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Research Article

Study of Thermophysical Properties at High Temperatures for Some Nanomaterials

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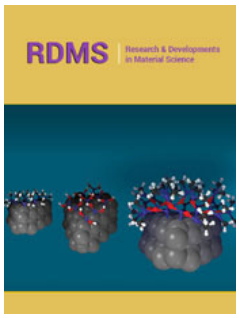

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Abstract

A simple theoretical model is developed to study the effect of temperature on nanomaterials. It is found that the volume thermal experimental data for nanomaterials under study can be reproduced satisfactorily with the help of Liu model, which takes into account the temperature dependence of the Anderson- Grüneisen parameter. The Anderson model for investigating the temperature dependence of volume expansion of some nanomaterials viz. Zirconia, Ag, ZnO, NiO and Al compounds have been used by Kumar model to obtain results in an approximately fair agreement with the available experimental data. The model used by them is based on the assumption that the Anderson-Gru¨neisen parameter does not depend on temperature.

Keywords: Nanomaterials; Volume thermal expansion; Anderson – Grüneisen parameter; Isobaric equation of state

Introduction

Nanomaterials are the central importance in the field of science and technology. The properties of nanomaterials are modified significantly at high temperatures [1,2]. Kumar et al. [3] have studied the temperature dependence of volume expansion of some nanomaterials viz. Zirconia, Ag, Zno, NiO and Al compounds using the Anderson formulation [4] which is based on the assumption that the Anderson- Grüneisen parameter δ_T is independent of temperature, i.e. δ_T does not change with the variation in temperature. It was found by Liu [5,6] that to take account of the temperature dependence of the Anderson- Grüneisen the Anderson formulation is necessary in order to improve the agreement between theoretical results and available experimental data.

Method of Analysis

Anderson and Zou [7] used the basic calculus to study the thermal properties of materials

$$\left(\frac{d\alpha}{dT}\right)_v = \left(\frac{d\alpha}{dT}\right)_P + \alpha B\left(\frac{d\alpha}{dP}\right)_T \quad (1)$$

Where α is the volume thermal expansion coefficient or simply the thermal Expansivity,

$$\alpha = \frac{1}{V}\left(\frac{dV}{dT}\right)_P \quad (2)$$

And B the isothermal bulk modulus given below

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (3)$$

Eq. (1) has the status of an identity. The Anderson-Grneisen parameter δ_T is related to the temperature derivative of bulk modulus as follows [4]

$$\delta_T = -\frac{1}{\alpha B}\left(\frac{dB}{dT}\right)_P \quad (4)$$

Using another identity between thermodynamic quantities [8,9]

$$\left(\frac{d\alpha}{dP}\right)_T = \frac{1}{B^2}\left(\frac{dB}{dT}\right)_P \quad (5)$$

In Eq. (4), we get

$$\left(\frac{d\alpha}{dP}\right)_T = -\frac{\alpha\delta_T}{B} \quad (6)$$

Using Eq. (5) in Eq. (1), we get

$$B\left(\frac{d\alpha}{dT}\right)_V = \left[\frac{d(\alpha B)}{dT}\right]_P \quad (7)$$

For most of the materials, the product remains constant in the high temperature region above the Debye temperature. Hence, Eq. (7) gives $(d\alpha/dT)_V = 0$, and then Eq. (1) yields.

$$\left(\frac{d\alpha}{dT}\right)_P = -\alpha B\left(\frac{d\alpha}{dP}\right)_T \quad (8)$$

Equations (6) and (8) takes together yield

$$\left(\frac{d\alpha}{dT}\right)_P = \alpha^2\delta_T \quad (9)$$

On integrating Eq. (9) with respect to temperature T between the limits T_0 and a value of high temperature T, and taking a constant value of δ_T equal to δ_T^0, we get

$$\frac{\alpha}{\alpha_0} = \frac{1}{\left[1-\alpha_0\delta_T^0(T-T_0)\right]} \quad (10)$$

Taking Eq. (2) in Eq. (10), and then further integrating, we find

$$\frac{V}{V_0} = \left[1-\alpha_0\delta_T^0(T-T_0)\right]^{-1/\delta_T^0} \quad (11)$$

Where V_0 is the volume V at $T-T_0$, unified temperature. It is found [3] that the results for volume thermal expansion versus temperature calculated from Eq. (11) for the nanomaterials under study derivative significantly from the experimental data. This discrepancy appears due to the assumption that δ_T giving the following expression [5]

$$\int_{V_0}^{V}\frac{1}{V}\exp\left[\left(\frac{\delta_T^0}{s}\right)\left(1-\left(\frac{V}{V_0}\right)^s\right)\right]dv = \alpha_0(T-T_0) \quad (12)$$

$$\left(1+\frac{\delta_T^0}{s}+\frac{\delta_T^{02}}{2s^2}\right)\ln\frac{V}{V_0}+\frac{\delta_T^0}{s^2}\left(\frac{\delta_T^0}{s}+1\right)\left[1-\left(\frac{V}{V_0}\right)^s\right]-\frac{\delta_T^{02}}{4s^3}\left[1-\left(\frac{V}{V_0}\right)^{2s}\right] = \alpha_0(T-T_0) \quad (12a)$$

As in Eq. (12) the integral on left hand side, cannot be evaluated exactly with the help of an analytical method, and therefore [5,10] used an approximation procedure by truncating the expansion of the exponential function up to quadratic term in

$$\left(1+\frac{\delta_T^0}{s}+\frac{\delta_T^0}{s^2}\right)\left[\left(\frac{V}{V_0}\right)^s-1\right] = \alpha_0(T-T_0) \quad (13)$$

Where $s = (d\ln\delta_T / d\ln V)_P$. "s" is the dimensionless thermoelastic parameter whose [4] value is about s = +2, Eq. (12a) is in fact an isobaric equation of state determining V/V_0 as a function of temperature along an isobar at P = 0 for different types of materials.

Discussion and conclusion

Value of δ_T^0, the Anderson- Grneisen at room temperature and atmospheric pressure remain almost between 4 and 6 for different types of materials [7]. For nanomaterials, accurate values of δ_T^0 are not known, we have calculated $\frac{V}{V_0}$, taken three representative values of δ_T^0 equal to 4, 5, and 6 for each material. Values of α_0 used as input in calculations are given in Table 1 of Kumar et al. [3],[11].

Table 1: Value of input parameters used in present work [3,11].

Nanomaterials	$\alpha_0(10^{-4}K^{-1})$
Zirconia	3.46
Ag	1.8
ZnO	1.04
NiO	3.77
Al	7.8
11% AlN/Al	5.88
39% AlN/Al	4.2

In order to demonstrate the validity of Eq. (13) and (11) are calculated as a function of temperature. Because one should check for consistencies using the same set only with Eq. (11) with experimental data [3], here we have used seven nanomaterials in present study, the value of α_0, δ_T^0 are used as input parameters which are given in Table 1. Eq. (13) and (11) are used to compute temperature dependence of V/Vo at different temperature of nanomaterials. The result are compared with experimental data [3] we found Liu Model (13) is very consistent with experimental data [3] we can say that Liu Model can reproduced the experimental data in figure of merit The present work is simple and straightforward method to study the effect of temperature on nanomaterials due to the simplicity and applicability it may be the current interest to the researchers engaged in this field. To the best of our knowledge such simple methods are not yet available in the literature for nanomaterials (Tables 2-4; Figures 1-3).

Table 2: Temperature dependence of V/Vo of Eqs. (13) and (11) with the value $\delta_T^0 = 4$.

Zirconia				Ag			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
425	1.005	1.006	1.005	360	1.0013	1.001	1.001
575	1.012	1.012	1.009	460	1.003	1.003	1.0029
750	1.019	1.018	1.016	560	1.005	1.005	1.0047
900	1.025	1.024	1.021	670	1.0075	1.0076	1.0067
1000	1.03	1.029	1.025	775	1.01	1.01	1.0087
1200	1.038	1.037	1.033	880	1.013	1.013	1.0107
1300	1.042	1.041	1.037	975	1.015	1.015	1.0125

1500	1.05	1.049	1.046				
1650	1.056	1.055	1.053				
ZnO				**NiO**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
500	1.002	1.002	1.002	600	1.014	1.013	1.0116
600	1.004	1.004	1.0031	700	1.018	1.018	1.0156
700	1.005	1.005	1.0042	800	1.023	1.022	1.0197
820	1.0067	1.0065	1.0054	900	1.027	1.027	1.0239
920	1.008	1.0079	1.0065	1000	1.032	1.031	1.0292
1020	1.0093	1.0092	1.0076	1100	1.037	1.036	1.0326
1120	1.011	1.011	1.0087	1200	1.041	1.04	1.0371
1220	1.012	1.012	1.0098	1400	1.05	1.049	1.0463
1320	1.013	1.013	1.0108	1500	1.055	1.053	1.0511
1450	1.015	1.015	1.0123				
1550	1.016	1.016	1.0134				
Al				**AlN/Al 11%**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
325	1.0024	1.0024	1.0019	325	1.0018	1.0019	1.0014
375	1.007	1.007	1.0059	375	1.0054	1.0053	1.0044
425	1.012	1.012	1.0099	425	1.0091	1.009	1.0074
475	1.016	1.016	1.0141	475	1.012	1.012	1.0105
575	1.026	1.025	1.0226	525	1.016	1.015	1.0136
AlN/Al 39%							
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)				
325	1.002	1.002	1.002				
375	1.003	1.003	1.0031				
425	1.006	1.006	1.0053				
475	1.0082	1.008	1.0074				
525	1.01	1.01	1.0096				

Table 3: Temperature dependence of V/Vo of Eqs. (13) and (11) with the value $\delta_T^0 = 5$.

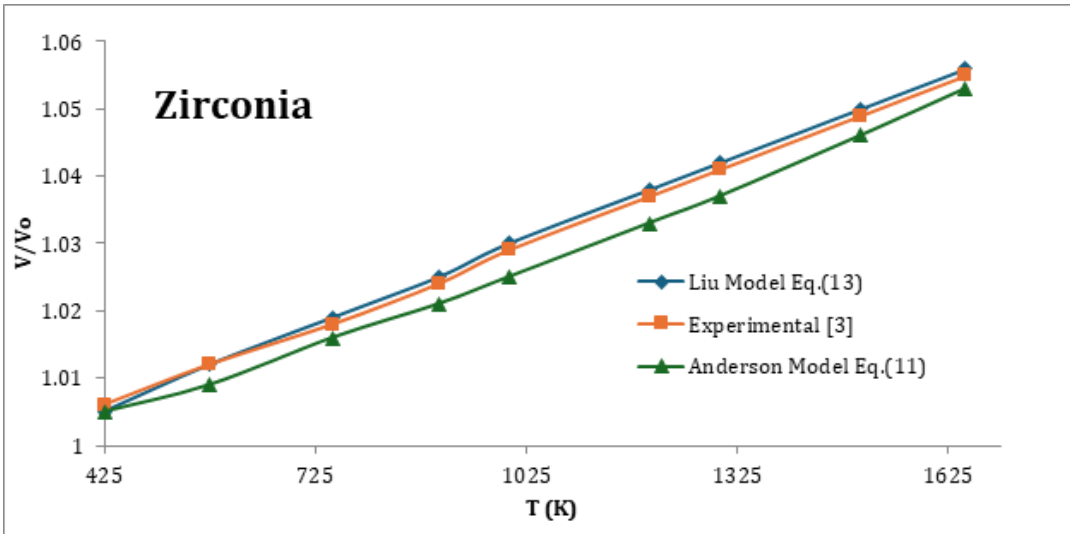
Zirconia				**Ag**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
425	1.005	1.006	1.005	360	1.001	1.0012	1.001
575	1.01	1.01	1.009	460	1.003	1.0031	1.0029
750	1.016	1.017	1.016	560	1.006	1.0057	1.0047
900	1.022	1.023	1.021	670	1.008	1.0078	1.0067
1000	1.028	1.029	1.025	775	1.01	1.01	1.0087
1200	1.035	1.036	1.033	880	1.012	1.012	1.0107
1300	1.039	1.04	1.037	975	1.014	1.014	1.0125
1500	1.048	1.049	1.046				
1650	1.056	1.057	1.053				
ZnO				**NiO**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
500	1.002	1.002	1.002	600	1.012	1.013	1.012

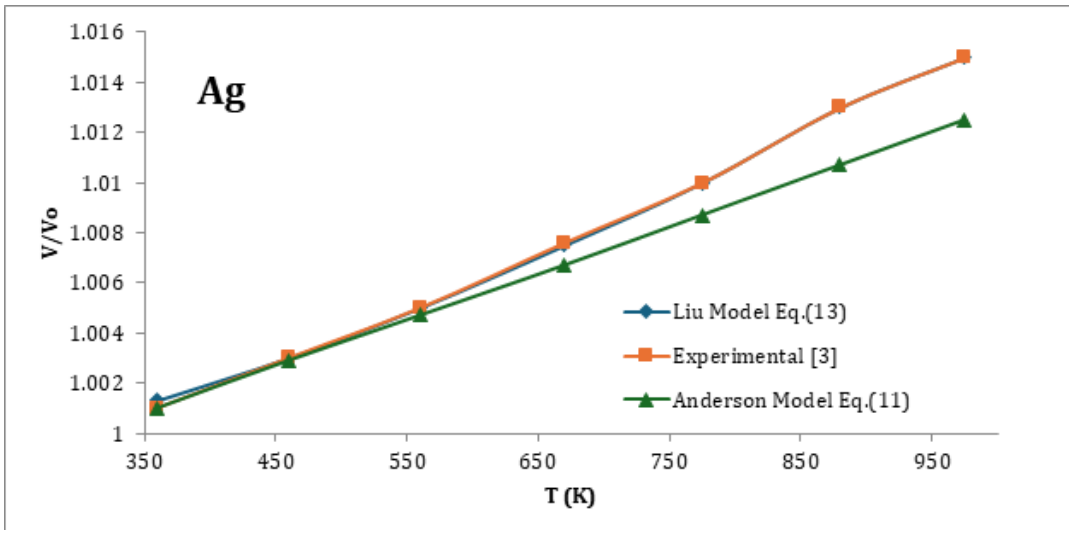
600	1.0035	1.0035	1.0031	700	1.016	1.017	1.02
700	1.0048	1.0047	1.0042	800	1.02	1.021	1.025
820	1.006	1.006	1.0054	900	1.025	1.026	1.03
920	1.007	1.0073	1.0065	1000	1.03	1.03	1.035
1020	1.0085	1.009	1.0076	1100	1.032	1.033	1.04
1120	1.01	1.01	1.0087	1200	1.035	1.036	1.045
1220	1.011	1.011	1.0098	1400	1.045	1.046	1.054
1320	1.012	1.012	1.0108	1500	1.05	1.051	1.055
1450	1.014	1.014	1.0123				
1550	1.015	1.015	1.0134				
Al				**AlN/Al 11%**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
325	1.002	1.002	1.0019	325	1.0017	1.0019	1.0014
375	1.0065	1.007	1.0059	375	1.0052	1.0053	1.0044
425	1.012	1.012	1.0099	425	1.009	1.009	1.0074
475	1.016	1.016	1.0141	475	1.012	1.012	1.0105
575	1.026	1.026	1.0226	525	1.015	1.015	1.0136
AlN/Al 39%							
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)				
325	1.001	1.0012	1.001				
375	1.003	1.003	1.0031				
425	1.006	1.006	1.0053				
475	1.008	1.008	1.0074				
525	1.01	1.01	1.0096				

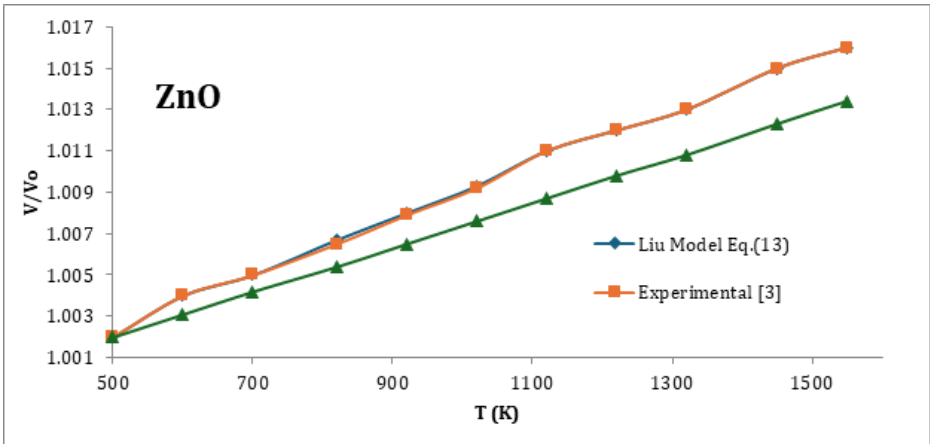
Table 4: Temperature dependence of V/Vo of Eqs. (13) and (11) with the value $\delta_T^0 = 6$.

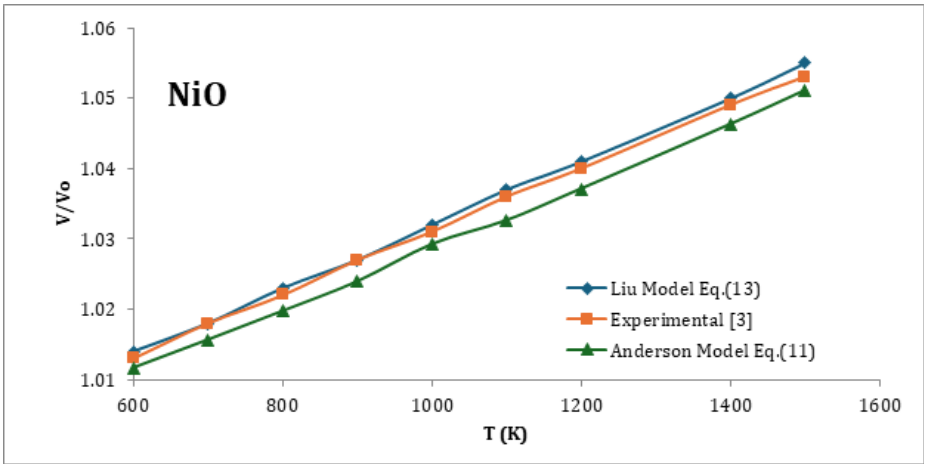
Zirconia				**Ag**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
425	1.004	1.005	1.005	360	1.001	1.0012	1.001
575	1.009	1.01	1.009	460	1.003	1.003	1.0029
750	1.014	1.015	1.016	560	1.0045	1.005	1.0047
900	1.019	1.02	1.021	670	1.0068	1.007	1.0067
1000	1.022	1.023	1.025	775	1.01	1.01	1.0087
1200	1.029	1.03	1.033	880	1.012	1.012	1.0107
1300	1.033	1.033	1.037	975	1.014	1.014	1.0125
1500	1.039	1.04	1.046				
1650	1.045	1.046	1.053				
ZnO				**NiO**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
500	1.002	1.002	1.002	600	1.01	1.01	1.0116
600	1.003	1.003	1.0031	700	1.015	1.016	1.0156
700	1.004	1.004	1.0042	800	1.017	1.018	1.0197
820	1.005	1.005	1.0054	900	1.02	1.02	1.0239
920	1.006	1.006	1.0065	1000	1.024	1.025	1.0292
1020	1.007	1.007	1.0076	1100	1.027	1.028	1.0326
1120	1.008	1.0078	1.0087	1200	1.03	1.031	1.0371

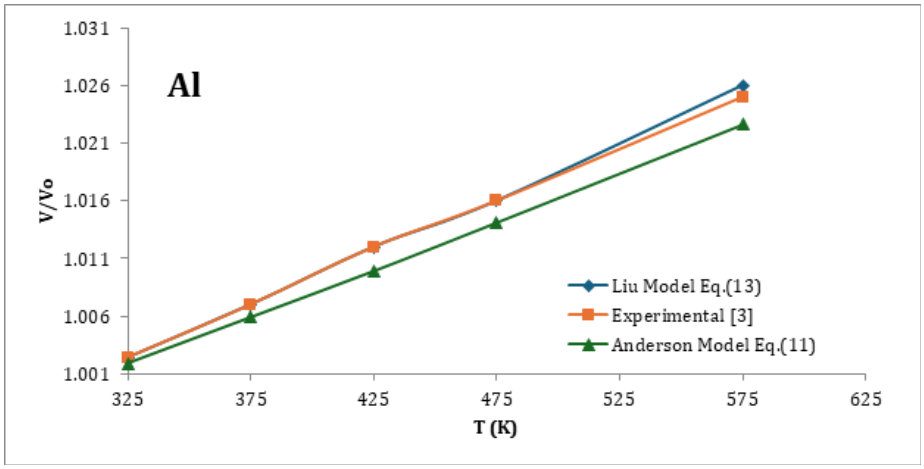
1220	1.009	1.009	1.0098	1400	1.037	1.038	1.0463
1320	1.01	1.01	1.0108	1500	1.04	1.041	1.0511
1450	1.011	1.011	1.0123				
1550	1.012	1.012	1.0134				
Al				**AlN/Al 11%**			
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)	T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)
325	1.0023	1.0024	1.0019	325	1.0017	1.0019	1.0014
375	1.005	1.0045	1.0059	375	1.005	1.0053	1.0044
425	1.009	1.0091	1.0099	425	1.009	1.009	1.0074
475	1.012	1.012	1.0141	475	1.012	1.012	1.0105
AlN/Al 39%							
T(K)	Liu Model Eq. (13)	Experimental [3]	Anderson Model Eq. (11)				
325	1.001	1.0012	1.001				
375	1.003	1.003	1.0031				
425	1.0058	1.006	1.0053				
475	1.0078	1.008	1.0074				
525	1.0098	1.01	1.0096				

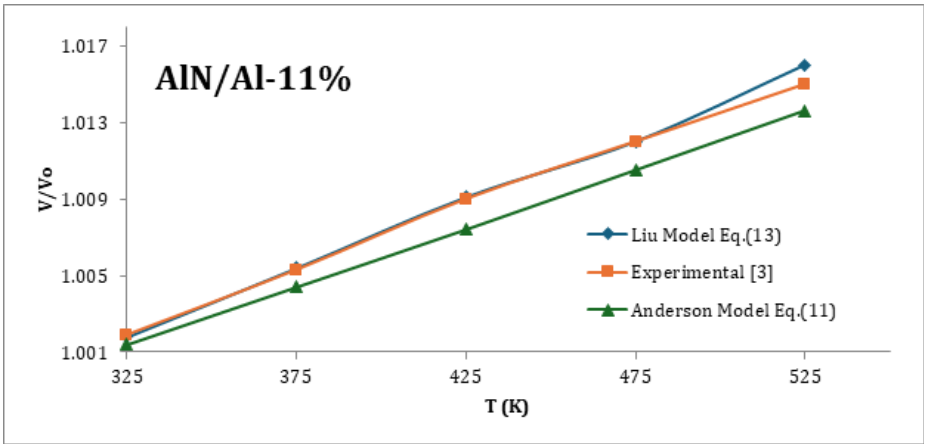


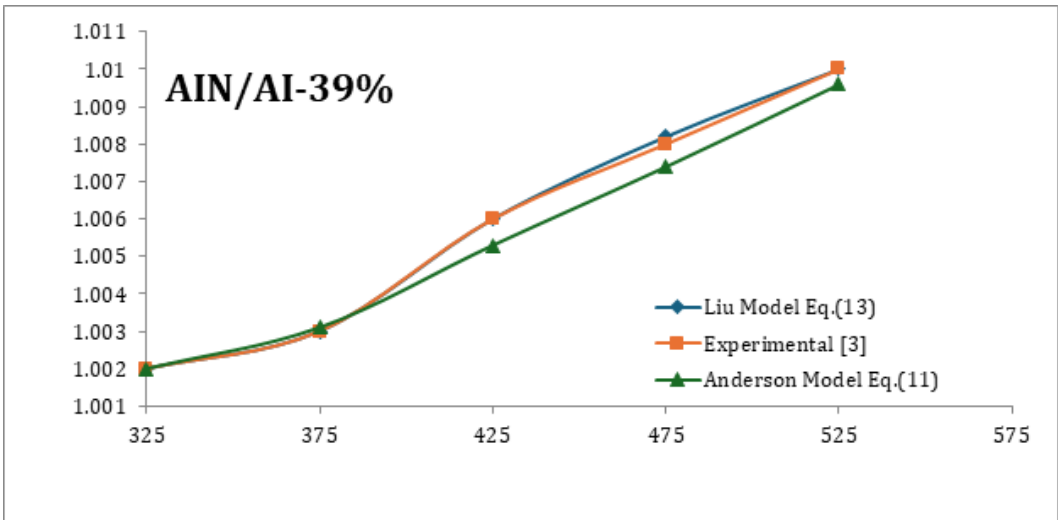












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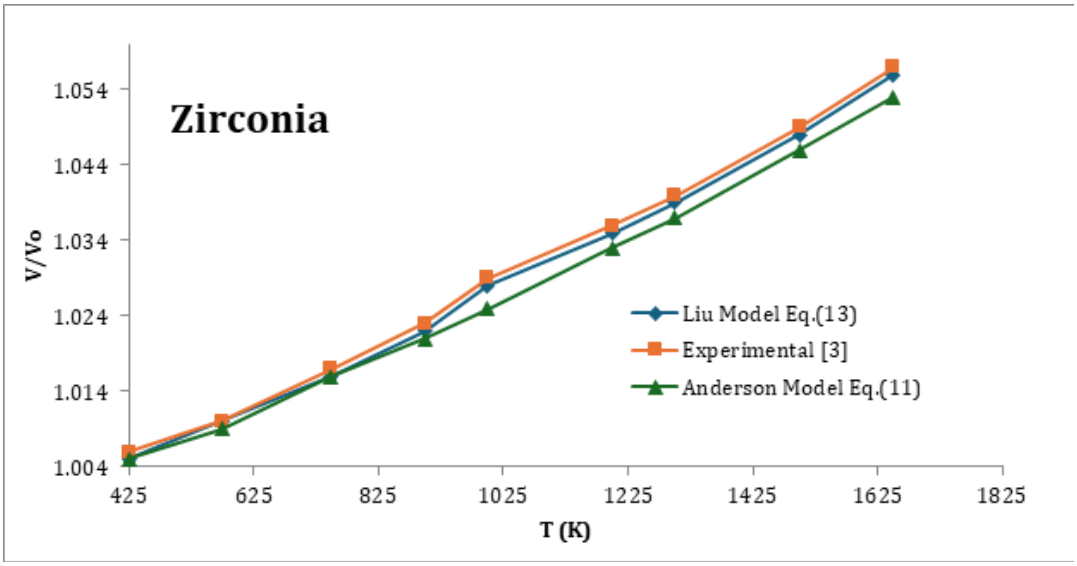

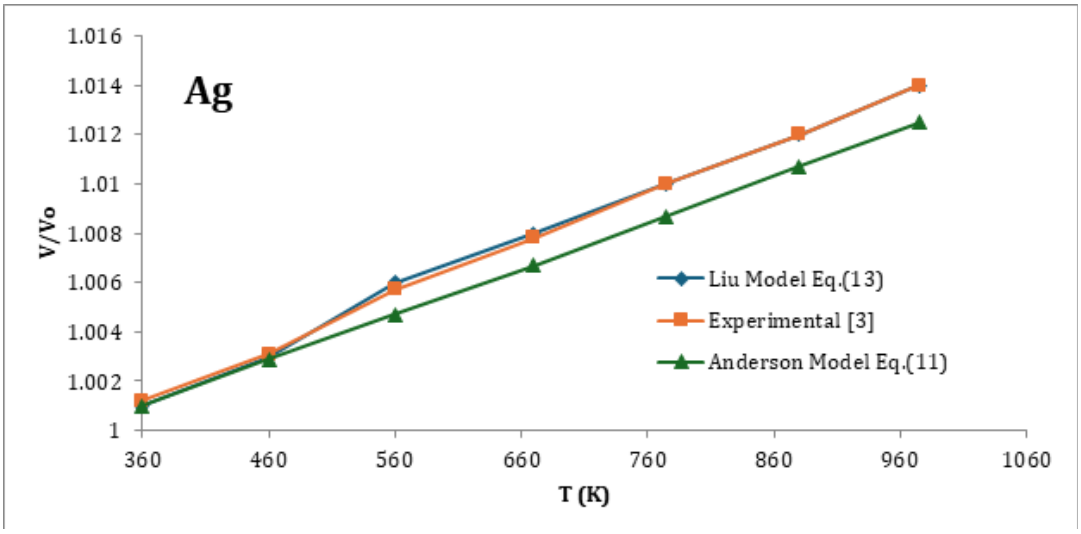

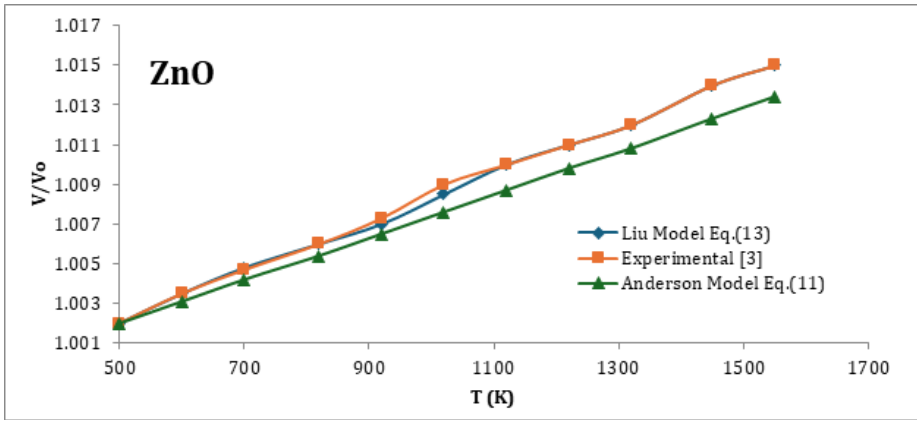

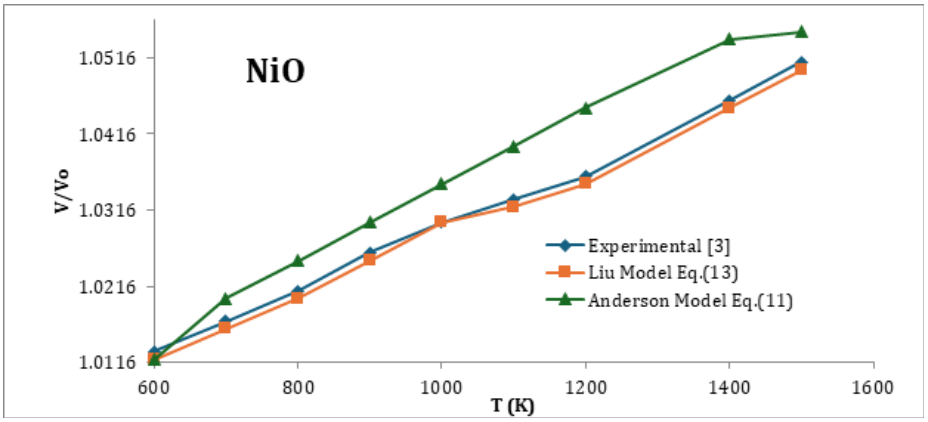

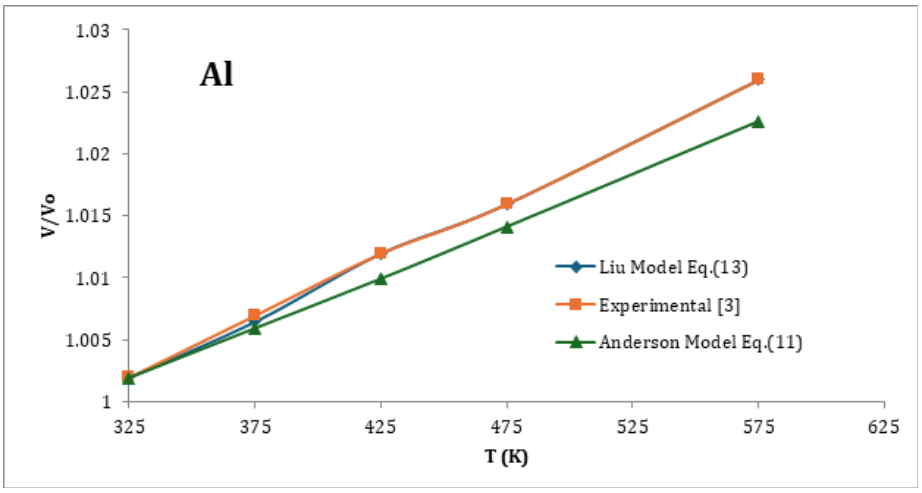

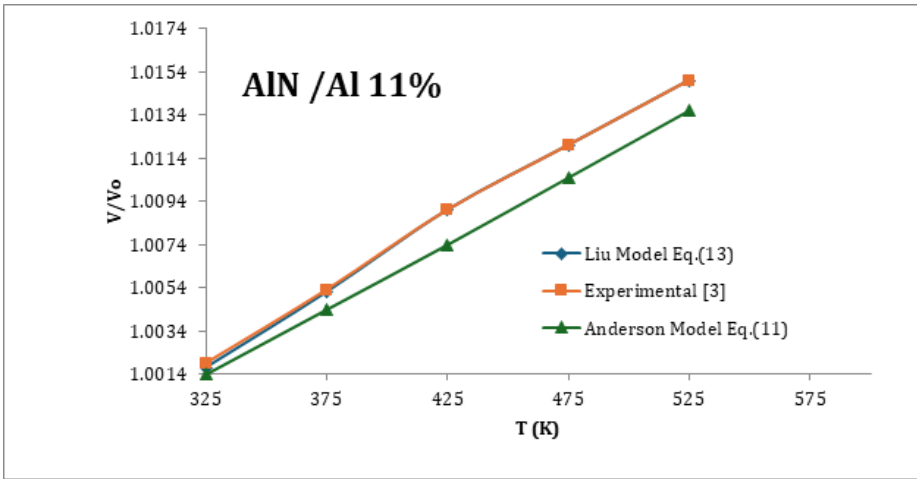

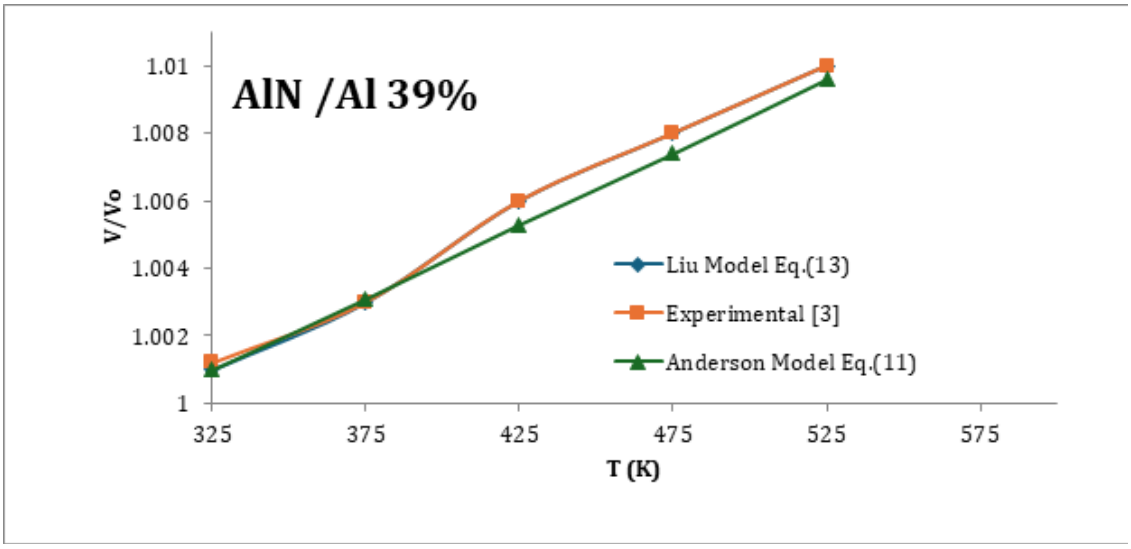

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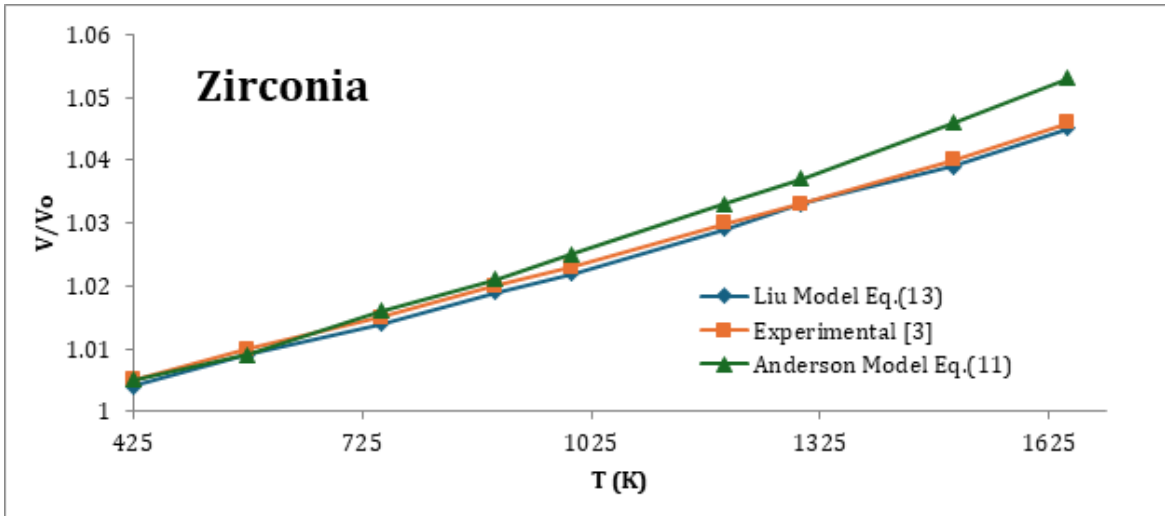

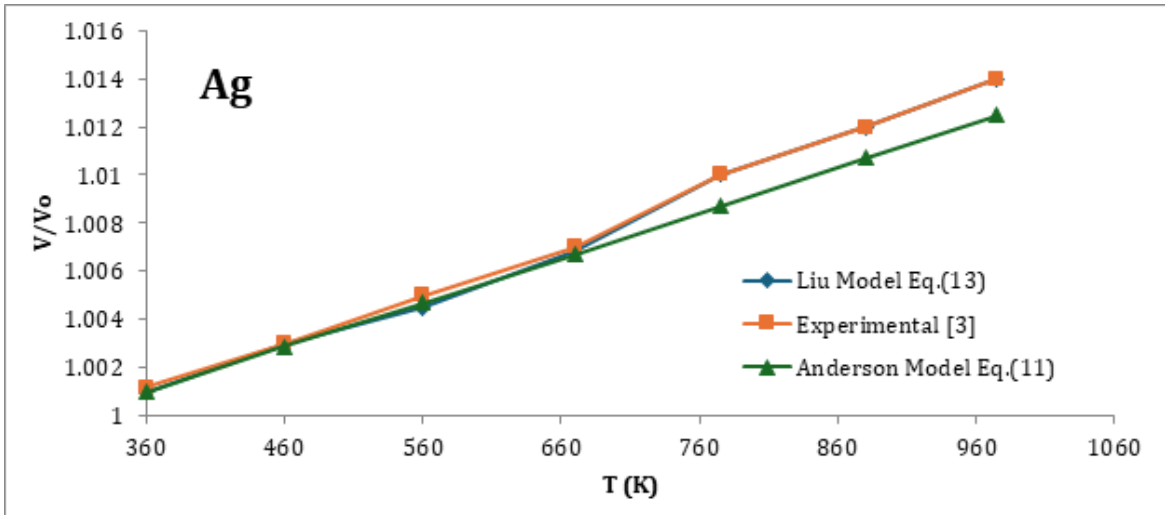

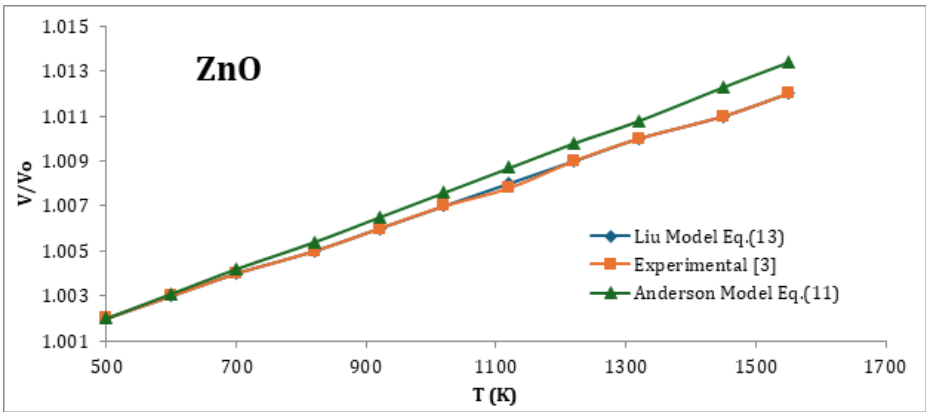

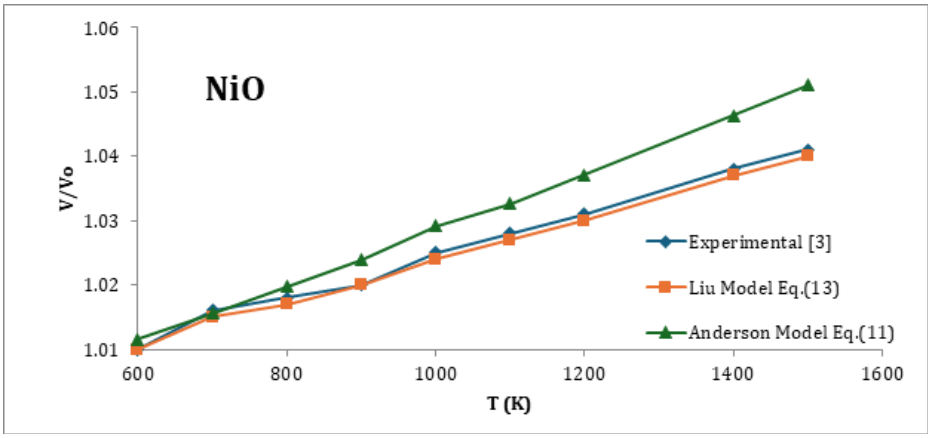

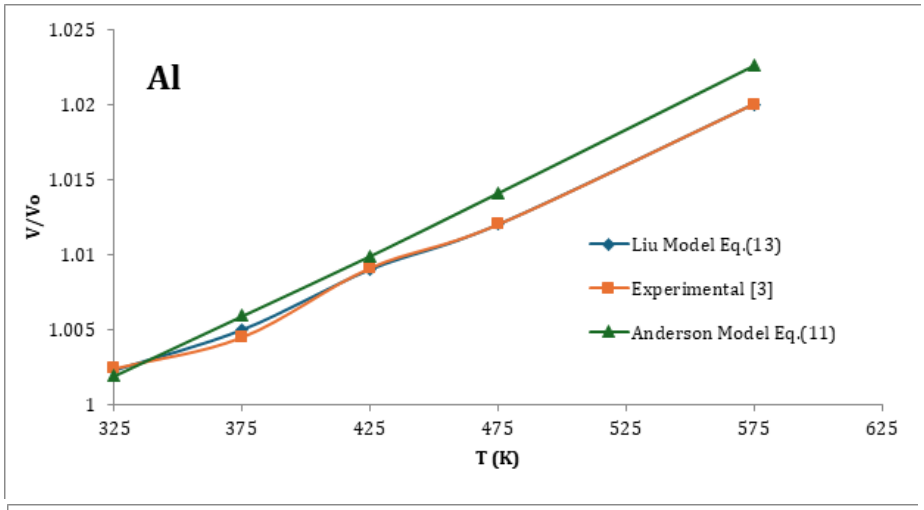

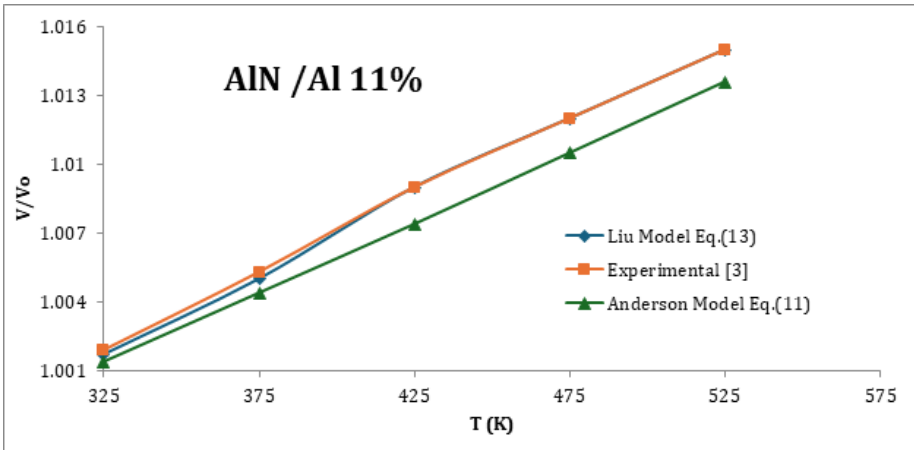

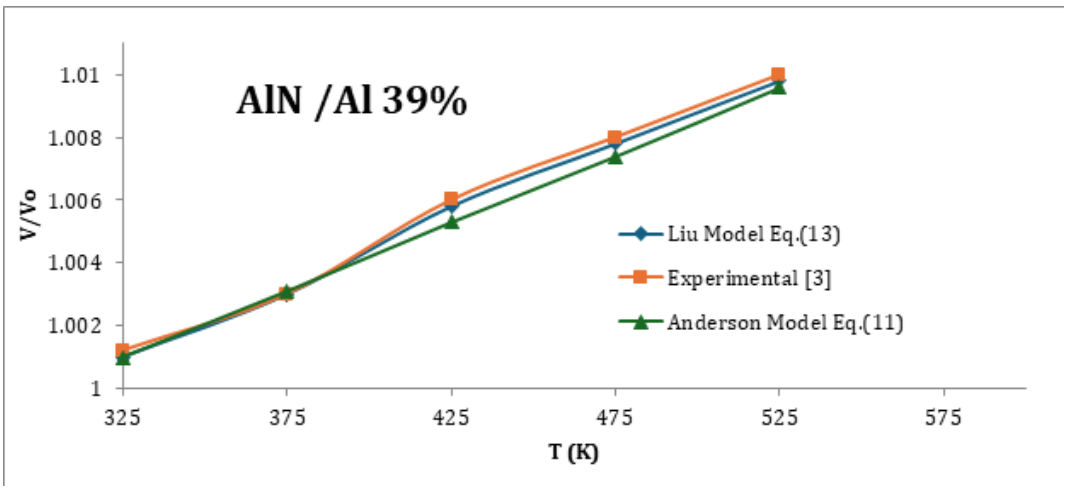

Figure 3:

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