.71027E+17	-9.58929E+16	-2.30933E+17	-2.41783E+17	-2.3813E+17
84	FINAL VAUE OF Q	3.37	3.378	3.376	3.379	3.373

	A	B	C	D	E	F	G
88	HOW TO CALCULATE IF P AND Q ARE CONSISTENT WITH N OF TB-SMA						
89	CONSTANTS/CALCULATED PARAMETERS	1NN	2NN	3NN	4NN	5NN	
90	A	3.92E-08	4.08E-08	3.89E-08	3.89E-08	4.07E+08	
91	E1	1.60E-12	1.60E-12	1.60E-12	1.60E-12	1.60E-12	
92	E	1.5	1.1	1.4	1.4	0.9	
93	Uo	-5.85	-2.96	-3.94	-3.74	-3.79	
94	C12	2.54E+12	9.70E+12	1.76E+12	1.75E+12	1.55E+12	
95	C44	7.70E+12	5.10E+12	7.10E+12	-7.10E+12	4.50E+12	
96	Bo	2.85E+12	1.08E+12	1.95E+12	1.98E+12	1.66E+12	
97	Ro	2.77E-08	2.88E-08	2.75E-08	2.75E-08	2.88E+08	
98	N	6.13E-01	6.19E-01	7.15E-01	7.14E-01	6.32E-01	
99	P	9.19E+00	9.25E+00	8.43E+00	8.45E+00	8.82E+00	
100	Q	3.70E+00	3.00E+00	3.31E+00	3.32E+00	3.67E+00	
101	T1	3.14E+17	1.24E+17	2.13E+17	2.16E+17	2.79E+50	
102	R1	1.20E+01	1.20E+01	1.20E+01	1.20E+01	1.20E+01	
103	R2	4.80E+01	4.80E+01	4.80E+01	4.80E+01	4.80E+01	
104	M1	1.21E+01	1.21E+01	1.22E+01	1.22E+01	1.22E+01	
105	M2	2.32E+36	4.02E+36	2.84E+33	3.36E+33	9.03E+34	
106	S	4.80E+02	1.76E+02	3.74E+02	3.36E+02	3.34E+02	
107	R	2.59E-35	1.49E-35	2.11E-32	1.79E-32	6.64E-34	
108	T2	1.25E-32	2.63E-33	7.91E-30	6.02E-30	2.22E-31	
109	S1	-7.07E+00	-3.10E+00	-6.59E+00	-6.04E+00	-5.11E+00	
110	V1	1.59E+01	1.90E+01	1.74E+01	1.74E+01	1.60E+01	
111	V2	4.23E-02	1.89E-01	9.67E-02	9.49E-02	4.50E-02	
112	W1	1.23E+01	1.25E+01	1.24E+01	1.24E+01	1.23E+01	
113	W2	2.40E+01	2.41E+01	2.40E+01	2.40E+01	2.40E+01	
114	V	2.41E+01	1.89E+01	2.11E+01	2.12E+01	2.38E+01	
115	T3	-1.70E+02	-5.87E+01	-1.39E+02	-1.28E+02	-1.22E+02	
116	T4	3.14E+17	1.24E+17	2.13E+17	2.16E+17	2.79E+50	
117	T	6.28E+17	2.48E+17	4.26E+17	4.33E+17	5.59E+50	

CHAPTER FIVE

FINDINGS, CONCLUSION AND SUGGESTIONS FOR FURTHER STUDIES

5.1 FINDINGS

From this research the following findings were made;

1. The assumed value of **n** is not constant
2. The value of **n** varies for the three FCC Metals (Palladium **Pd**, Platinum **Pt** and Silver **Ag**)

5.2 CONCLUSION

This study has used the recently established combination between EAM and the TB-SMA scheme to calculate the n, p, values for the three FCC metals. Our calculated value of n for Pd is in accordance with result obtained by Guevara et al, (1995). This project work also established the fact that n varies for different metals instead of assumed constant values of ½ and 2/3 as assumed by Cleri and Rosato. [2] and Guevara et al. [7]

5.3 SUGGESTIONS FOR FURTHER STUDIES

The results are preparatory findings to the study of FCC metals and it is recommended that more work be carried out on these or other FCC as well as BCC or HCP metals. The work should especially be directed towards answering the following questions:

(i) How well do the TB-SMA parameters, obtained via the workings shown in this study, perform in reproducing a better results of ab initio total energy calculation methods? It must be recalled that the parameters of the TB-SMA scheme are often determined by reference to ab initio total energy calculations.

(ii) How well do the parameters of the new generalized TB-SMA scheme perform in correctly reproducing the various physical properties of pure FCC metals, alloys and defects?

(iii) How sensitive are the parameters (and calculated results) to the number of neighbours taken into account in the definition of the functions $F(\rho)$, $\Phi 1(r)$, and $\rho(r)$ In this study the summation over j in these equations was carried out up to the 5th nearest-neighbour.

(iv) How compatible and effective will this new generalized scheme work for BCC metals?

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