Title: Crystallinity, Magnetic and Electrical Properties of Doped Perovskite-Oxid

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Abstract: Sepiedeh Pirasteh

Crystallinity, Magnetic and Electrical Properties of Doped Perovskite-Oxid ($LaVO_3$)

Sepiedeh Pirasteh

Supervisor: Prof. F. Razavi

Contents:

- Introduction of Perovskite Oxide
- Bi as doping element
- Method of the Preparation
- Crystal Structure Measurement
- Magnetic Measurement
- Resistivity Measurement
- Future works
- Conclusion
- References

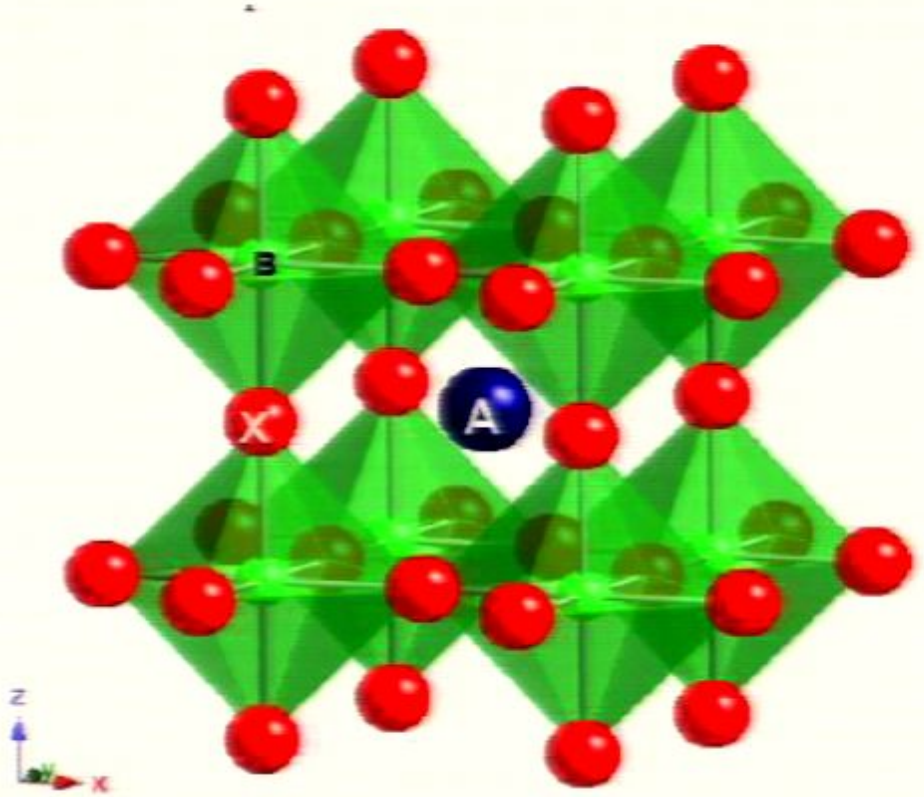
Discovery of high Tc superconductivity in Ba-doped La_2CuO_4 was the reason that study in perovskite arrangement is interesting for research works.

ABO_3

O=oxygen

B=transition metal ion.

A=rare-earth element



The perovskite unit cell.
The **A** ions are on the corners of the cube and the **B** ion is at body center.

The oxygen ions are at face center

Some important properties of LaVO3:

- Above Neel temperature shows Orthorhombic symmetry below this temperature it's considered to be mono-clinic (as reported by R.T.A.Khan.J.Bashir. Materials Letters 58. 1737(2004)).
- Magnetic transition from paramagnetic to anti-ferromagnetic at 140 K when cooled under a high magnetic field.
- Metal-Insulator transition by doping Ca in LaVO3 (as obtained by C.N Hoan.J.B.Goodenough.Phys.Rev.B 52.324(1995))
- Most of perovskite compounds like LaVO3 are able for doping of charge carriers over large rang of compositions without breaking the crystal structure. (K Maiti.N Y Vasanthacharya.J.Phys.Condens.Matter 9.7507-7514(1997))

Doped $LaVO_3$:

- Bi as doping element to substitute at La site :

  Bi is semi-metal element with electron configuration

  Bi_{83}:[Xe]4f14.5d10.**6s2.6p3**

- In $La_{1-x}Bi_xVO_3$ the V3+ is a paramagnetic ion(magnetic ion)with S=1 but La3+ and Bi3+ can't be consider as magnetic ions because spin is zero
- Ionic radius of Bismuth is comparable to ionic radius of A site.

  ionic radius Bi3+ = 1.03 A

  ionic radius La3+ = 1.06 A

- Oxidation state of La and Bi is same, Bi_2O_3, La_2O_3.
- Bi3+ substitution in $LaVO_3$ dopes extra electrons which are not bonded,so some physical properties changes, such as magnetic and electric properties.

Preparation of the ceramic samples of $La_{1-x}Bi_xVO_3$:

- Polycrystalline samples of La1-xBixVO4 were obtained by standard solid reaction in air

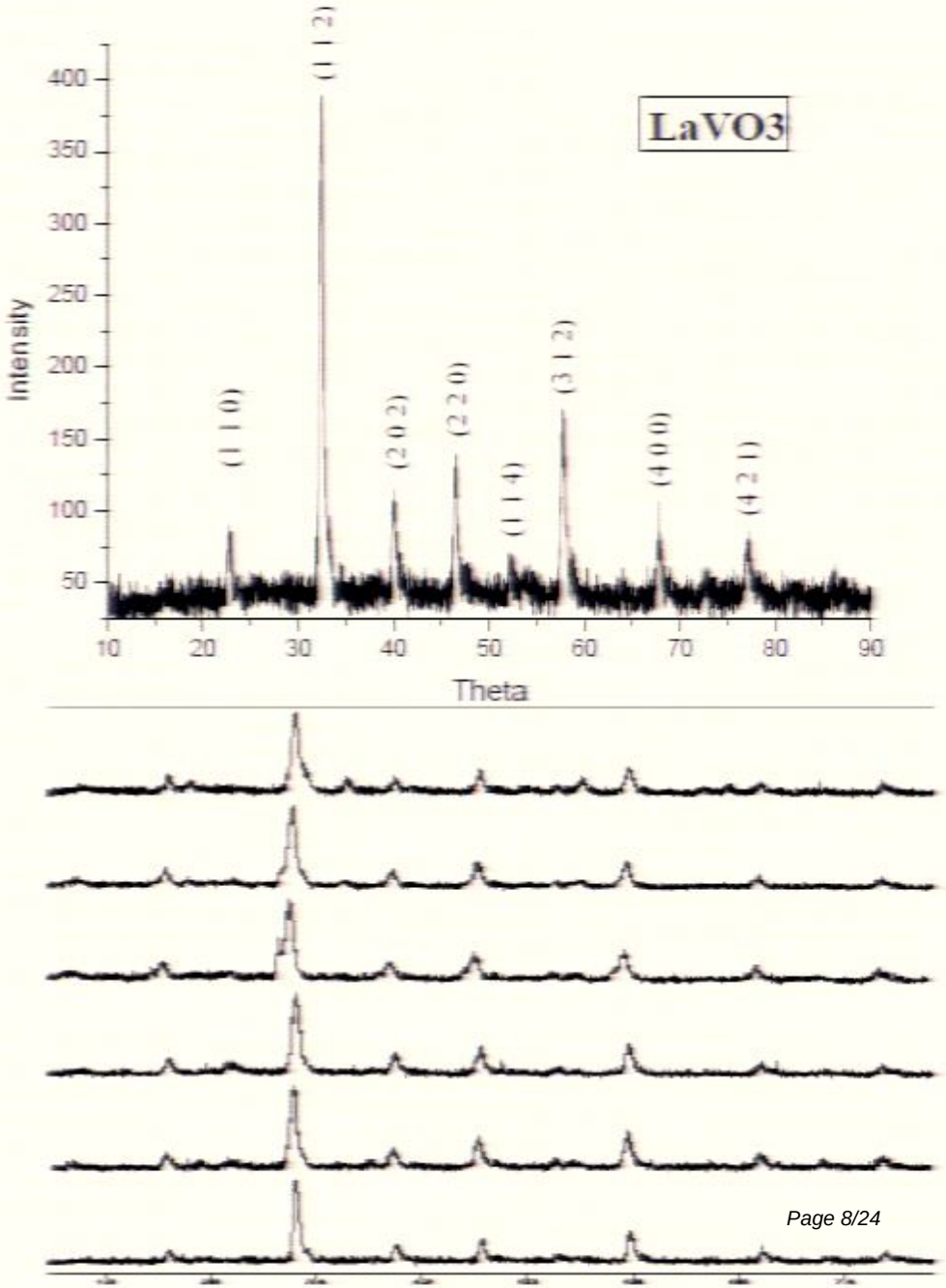
  $(1-x)/2\ La_2O_3 + 1/2\ V_2O_5 + x/2\ Bi_2O_3 \Longrightarrow La_{1-x}Bi_xVO_4$

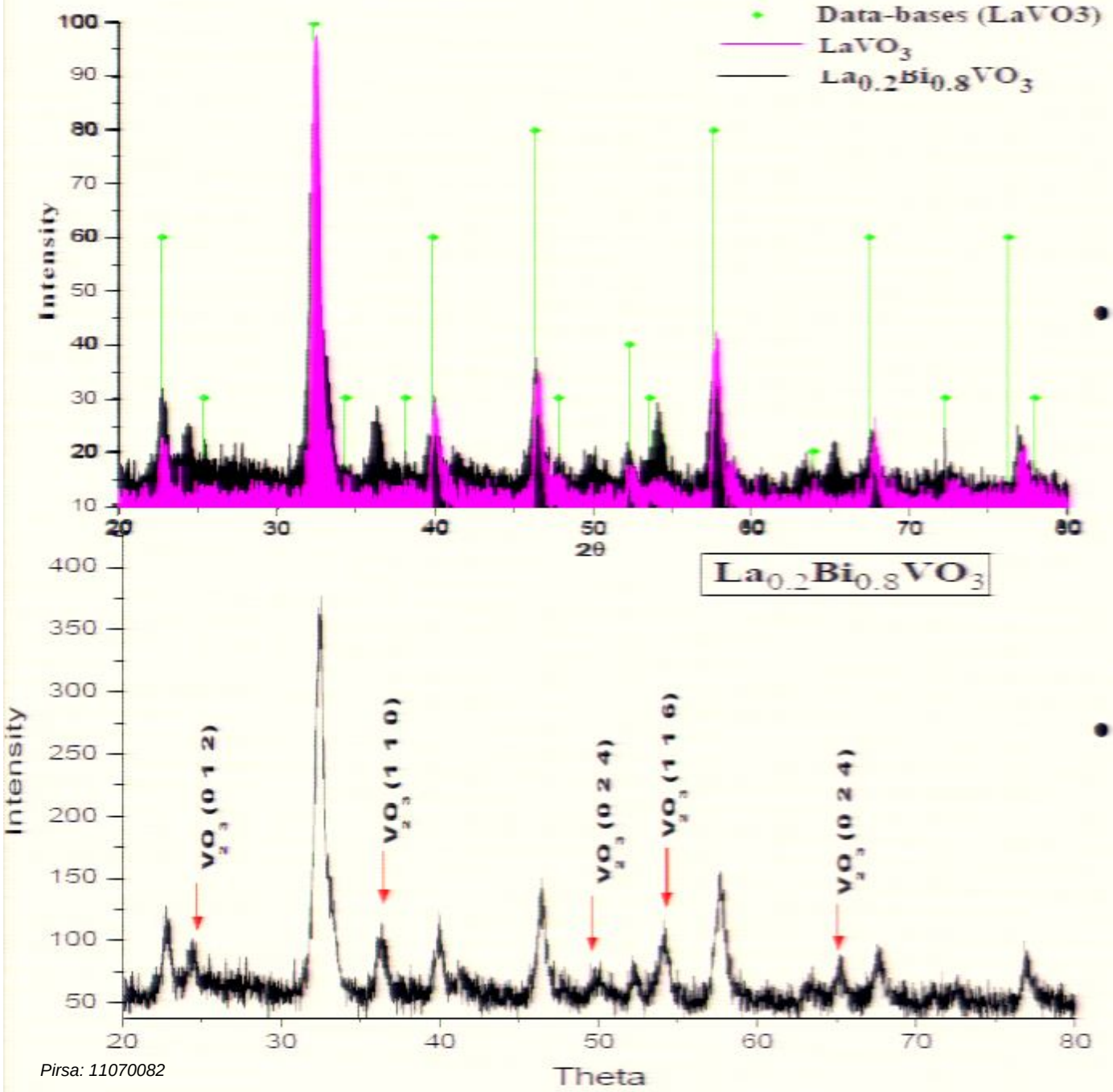
- They were grinded and the powder was pressed into pellets

- To get the $La_{1-x}Bi_xVO_3$ phase, La1-xBixVO4 pellet was prepared by reduction reaction at 1323° K for 10 hours in Argon and Hydrogen(10%) furnace.

Crystal Structure:

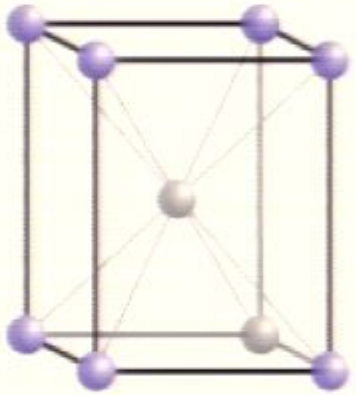
- X-ray diffraction measurement was studied to find crystal structure,
- It is clear that the entry of Bi ions for different context ($x<0.6$) brings no change in the internal structure of crystals.
- Calculation of cell parameters shows that all compounds belong to Tetragonal crystal system. (CuKa: 1.5418A.Reference:Kestigian. J.Am. Chem. Soc. 79.5598(1957) last modification Date:01/24/2009)





- Phase segregation To V_2O_3 and $La_{1-x}Bi_xVO_3$ by doping Bi more than 60 % .
- Crystal Structure is changed at $x \geq 0.6$.

Cell Parameters



Tetragonal structure is found for four samples

α: 90 ß:90 γ:90 a = b ≠ c

Sample	a(°A)	b(°A)	c(°A)	V(°A)
LaVO3	5.63	5.63	7.96	252.31
$La_{0.9}Bi_{0.1}VO3$	5.61	5.61	7.91	248.94
$La_{0.8}Bi_{0.2}VO3$	5.63	5.63	7.93	251.36
$La_{0.6}Bi_{0.4}VO3$	5.62	5.62	7.92	250.15

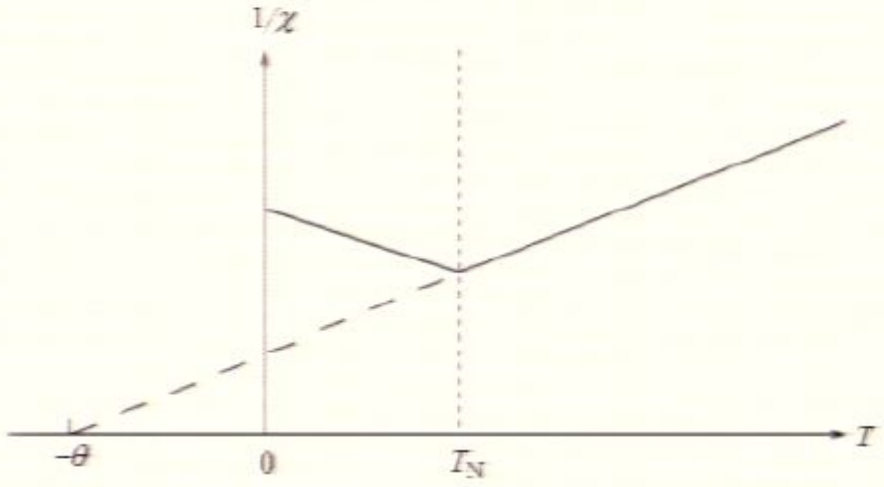
Magnetization Measurement:

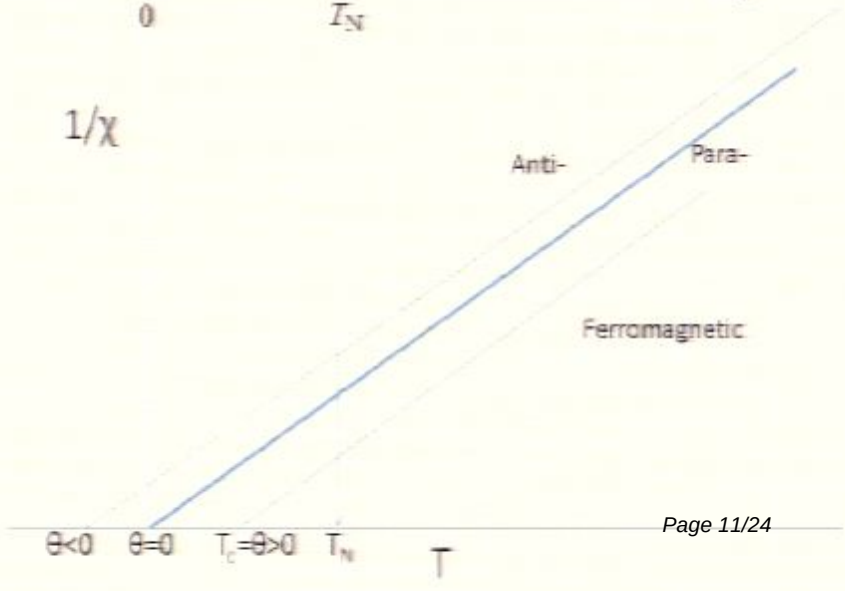
The reason that many researchers are focused on study of perovskite oxide. such as LaVO3. is because of their unusual Electric and Magnetic properties.

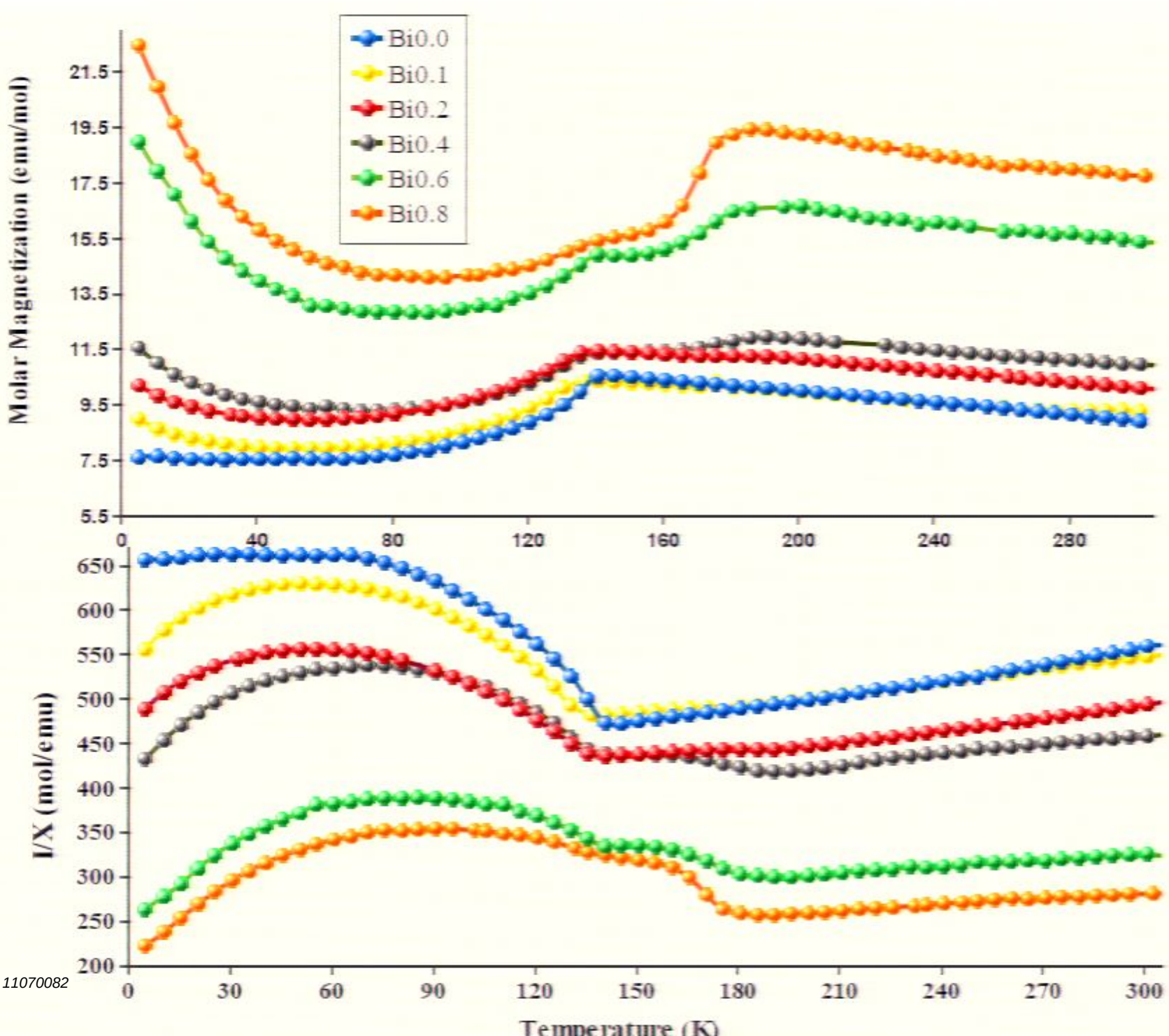
$$\boldsymbol{M} = C\frac{\boldsymbol{H}}{T-\theta}$$

$$\chi = \frac{Ng^2 J(J+1)\mu_B^2}{3k_B T} = \frac{C}{T}.$$

$$\mathbf{1/\chi = T/Cm - \Theta/Cm}$$






Bi0.0
Bi0.1
Bi0.2
Bi0.4
Bi0.6
Bi0.8
Molar Magnetization (emu/mol)
21.5
19.5
17.5
15.5
13.5
11.5
9.5
7.5
5.5
0
40
80
120
160
200
240
280
I/X (mol/emu)
650
600
550
500
450
400
350
300
250
200
0
30
60
90
120
150
180
210
240
270
300
Temperature (K)

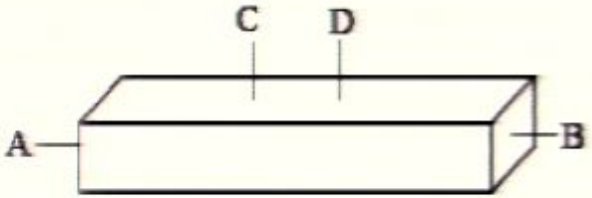
Sample	T_N (°K)	C (emu.K.mol-1)	Θ (°K)	μeff(μB)
LaVO3	≈ 140	1.8022239	-701.9	3.786
La0.9Bi0.1VO3	≈ 140	2.3776689	-997.0	4.348
La0.8Bi0.2VO3	≈ 140	2.0909566	-732.8	4.077
La0.6Bi0.4VO3	≈ 170	2.9309183	-1035.7	4.828
La0.4Bi0.6VO3	≈ 170	4.6232085	-1195.9	6.063
La0.2Bi0.8VO3	≈ 170	4.81602	-1055.7	6.188

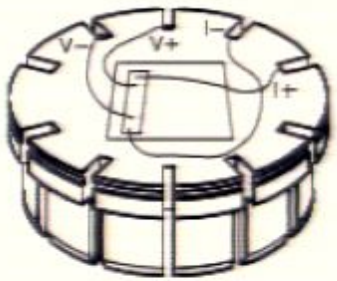
Resistivity Measurement of $La_{1-x}Bi_xVO_3$

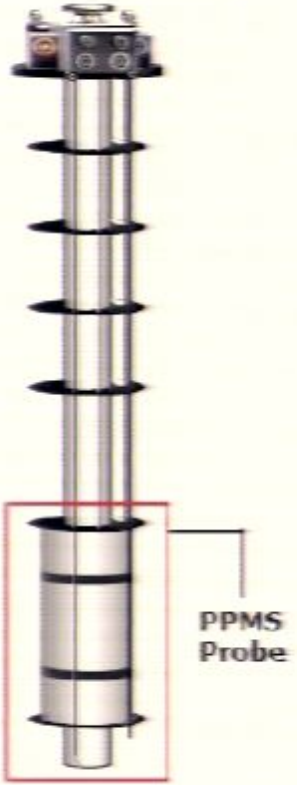
- In order to understand the conductivity properties of ceramic sample,the resistivity measurement was studied at 50 – 400 °K.

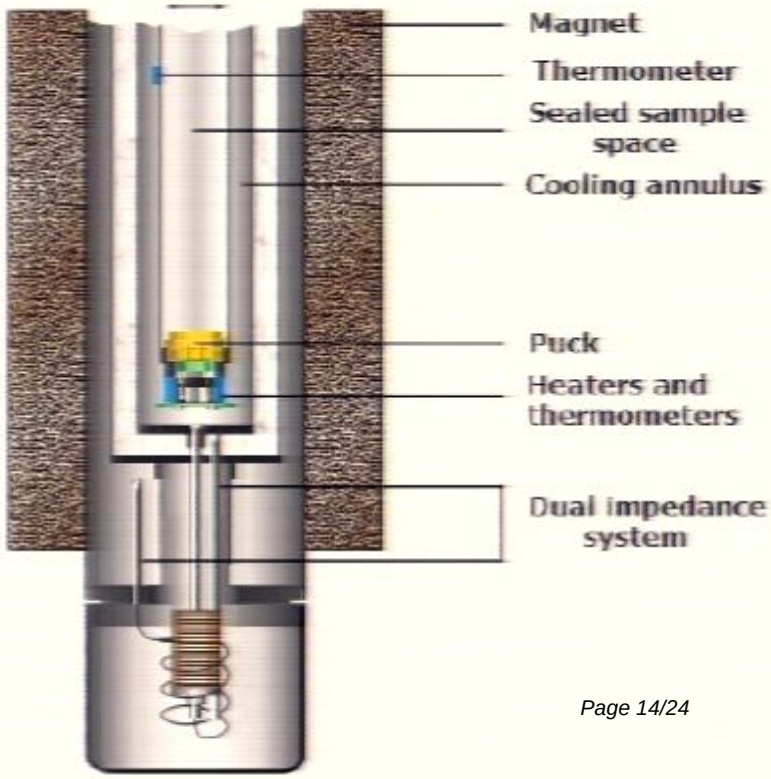
- Physical Properties Measurement System was used by crossing constant current into the sample and using Ohm'law to measure resistance.

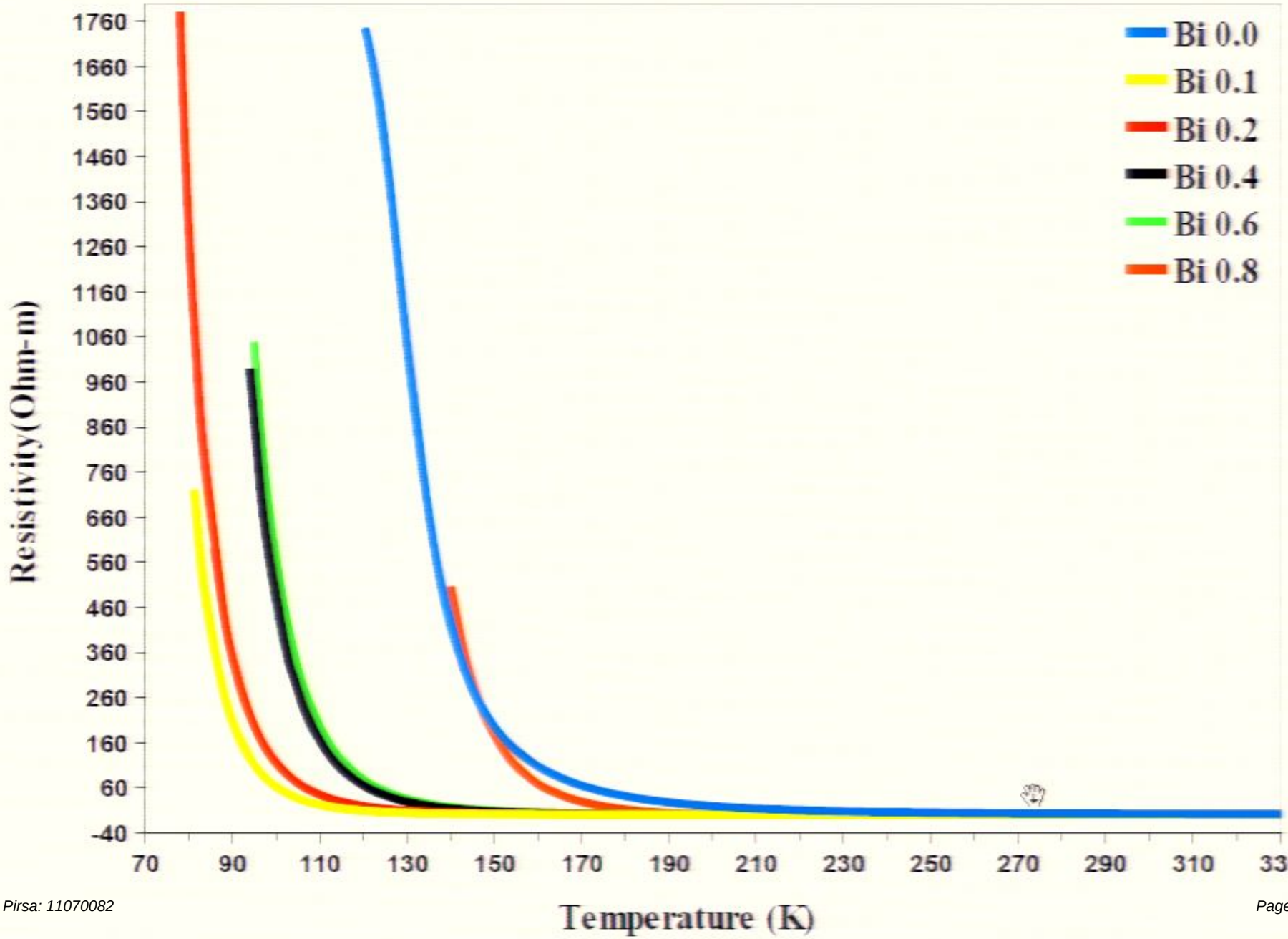
$$\rho = R(A/L)$$









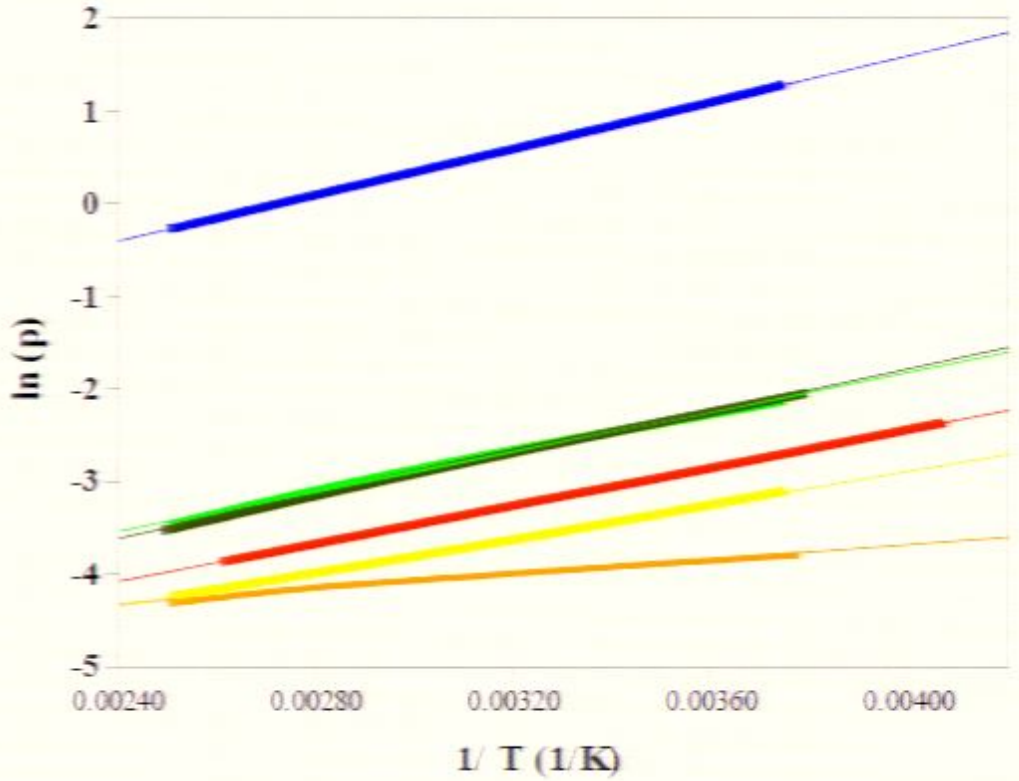

Bi 0.0
Bi 0.1
Bi 0.2
Bi 0.4
Bi 0.6
Bi 0.8
Resistivity(Ohm-m)
1760
1660
1560
1460
1360
1260
1160
1060
960
860
760
660
560
460
360
260
160
60
-40
70
90
110
130
150
170
190
210
230
250
270
290
310
330
Temperature (K)

Energy Gap :

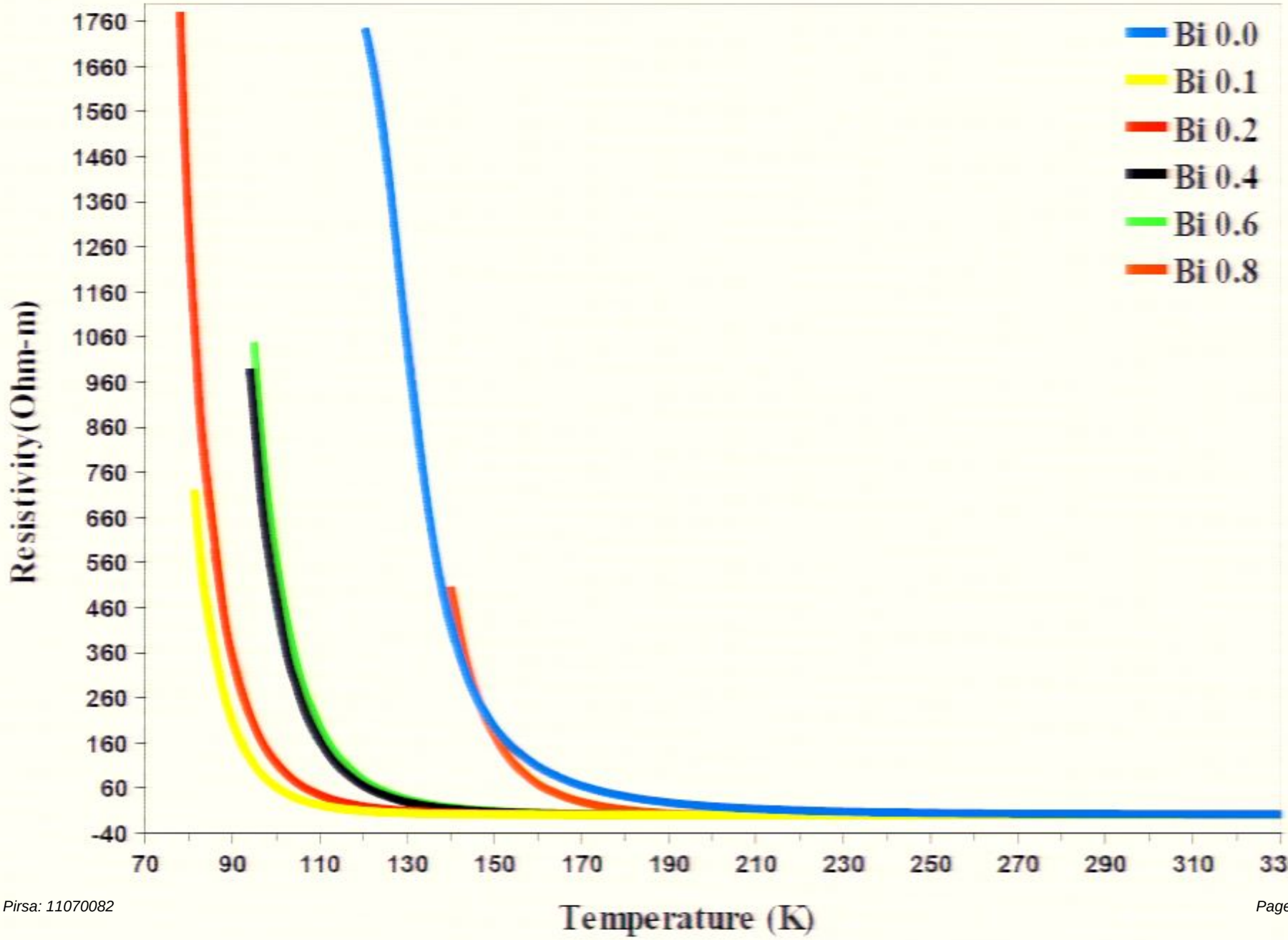
- Temperature dependence at higher values(250-400 K) follows the Arrhenius law and is given by:

$\rho=\rho_0 \exp(E_a/K_B.T)$

$E_g=2E_a$



Sample	LaVO3	La0.9Bi0.1VO3	La0.8Bi0.2VO3	La0.6Bi0.4VO3	La0.4Bi0.6VO3	La0.2Bi0.8VO3
Eg(ev)	0.216	0.157	0.177	0.197	0.185	0.069


Bi 0.0
Bi 0.1
Bi 0.2
Bi 0.4
Bi 0.6
Bi 0.8
Resistivity(Ohm-m)
1760
1660
1560
1460
1360
1260
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960
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760
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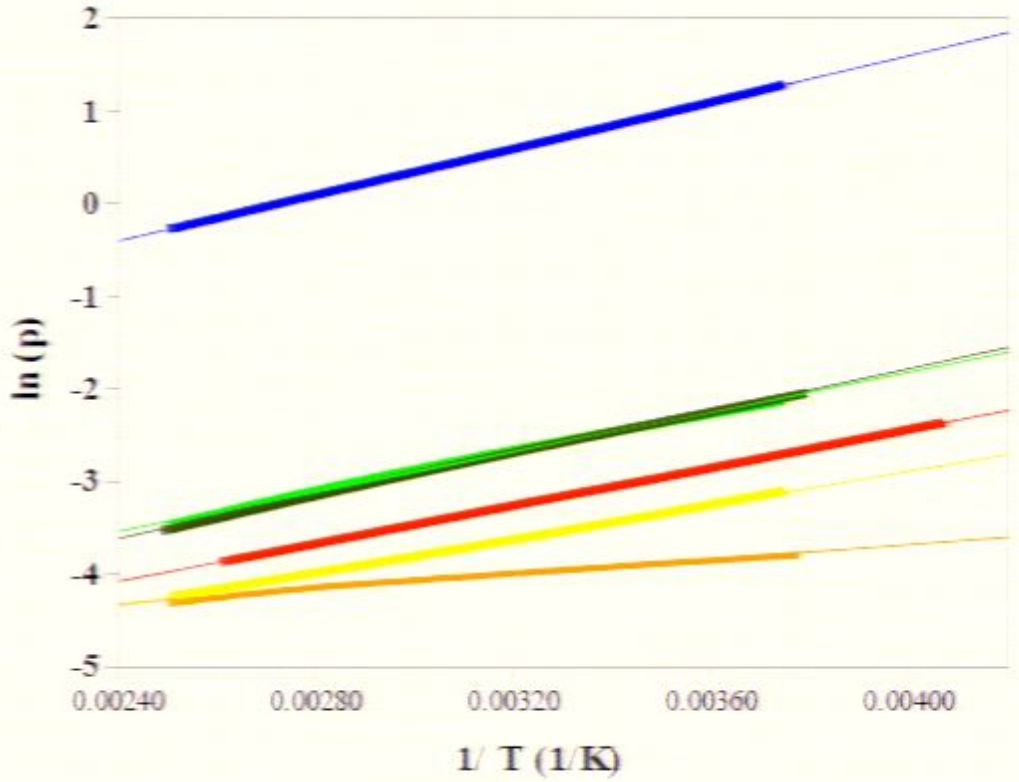

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Eg(ev)	0.216	0.157	0.177	0.197	0.185	0.069

Conclusion:

1. The temperature dependence of conductivity for doped $LaVO_3$ was measured with semiconductor behavior.

2. Neel Temperature was changed by doping Bismuth.

3. Crystal structure is Tetragonal for all concentration of Bismuth less 60%

4. Effective magnetic moment increase by doping more Bi

Next work:

1. Thermal Conductivity Measurement for these compounds due to determine effects of doped $LaVO_3$ to this property.

2. Applicable for electro-thermal devices in which to find high efficiency

References:

1.Mustafa Okutana., Halil I. Bakanb. Kemal Korkmazc. Fahrettin. Yakuphanoglud.Physica B 355 (2005) 176–181.accepted 23 October 2004

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9.Physical Property Measurement System.Resistivity Option User's Manual

Thank You

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