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Research Article

POINT DEFECT GRAPHIC MODEL USING SPREADSHEET PROGRAM

Fita Permata Sari[1]*., Danis Alif Oktavia[2] and Heru Kuswanto[3]

[1,2]Physics Education Student, Postgraduate Program, Yogyakarta State University
[3]Physics Education Lecturer, Yogyakarta State University

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ABSTRACT

Point Defect is known as imperfections, grouped by space.Point defects have zero dimension; line defects, also known as dislocations, are one dimensional; and planar defects such as surface defects and grain boundary defects have two dimensions. Point defects have equilibrium concentrations that are determined by temperature, pressure, and composition. Point Defect on semiconductors and insulators govern a variety of mechanical, transport, electronic, and optoelectronic properties. This article describes how to know Point Defect values of some metals in the form of graphs using the Spreadsheet application. Point Defect value against temperature is seen through graph. The value of some metals can be known. The data entered produces a different graph, ie Al metal has the largest Point Defect value among Au, Cu, and Pt metals.

INTRODUCTION

Now that the most important aspects of perfect crystals have been described, it is time to recognize that things are not always perfect, even in the world of space lattices**.** This is not necessarily a bad thing**.** As we will see, many important materials phenomena that are based on defective structures can be exploited for very important uses**.** These defects, also known as imperfections, are grouped according to spatial extent. Point defects have zero dimension; line defects, also known as dislocations, are one dimensional; and planar defects such as surface defects and grain boundary defects have two dimensions. These defects may occur individually or in combination.

Point defects have equilibrium concentrations that are determined by temperature, pressure, and composition. This is not true of all types of dimensional defects that we will study.

$$N_d = \mathrm{N} \exp(E_d/k_B T) \quad (1)$$

In equation (1), $N_d$is the equilibrium number of point defects**, N**is the total number of atomic sites per volume or mole**,** $\boldsymbol{E_d}$is the activation energy for formation of the defect**,** $\boldsymbol{k_B}$ is Boltzmann's constant (1,38 x 10^{-23} J/atom.K), and T is absolute temperature. Equation (1) is an *Arrhenius-type expression* and many of these Arrhenius expressions can be derived from the Gibbs free energy,ΔG(Mitchell, 2004).

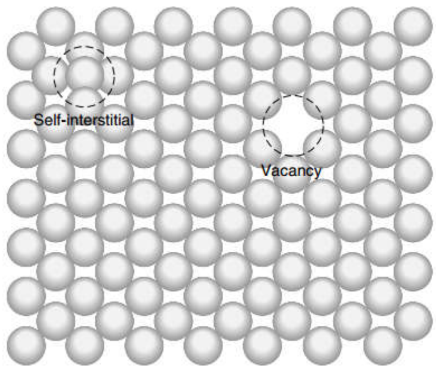


Figure 1 Representation of a vacancy and self-interstitial in a crystalline solid. FromK. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of JohnWiley & Sons, Inc.

Corresponding author:* **Fita Permata Sari
Physics Education Student, Postgraduate Program, Yogyakarta State University

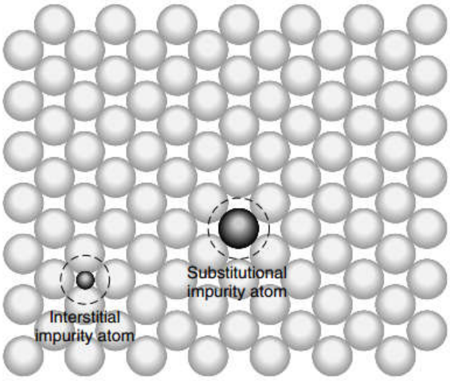


Figure 2 Representation of interstitial and substitutional impurity atoms in a crystalline solid. From K. M. Ralls, T. H. Courtney, and J. Wulff, *Introduction to Materials Science and Engineering*. Copyright © 1976 by John Wiley & Sons, Inc. This material is used by permission of John Wiley & Sons, Inc.

Point Defect is a defect that only happens around a single lattice point. Point Defect on semiconductors and insulators govern a variety of mechanical, transport, electronic, and optoelectronic properties. The fact that the properties of Point Defect is difficult to fully characterize from the experiments of computing tools that have been widely applied. Point defects have a strong impact on the performance of semiconductor and insulator materials used in technological applications, spanning microelectronics to energy conversion and storage (Broberg, Medasani, Zimmermann, Yu, Canning, Haranczyk, Asta,& Hautier, 2018). The collective behavior of point defects formed on the free surfaces of ionic crystals under redox conditions can lead to initiation of local breakdown by pitting(Herbert, Krishnamoorthy, Ma, Van Vliet, & Yildiz, 2014).

The chart is the visualization of the observed data table. Graphs are a useful type of representation in summarizing data, processing and interpreting new information from complex data. Chartsare often regarded as mathematical devices, because communicating through graphical representations requires math competencies such as visual perception, logical thinking, data ploting, line movement improvements, deduction of relationships between variables and others(Subali, Rusdiana, Firman, & Kaniawati, 2015).

Chart is a form of representation used to describe material concepts and phenomena in physics learning (Docktor & Mestre, 2014). Interpretations using graphs are influenced by several factors such as aspects of characteristics, content, and knowledge of graphs (Glazer, 2011). It is as written in the results of research (Nixon, Godfrey, Mayhew, & Wiegert, 2016) which shows that interpretation of data using graphs can be used to reduce experimental errors, determine the value of a variable, and explain the relationship between variables. The results (Susac, Bubic, Martinjak, Planinic, & Palmovic, 2017)suggest that graphic representation has advantages in interpreting measurement data and comparison data. Problems in physics learning such as mathematical formulas can be interpreted using charts using Spreadsheet. Based on the description above, the authors want to know the value of Point Defect some metal in the form of graphics by using Spreadsheet application. Spreadsheets have been around since the 1970s and have become an important part of teaching and learning tools because they are transparent, dynamic and easily modified (LoSchiavo, 2016).

METHODS

This section shows how the spreadsheet program can be used to simulate a physics problem.

Table 1 Energy Establishment of Vacancies for Selected Elements and Equilibrium Concentrations at Various Temperatures

Element	E_d(kJ/mol)	Melting Point, T_m (°C)	N_d (vacancies/cm^3) 25°C	300°C	600°C	T_m
Ag	106.1	960	$1.5x10^4$	$1.5x10^{13}$	$3.0x10^{16}$	$7.8x10^{17}$
Al	73.3	660	$1.0x10^{10}$	$1.2x10^{16}$	$2.4x10^{18}$	$5.0x10^{18}$
Au	94.5	1063	$1.5x10^6$	$1.5x10^{14}$	$1.5x10^{17}$	$1.2x10^{19}$
Cu	96.4	1083	$1.1x10^6$	$1.4x10^{14}$	$1.4x10^{17}$	$9.0x10^{18}$
Ge	192.9	958	<1	$1.3x10^5$	$1.3x10^{11}$	$8.2x10^{13}$
K	38.6	63	$2.1x10^{15}$	-	-	$1.3x10^{16}$
Li	39.5	186	$4.7x10^{15}$	-	-	$1.4x10^{18}$
Mg	85.8	650	$4.4x10^7$	$6.4x10^{14}$	$3.5x1010^{17}$	$5.7x10^{17}$
Na	38.6	98	$4.0x10^{15}$	-	-	$1.0x10^{17}$
Pt	125.4	1769	8.7	$2.7x10^{11}$	$2.0x10^{15}$	$4.2x10^{19}$
Si	221.8	1412	<1	$3.1x10^2$	$2.5x10^5$	$8.0x10^{15}$

From equations (1) and Table 1 we can determine the value of each variable by varying the temperature of each element. Analysis using spreadsheet program. The energy formation of the vacancy of each element is selected and the equilibrium concentration at various temperatures.

The steps used to determine the number of points of equilibrium defects are shown in the following figure:

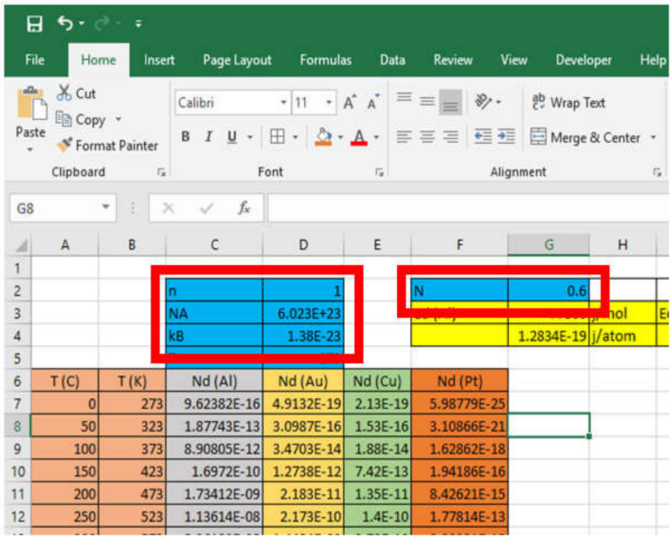


Figure 3 Variables That Are Not Varied n, N_A, k_B, and N.

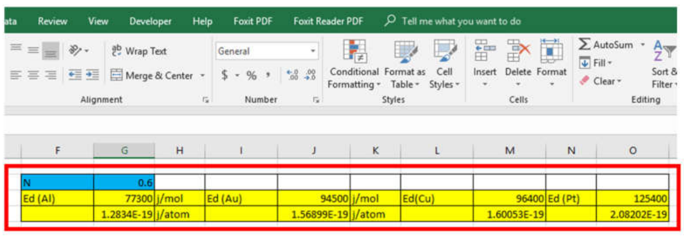
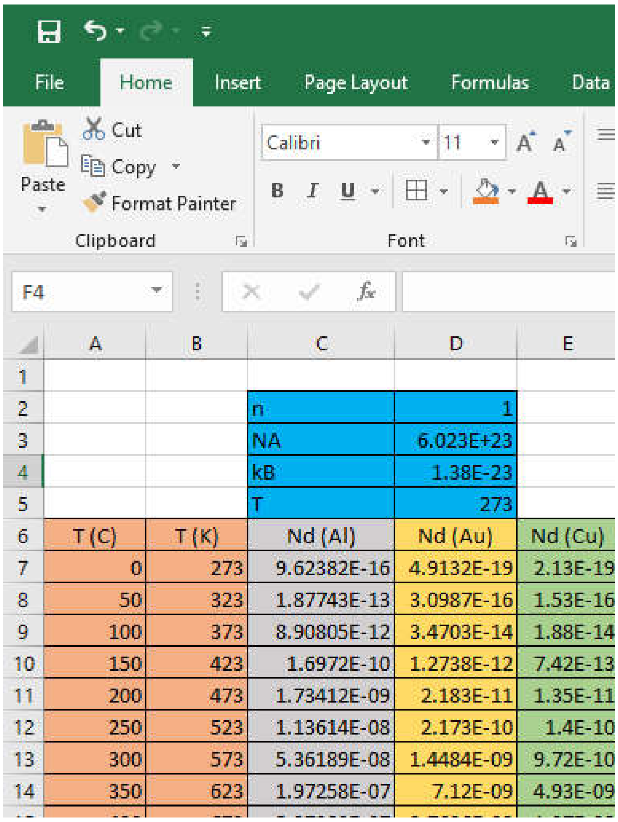
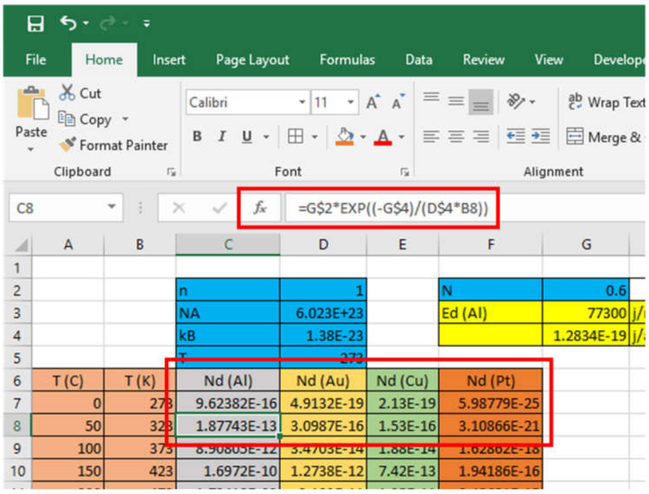


Figure 4 Input The Activation Energy



	A	B	C	D	E
1					
2			n	1	
3			NA	6.023E+23	
4			kB	1.38E-23	
5			T	273	
6	T (C)	T (K)	Nd (Al)	Nd (Au)	Nd (Cu)
7	0	273	9.62382E-16	4.9132E-19	2.13E-19
8	50	323	1.87743E-13	3.0987E-16	1.53E-16
9	100	373	8.90805E-12	3.4703E-14	1.88E-14
10	150	423	1.6972E-10	1.2738E-12	7.42E-13
11	200	473	1.73412E-09	2.183E-11	1.35E-11
12	250	523	1.13614E-08	2.173E-10	1.4E-10
13	300	573	5.36189E-08	1.4484E-09	9.72E-10
14	350	623	1.97258E-07	7.12E-09	4.93E-09

Figure 5 Input Temperature Variations

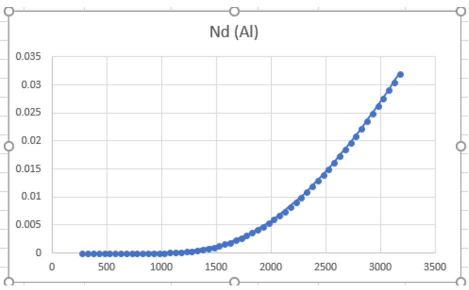


	A	B	C	D	E	F	G
1							
2			n	1		N	0.6
3			NA	6.023E+23		Ed (Al)	77300 j/
4			kB	1.38E-23			1.2834E-19 j/
5			T	273			
6	T (C)	T (K)	Nd (Al)	Nd (Au)	Nd (Cu)	Nd (Pt)	
7	0	273	9.62382E-16	4.9132E-19	2.13E-19	5.98779E-25	
8	50	323	1.87743E-13	3.0987E-16	1.53E-16	3.10866E-21	
9	100	373	8.90805E-12	3.4703E-14	1.88E-14	1.62802E-18	
10	150	423	1.6972E-10	1.2738E-12	7.42E-13	1.94186E-16	

Figure 6 Equations and Results The Equilibrium Number of Point Defects

RESULTS AND DISCUSSION

Each variable is determined from Equations (1) and Table 1, so that it matches the value of Point Defect analyzed using the Spreadsheet application.



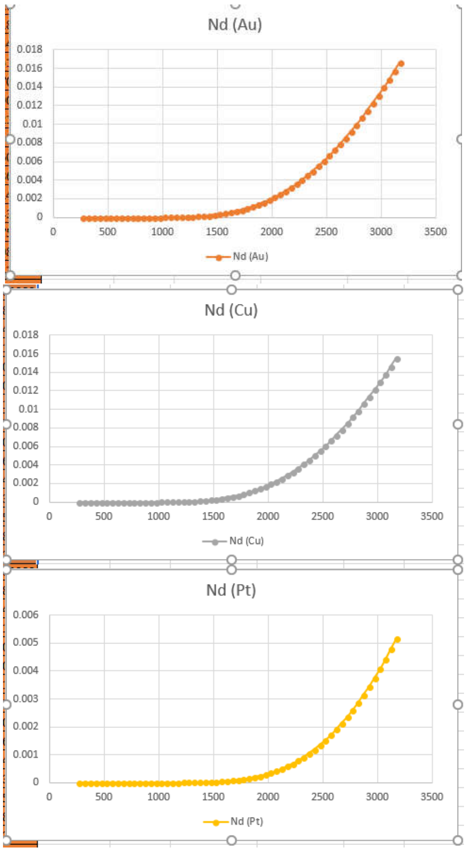


Figure 7 EachGraph The Equilibrium Number Of Point Defects (Al, Au, Cu, Pt)

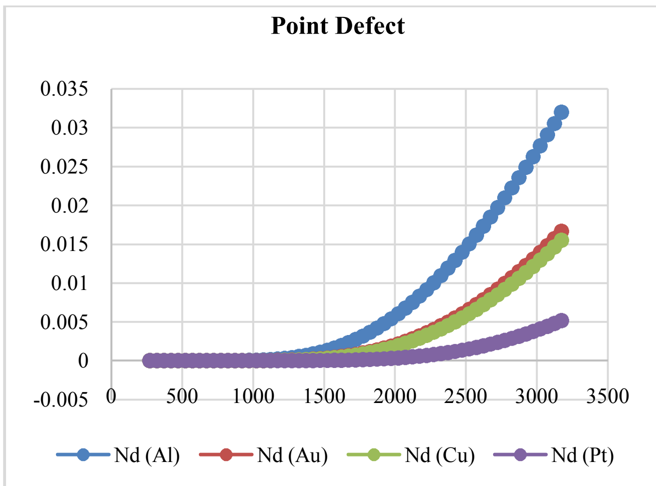


Figure 8 Combined Graph Point Defect

Point Defect value of some metals can be seen in Figure 8. Point Defect values vary depending on temperature, the greater the temperature the greater the Point Defect value. Al metal has the most significant Point Defect value among the others, of the four metal variations used. Then the next sequence is occupied by metal Au, Cu, and Pt. The chart above shows that Spreadsheets can be used easily in displaying data. Graphical depiction with Spreadsheet is more accurate and reliable because it can vary the variables quickly and easily. Various calculations can be done quickly and accurately by utilizing the facilities of internal functions available in the Spreadsheet application.

CONCLUSION

Spreadsheets can help in analyzing data in the form of graphs or simulations. Point Defect equations and known data are inserted into Microsoft Excel, by using the existing command, the result of a graph of differences in Point Defect appears and can be distinguished. Some metals can be known through the Point Defect value graph to temperature. According to the data and graphs discussed it is found that Al metal has the greatest Point Defect value among Au, Cu, and Pt metal.

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