Advanced Glass Science
(4016101)

Instructor: Asst.Prof.Dr. Jakrapong Kaewkhao

Course Outine:

Week 3: **Physical properties and advanced measurement/ calculation analysis**

- Density

Structural properties and advanced measurement/calculation analysis

- Molar volume
- FTIR
- XRD

Case studies from international publications

Book: A.K., Varshneya. ***Fundamentals of inorganic glasses***
A., Paul A, ***Chemistry of glasses***
J.E. Shelby, ***Introduction to glass science and technology***

Physical properties and advanced measurement/ calculation analysis

The density of a material is defined as the mass of the substance per unit of volume, or

$$\boxed{\rho = \frac{M}{V}}$$

ρ = Density of the sample (g/cm^3)
M = Mass of the sample (g)
V = Volume of the sample (cm^3)

- If the sample is free of bubbles, voids, or other defects, the calculated density is the *true density* of the material.
- If, however, the sample contains bubbles, which is occasionally the case for glasses, the calculated density will be less than that of the true density and is termed the apparent density.

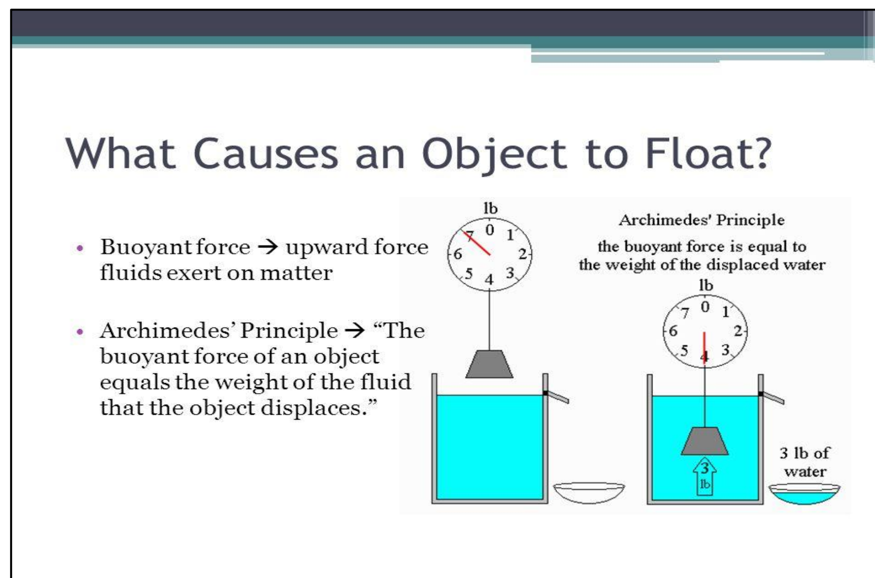
If the available samples do not have geometrics, we can use *Archimedes' principle* to determine the volume by liquid displacement.

$$\rho = \left(\frac{W_{air}}{W_{air} - W_{liquid}}\right) \times \rho_{liquid}$$

ρ	=	Density of glass (g/cm^3)
W_{air}	=	Weight of sample in air (g)
W_{liquid}	=	Weight of sample in liquid (g)
ρ_{liquid}	=	Density of liquid (g/cm^3)

*Generally accurate to ±0.001 g/cm^3

Analytical Balance
4 digit



Structural properties and advanced measurement/ calculation analysis (*Molar volume*)

The molar volume is defined as the volume occupied by one mole of a material and is obtained by dividing the molecular weight of a material by its density, or

$$\boxed{V_m = \frac{MW}{\rho}}$$

V_m = Molar volume of the sample (cm^3/mol)
MW = Molecular weight of the sample (g/mol)
ρ = Density of the sample (g/cm^3)

Where $MW = x_{Na_2O}z_{Na_2O} + x_{CaO}z_{CaO} + x_{SiO_2}z_{SiO_2} + x_{Cr_2O_3}z_{Cr_2O_3}$

X = mole of constituent oxide
Z = molecular weight of constituent oxide

Structural properties and advanced measurement/ calculation analysis (*FTIR*)

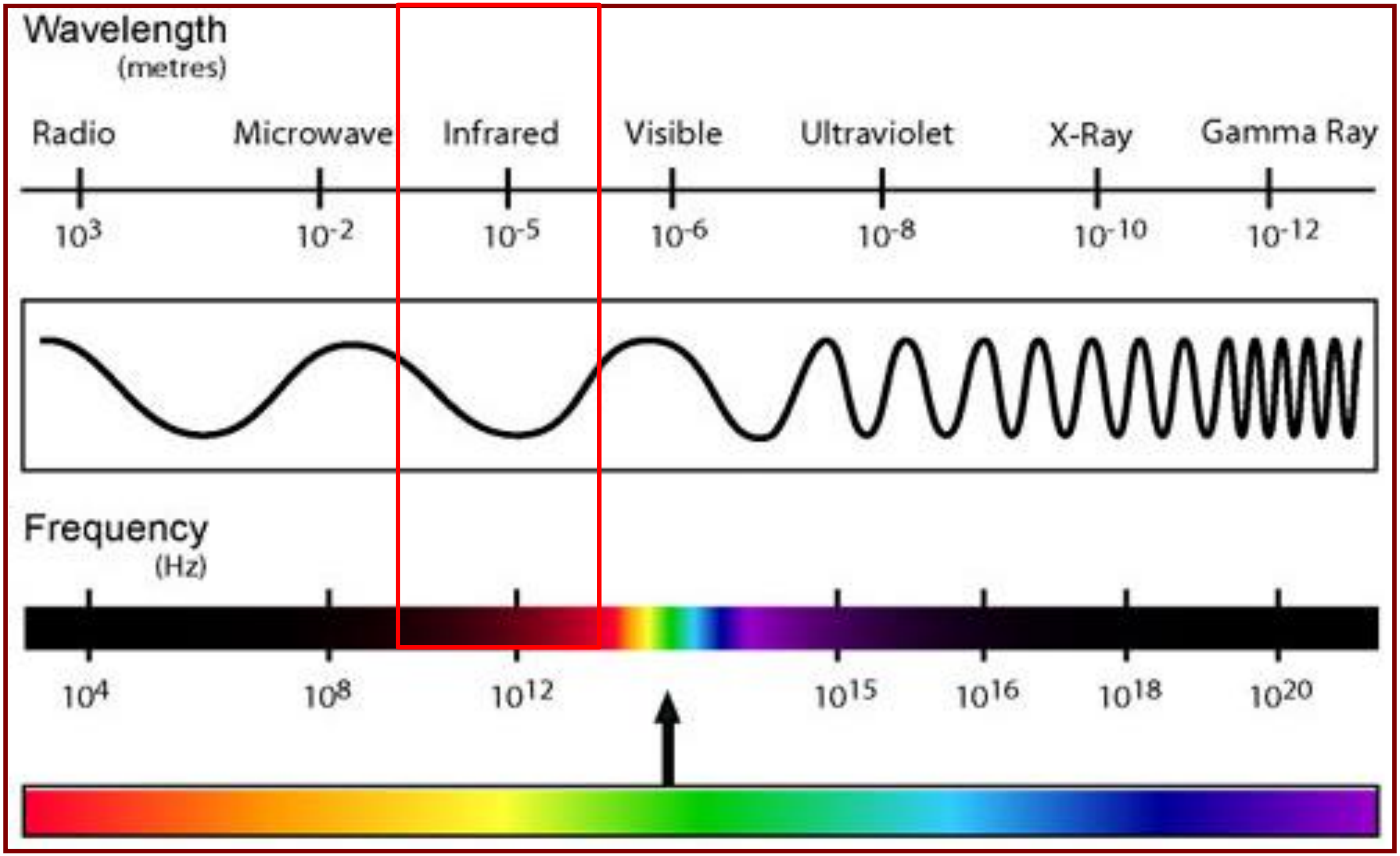


Fig. 1 Electromagnetic Spectrum

Structural properties and advanced measurement/ calculation analysis (*FTIR*)

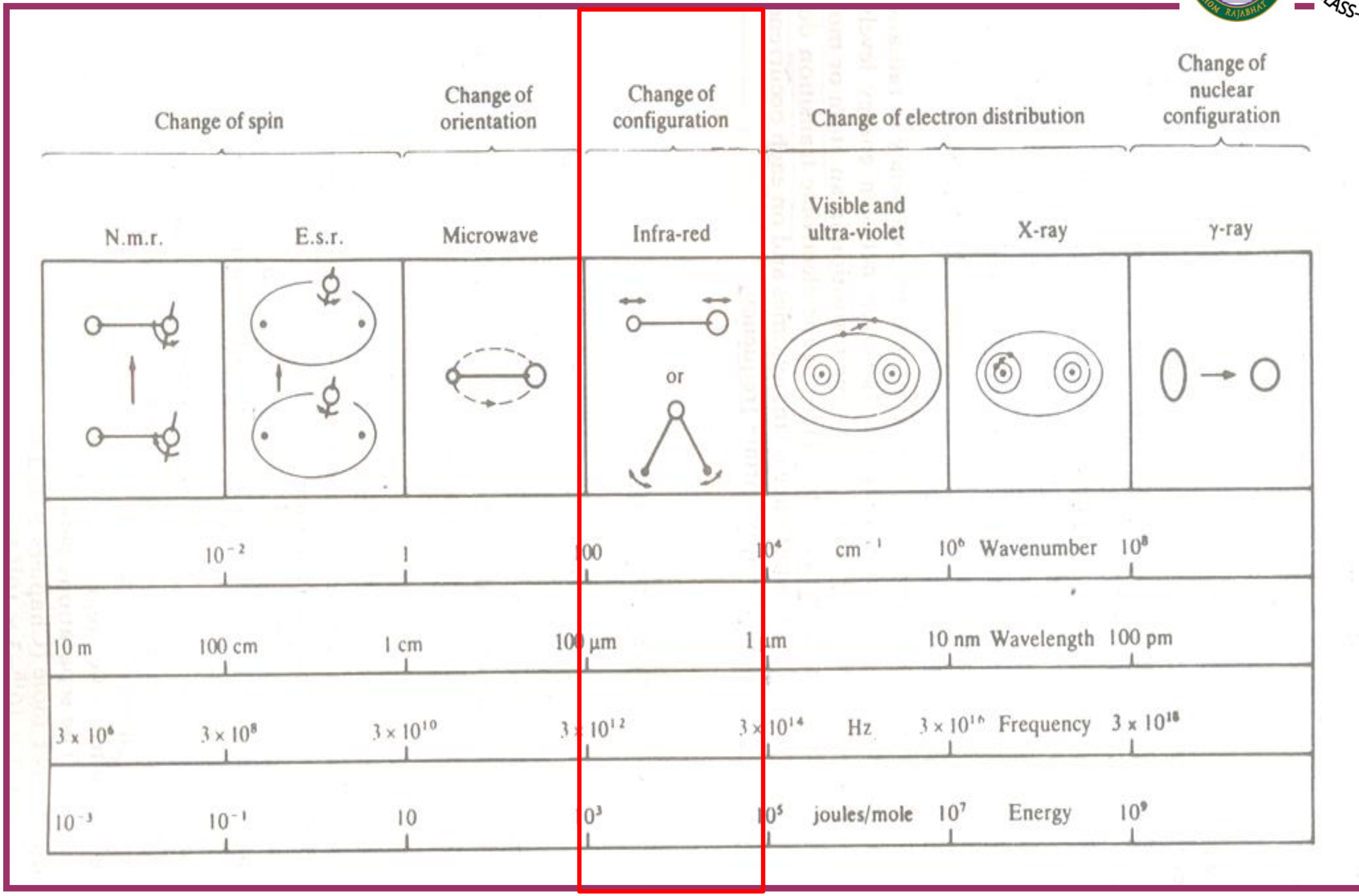


Fig. 2 Various regions of the Electromagnetic spectrum

Structural properties and advanced measurement/ calculation analysis (*FTIR*)

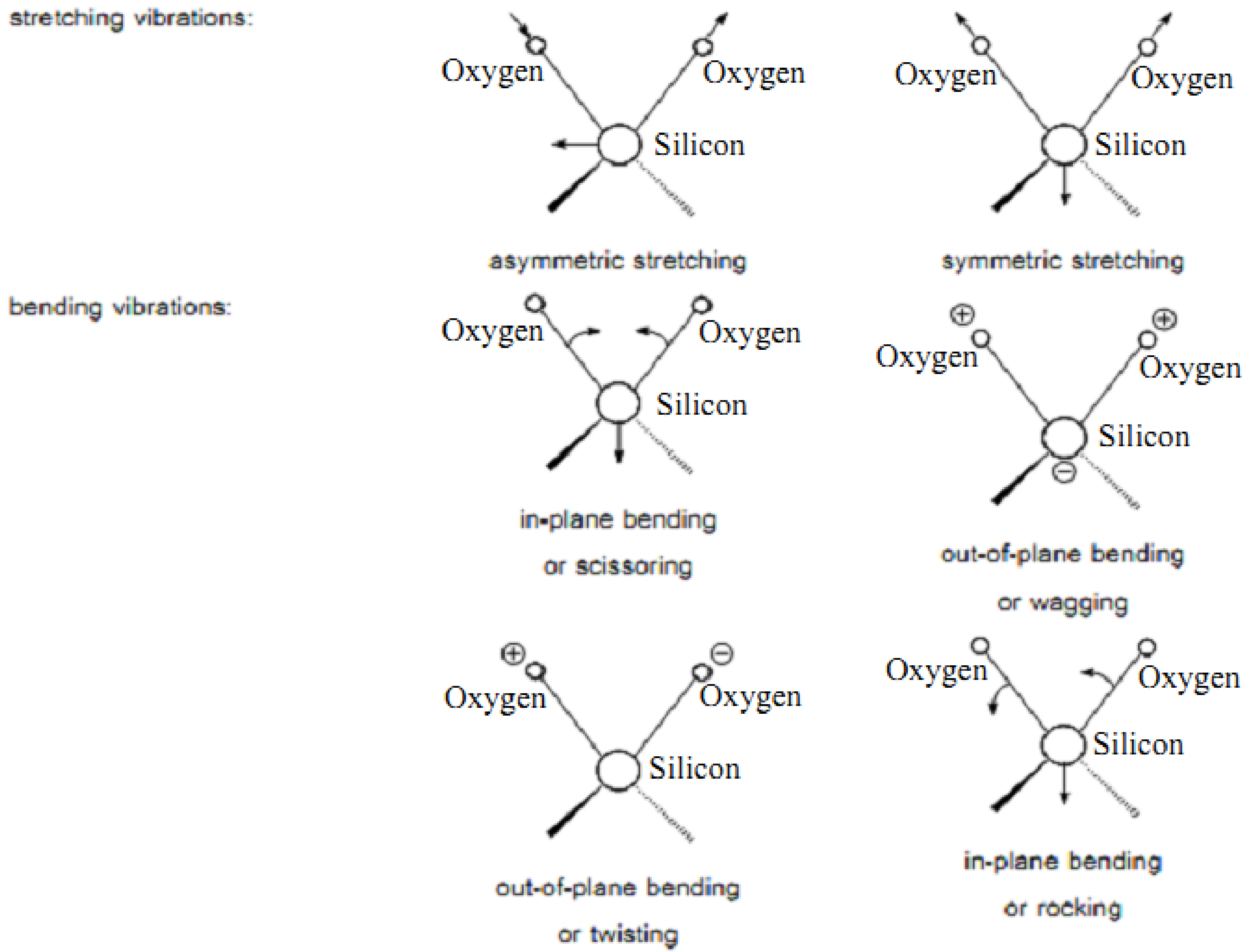


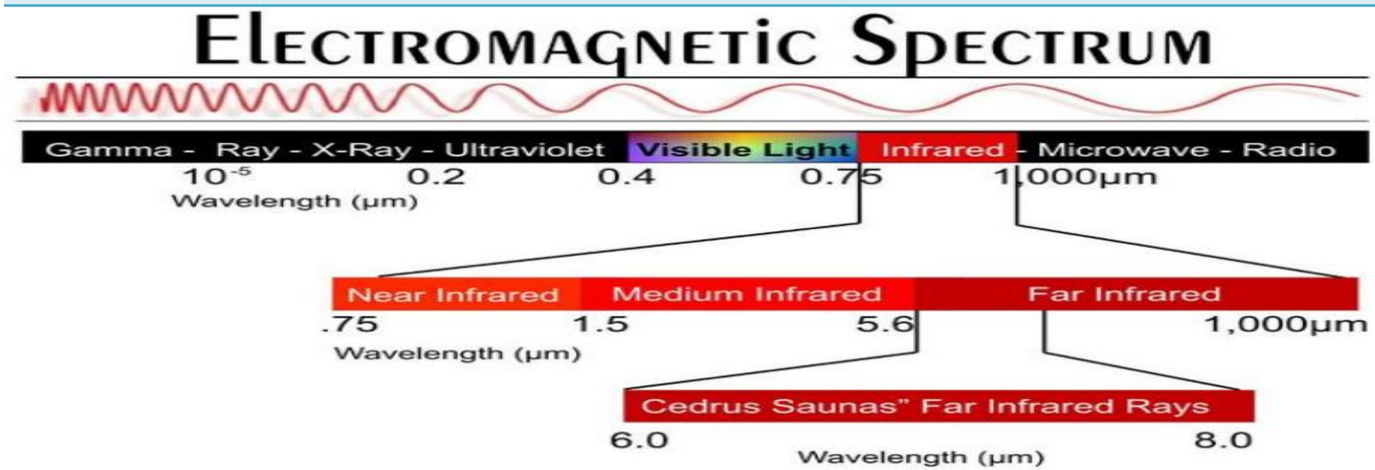
Fig. 3 The stretching and bending of SiO_2 group

Structural properties and advanced measurement/ calculation analysis (*FTIR*)

-Structural ideas: Can determine what chemical groups are in a specific compound

-Unit: Wavenumber (cm^{-1})

Region	Wavelength range (nm)	Wavenumber range (cm^{-1})
Near	780-2500	12800-4000
Middle	2500-50000	4000-200
Far	50000-1000000	200-10



Structural properties and advanced measurement/ calculation analysis (*XRD*)

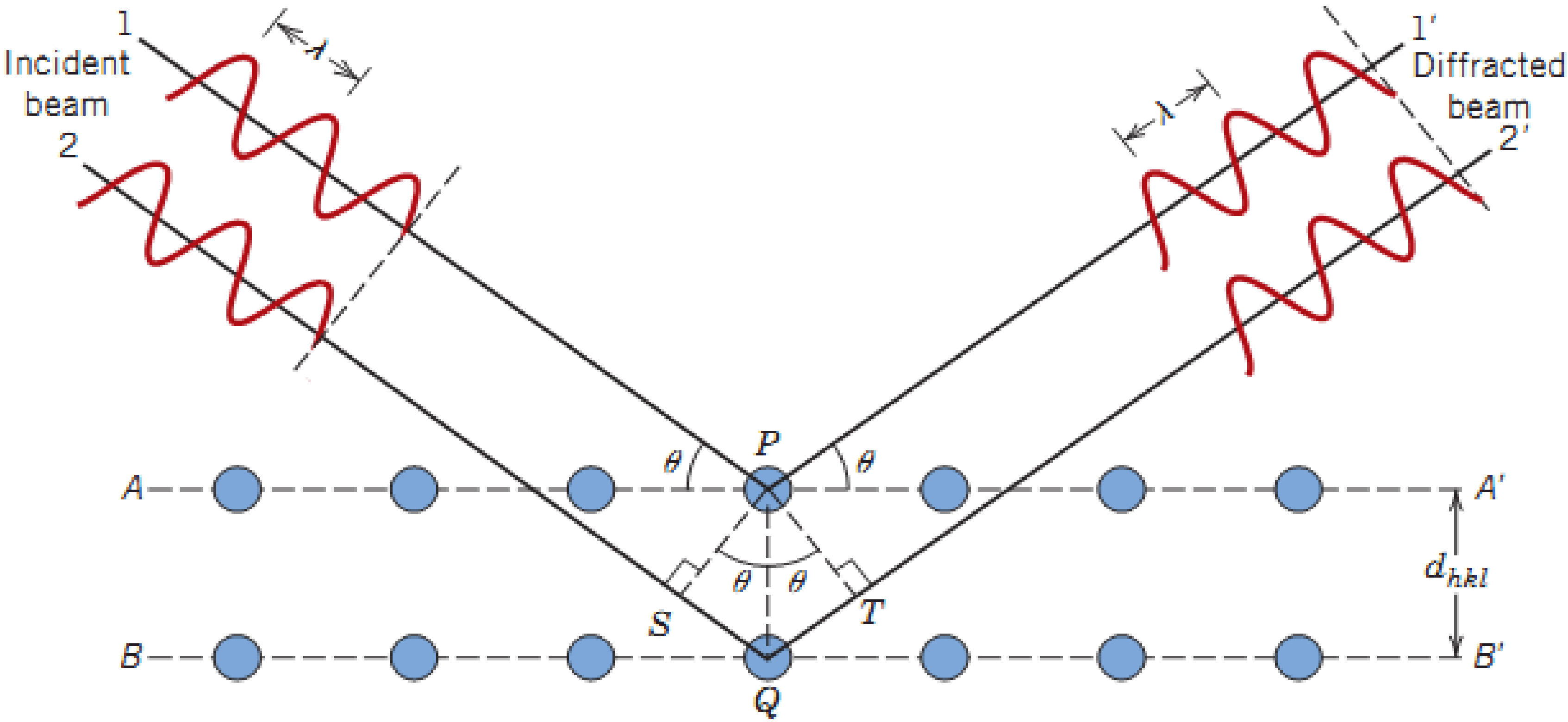


Fig. 4 Diffraction of x-rays by planes of atoms

Structural properties and advanced measurement/ calculation analysis (*XRD*)

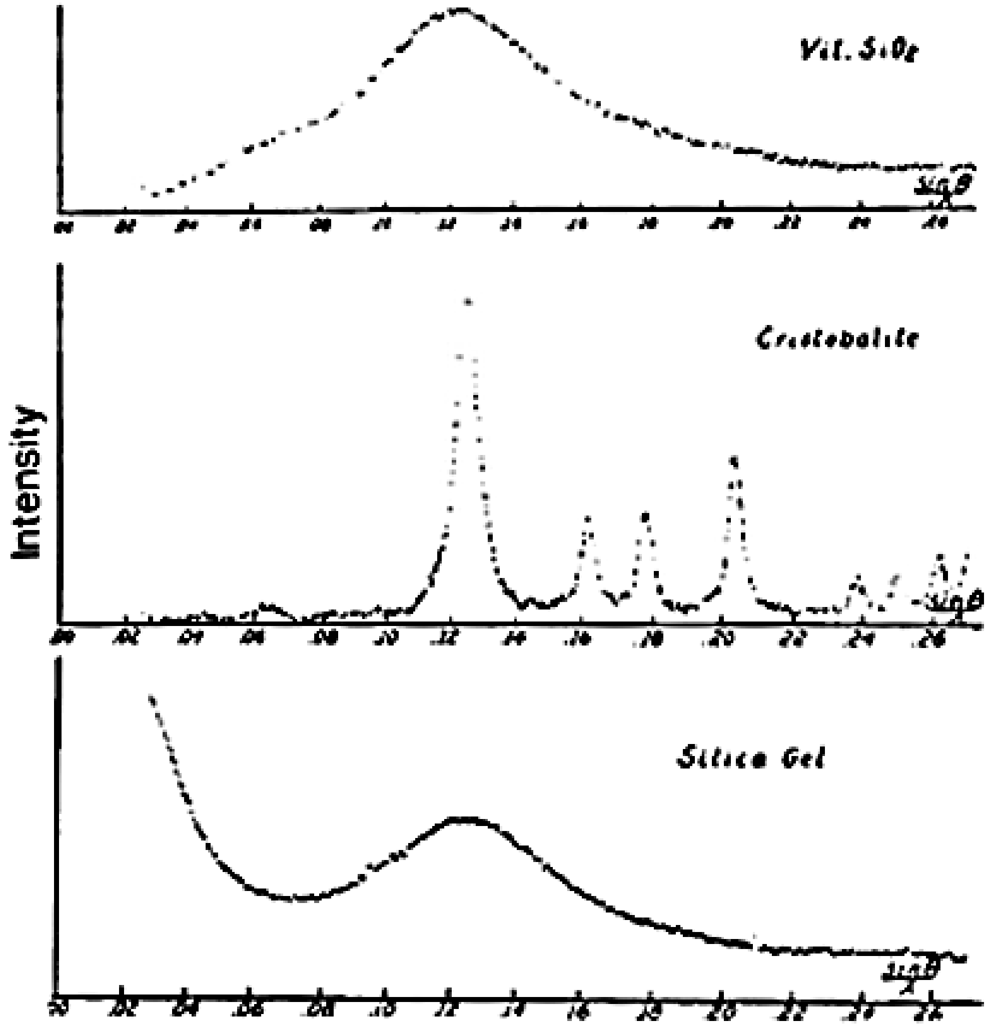


Fig. 5 Microphotometer record of x-ray diffraction patterns of vitreous silica, cristobalite, and dried silica gel

Case studies from international publications

Case 1

Advanced Materials Research Vol. 979 (2014) pp 98-101

doi:10.4028/www.scientific.net/AMR.979.98

Structural and optical properties of Ho^{3+} doped $ZnO\text{-}Bi_2O_3\text{-}B_2O_3$ glasses

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Case studies from international publications

- Composition: $10.0ZnO - 30.0Bi_2O_3 - (60.0\text{-}x)B_2O_3 - xHo_2O_3$ where x = 0.0, 0.2, 0.4, 0.6, 0.8 and 1.0 mol%
- MW of B_2O_3 = 69.6202 g/mol
- MW of Ho_2O_3 = 377.8588 g/mol

Ho_2O_3 concentrations (% mol)	0.0	0.20	0.40	0.60	0.80	1.0
Average molecular weight M_T (g)	189.6978	190.3142	190.9307	191.5472	192.1637	192.7801
Density ρ (g/cm^3)	3.9570	4.0033	4.0584	4.0680	4.0986	4.1540

$$V_m = \frac{MW}{\rho}$$

$$0.00\ \text{mol\%}\ ;\ V_m = \frac{189.6978}{3.9570} = 47.9398\ \text{cm}^3/\text{mol}$$

$$0.20\ \text{mol\%}\ ;\ V_m = \frac{190.3142}{4.0033} = 47.5393\ \text{cm}^3/\text{mol}$$

$$0.40\ \text{mol\%}\ ;\ V_m = \frac{190.9307}{4.0584} = 47.0458\ \text{cm}^3/\text{mol}$$

$$0.60\ \text{mol\%}\ ;\ V_m = \frac{191.5472}{4.0680} = 47.0863\ \text{cm}^3/\text{mol}$$

$$0.80\ \text{mol\%}\ ;\ V_m = \frac{192.1637}{4.0986} = 46.8852\ \text{cm}^3/\text{mol}$$

$$0.10\ \text{mol\%}\ ;\ V_m = \frac{192.7801}{4.1540} = 46.4083\ \text{cm}^3/\text{mol}$$

Case studies from international publications

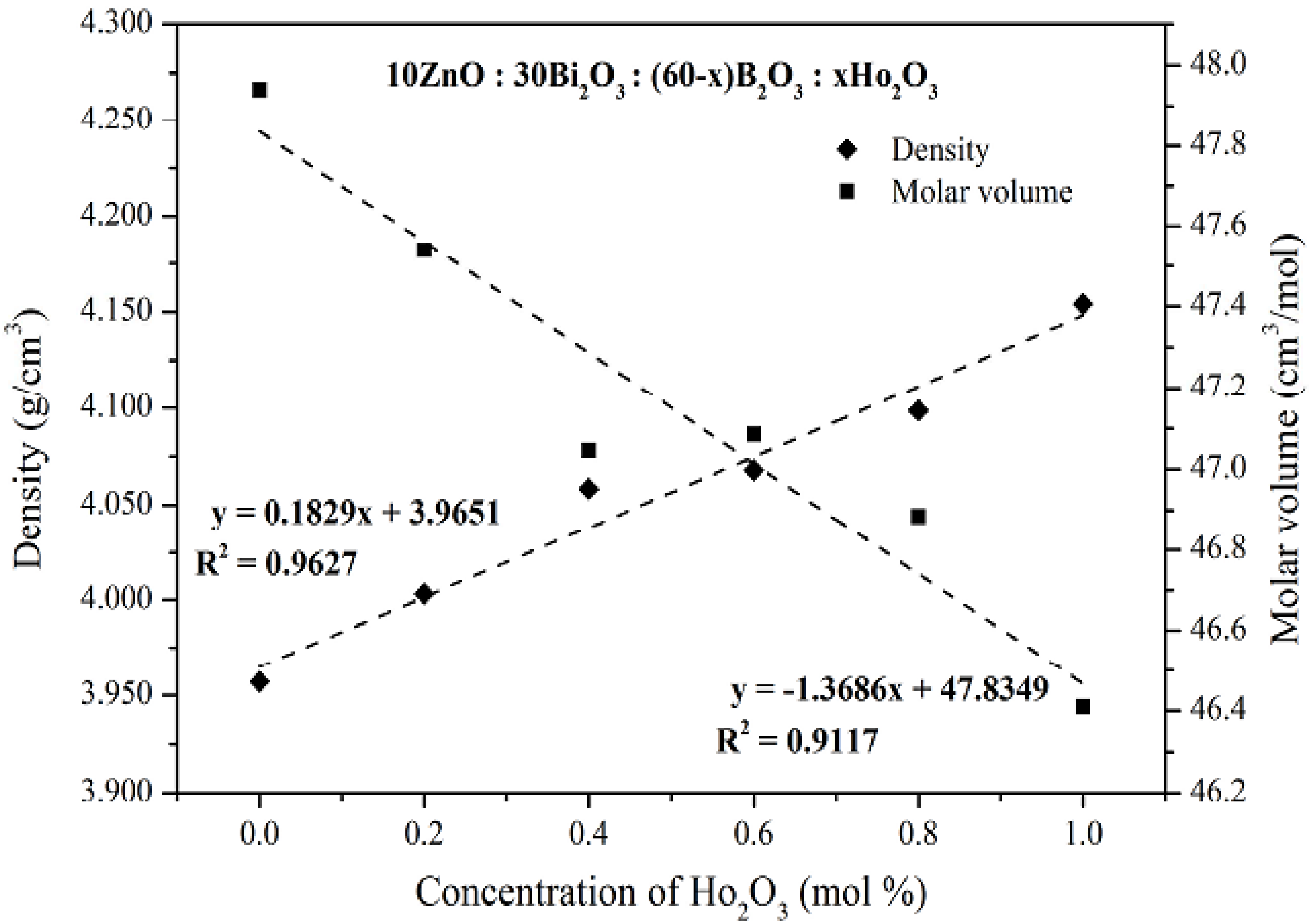

Fig. 6 Density and molar volume of $10.0ZnO : 30.0Bi_2O_3 : (60.0\text{-}x)B_2O_3 : xHo_2O_3$ glass system

Case studies from international publications

Case 2

Journal of Physics and Chemistry of Solids 71 (2010) 965–970

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

ELSEVIER

Optical and electronic polarizability investigation of Nd^{3+}-doped soda-lime silicate glasses

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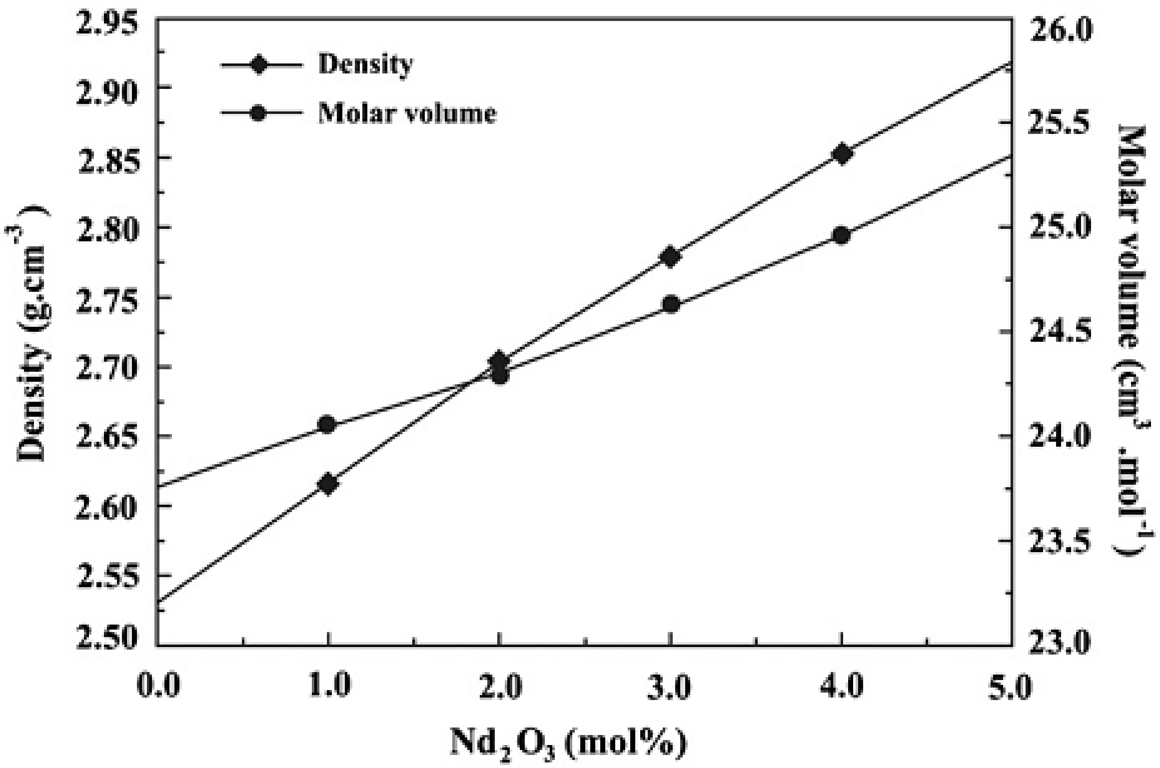
Case studies from international publications

- Composition: $25Na_2O$ - $10CaO$ - $(65\text{-}x)SiO_2$ - xNd_2O_3 where x = 0.00, 1.00, 2.00, 3.00, 4.00 and 5.00 mol%
- MW of SiO_2 = 60.0843 g/mol
- MW of Ho_2O_3 = 377.8588 g/mol



$$\boxed{V_m = \frac{MW}{\rho}}$$

NBO ↑

Fig. 7 Variation in the density and molar volume with Nd_2O_3 concentration

Case studies from international publications

Case 3

Journal of Physics and Chemistry of Solids 72 (2011) 245–251

Contents lists available at ScienceDirect

Journal of Physics and Chemistry of Solids

journal homepage: www.elsevier.com/locate/jpcs

Physical, optical, structural and gamma-ray shielding properties of lead sodium borate glasses

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Case studies from international publications

- Composition: $xPbO - 20Na_2O - (80-x)B_2O_3$ where x = 5, 10, 15, 20, 25, 30, 35, 40, 45, 50 and 55 mol%
- MW of B_2O_3 = 69.6202 g/mol
- MW of PbO = 223.1994 g/mol

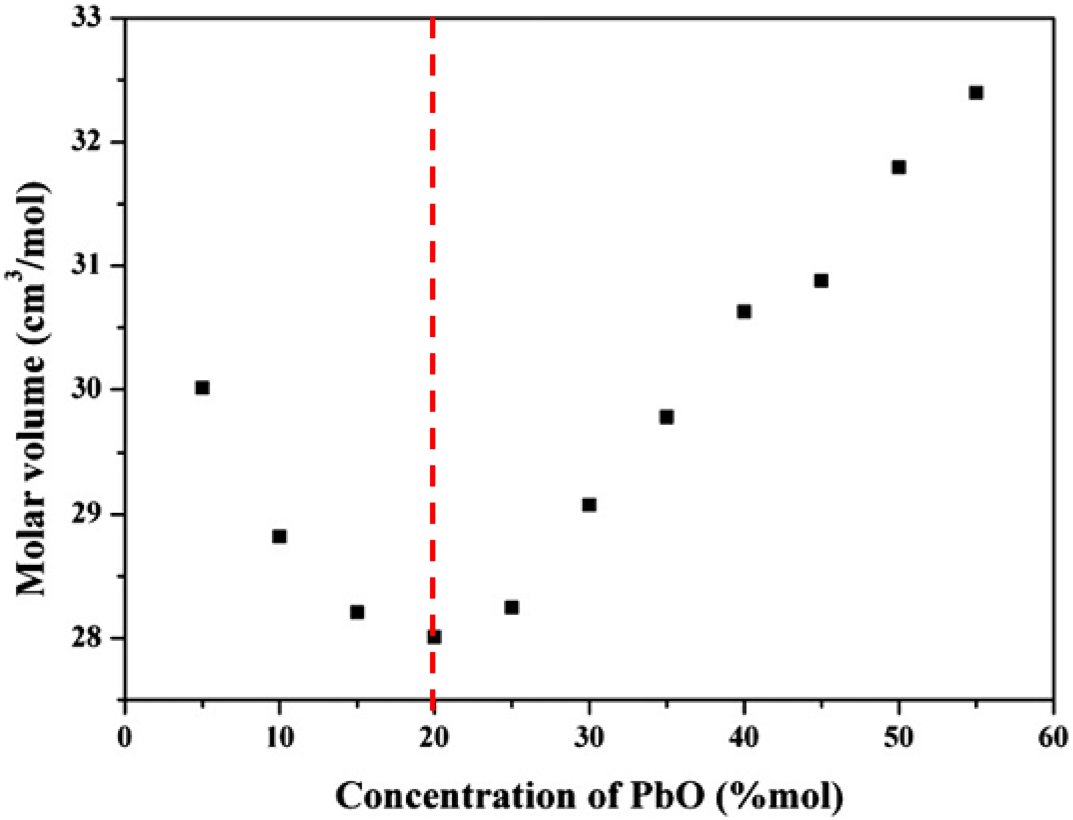

Fig. 8 Molar volume of lead sodium borate glasses

- 5-20 mol% PbO act as a ***network former***
- Beyond 20 mol% PbO act as ***a modifier***

Case studies from international publications

Case 4

Hindawi Publishing Corporation
Advances in Materials Science and Engineering
Volume 2014, Article ID 751973, 5 pages
http://dx.doi.org/10.1155/2014/751973

Research Article

Up- and Downconversion Luminescence Properties of Nd^{3+} Ions Doped in Bi_2O_3–BaO–B_2O_3 Glass System

R. Ruamnikhom,[1] P. Limsuwan,[1] M. Horprathum,[2] N. Chanthima,[3] H. J. Kim,[4] S. Ruengsri,[5] and J. Kaewkhao[3]

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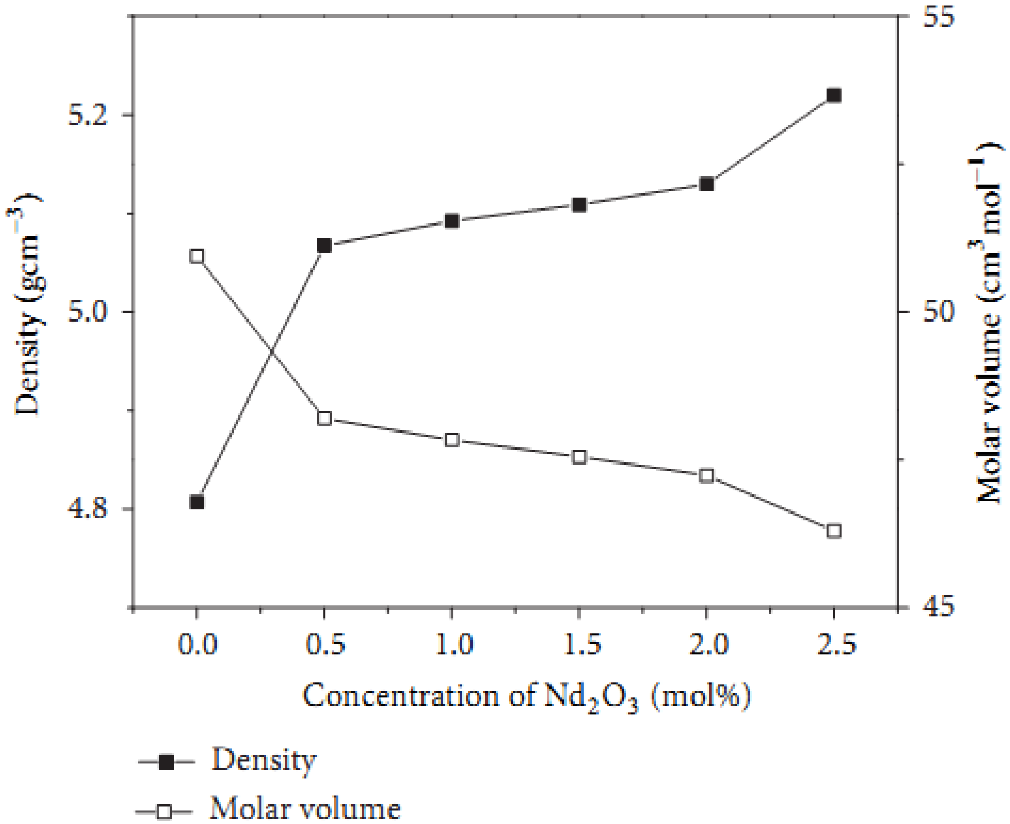
Case studies from international publications

- Composition: $40Bi_2O_3$-$20BaO$-$(40-x)B_2O_3$-xNd_2O_3 where x = 0.0, 0.5, 1.0, 1.5, 2.0 and 2.5 mol%
- MW of B_2O_3 = 69.6202 g/mol
- MW of PbO = 223.1994 g/mol



-Density is nonlinearly with increasing with composition of Nd_2O_3 due to different loss rates of Bi_2O_3 at high melting temperature process.

- Molar volume of glasses were decreased composition of Nd_2O_3 due to the decrease of average atomic separation.

Fig. 9 Density and molar volume of Nd^{3+} doped Bi_2O_3-BaO-B_2O_3 glasses

Case 5

Advanced Materials Research Vols. 93-94 (2010) pp 455-458

doi:10.4028/www.scientific.net/AMR.93-94.455

Effect of Nd^{3+} concentration on the Physical and Absorption Properties of Soda-Lime-Silicate Glasses

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Case studies from international publications

- Composition: $25Na_2O$ - $10CaO$ - $(65\text{-}x)SiO_2$ - xNd_2O_3 where x = 0.00, 1.00, 2.00, 3.00, 4.00 and 5.00 mol%

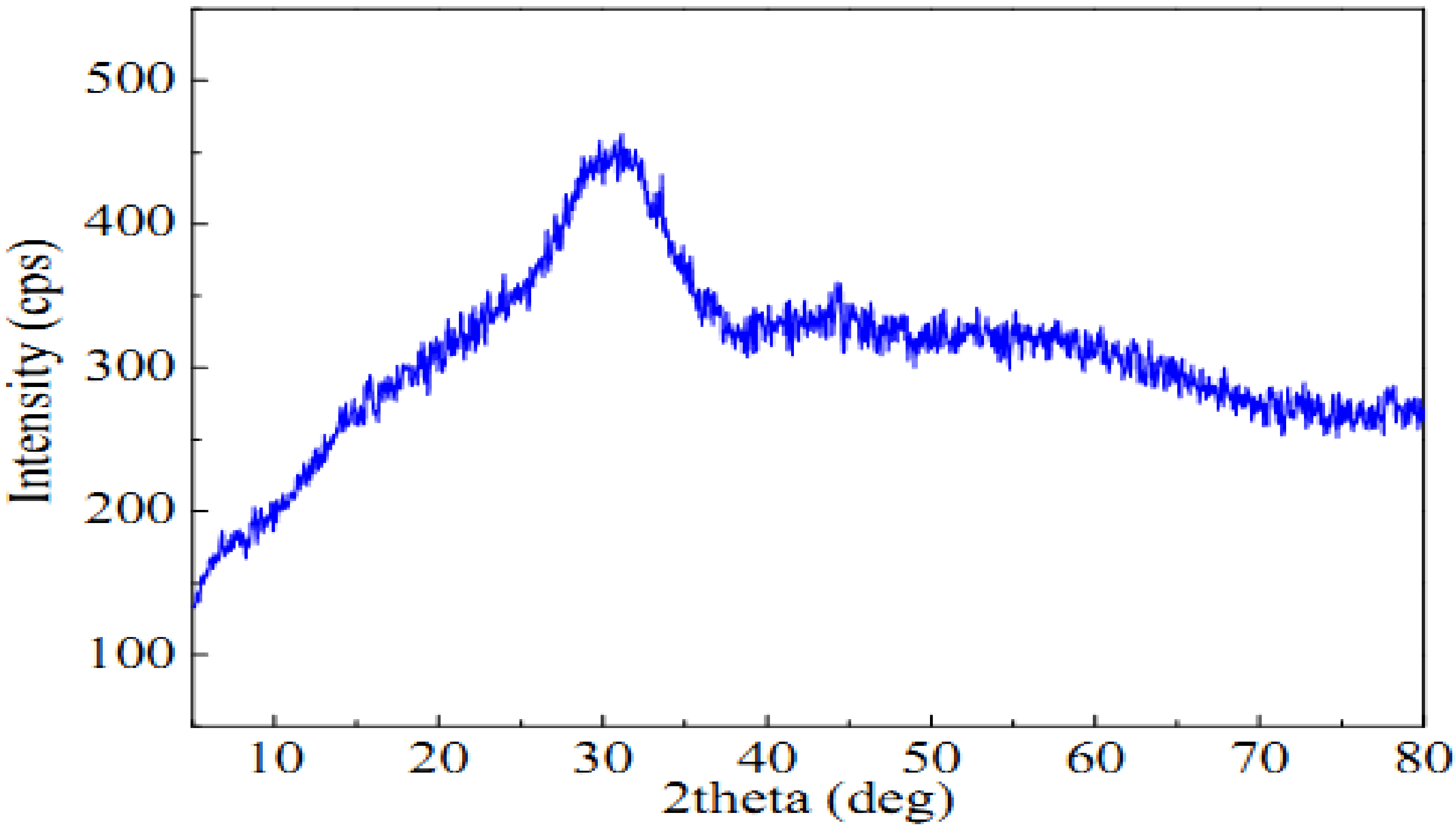

Fig. 10 XRD spectrum of the $25Na_2O$ - $10CaO$ - $65SiO_2$ - Nd_2O_3 glass

Case studies from international publications

Case 6

Advanced Materials Research Vols. 93-94 (2010) pp 439-442

doi:10.4028/www.scientific.net/AMR.93-94.439

Structural Studies of Lead Sodium Borate Glasses

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Case studies from international publications

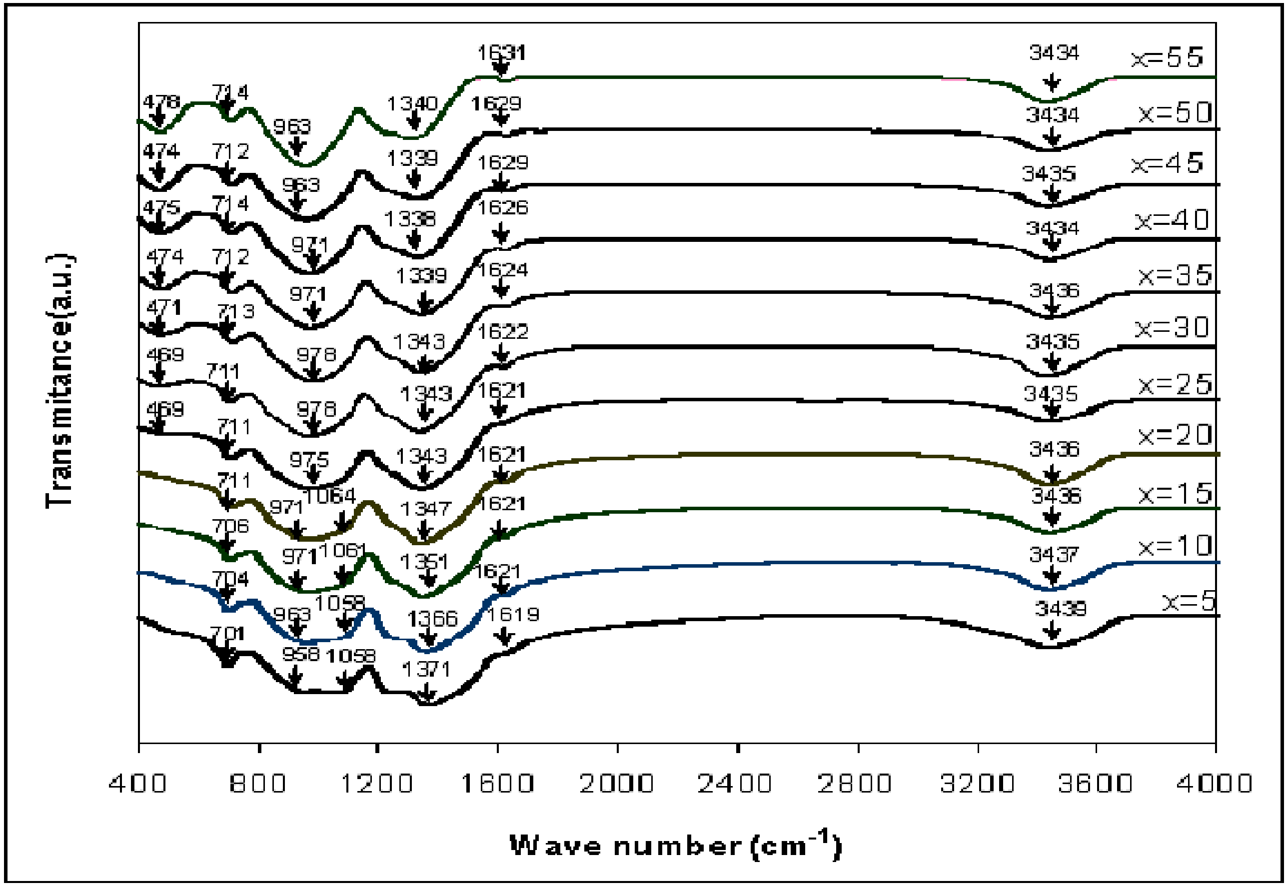
- Composition: $xPbO - 20NaO - (80\text{-}x)B_2O_3$ where x = 5, 10, 15, 20, 25, 30, 35, 40, 45, 50 and 55 mol%

Table 1 Chemical compositions, density and molar volume of glass samples

Composition (%mol)			Density (g/cm^3)	molar volume (cm^3/mol)
PbO(x)	Na_2O	B_2O_3(80-x)		
5	20	75	2.5248	30.011
10	20	70	2.8955	28.820
15	20	65	3.2305	28.209
20	20	60	3.5275	28.010
25	20	55	3.7697	28.248
30	20	50	3.9266	29.074
35	20	45	4.0911	29.782
40	20	40	4.2287	30.629
45	20	35	4.4432	30.878
50	20	30	4.5566	31.795
55	20	25	4.7086	32.400

Case studies from international publications

- Composition: $xPbO - 20NaO - (80-x)B_2O_3$ where x = 5, 10, 15, 20, 25, 30, 35, 40, 45, 50 and 55 mol%



470 cm^{-1} = Pb-O bond
710 cm^{-1} = B-O bending
960 cm^{-1} = B-O streching of BO_4 tetrahedra
1050 cm^{-1} = $[BO_4]$
1350 cm^{-1} = B-O streching of trigonal $(BO_3)^{3-}$
1620 cm^{-1} = H_2O bending
3435 cm^{-1} = OH streching

Fig. 11 Infrared transmission spectra of lead sodium borate glasses

Case studies from international publications

Case 7

Advanced Materials Research Vol. 506 (2012) pp 567-570

doi:10.4028/www.scientific.net/AMR.506.567

Preparation and Properties of Glass Produced from Palm ash

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Case studies from international publications

Table 2 Nominal compositions of palm petiole ash at different calcining temperature in oxide form

Compound	Calcining **Temperature (°C)**			
	400	**600**	**800**	**1000**
MgO	5.90	6.00	9.30	8.40
SiO_2	**65.70**	**67.70**	**60.30**	**65.20**
P_2O_5	2.27	2.43	3.21	0.99
SO_3	1.91	1.81	3.35	0.88
Cl	6.33	4.34	1.95	1.45
K_2O	4.42	4.60	3.67	2.42
CaO	12.4	12.00	15.88	15.97
TiO_2	0.05	0.05	0.07	0.07
MnO	0.72	0.68	0.80	0.84
Fe_2O_3	0.31	0.31	0.43	0.41
CuO	0.02	0.02	0.03	0.06
ZnO	0.02	0.02	0.02	0.02
Al_2O_3	-	-	0.98	0.99

Case studies from international publications

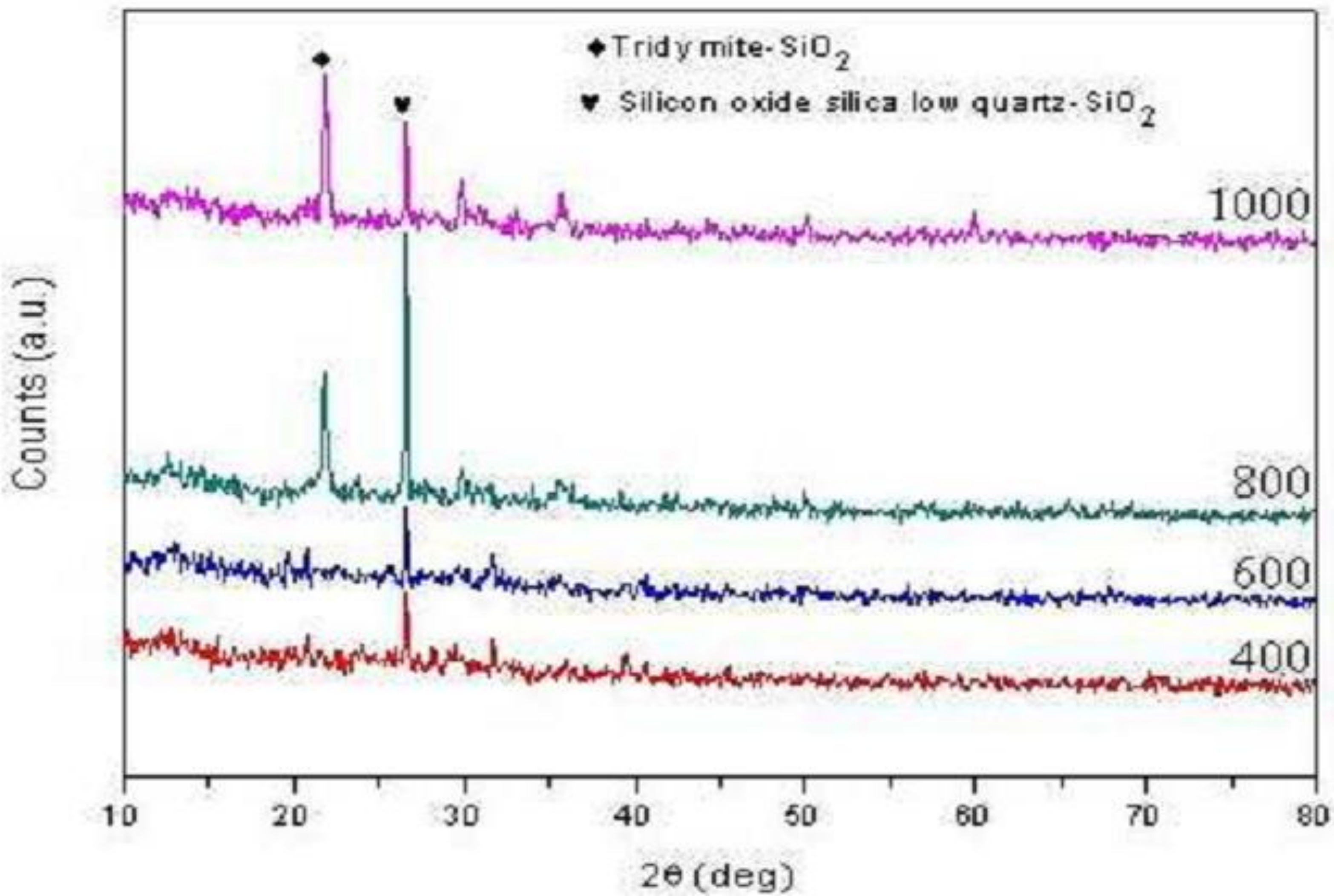

Fig. 12 XRD pattern of PPA at different burning temperature

Case studies from international publications

Case 8

Advanced Materials Research Vol. 748 (2013) pp 304-308
© (2013) Trans Tech Publications, Switzerland
doi:10.4028/www.scientific.net/AMR.748.304

Characterization of Rice Straw Ash and Utilization in Glass Production

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Case studies from international publications

Table 3 Compositions analysis of RSA at different calcining temperature in oxide form

Compound	Calcining temperatures (°C)			
	400	**600**	**800**	**1,000**
MgO	2.60	2.60	1.80	1.80
SiO_2	69.90	71.60	81.22	85.12
P_2O_5	1.54	1.52	1.71	1.93
SO_3	1.11	1.15	1.77	0.66
Cl	10.60	9.81	2.17	1.78
K_2O	9.94	9.81	5.75	3.50
CaO	3.90	3.15	4.90	4.40
TiO_2	0.01	0.01	0.02	0.02
MnO	0.23	0.19	0.33	0.42
Fe_2O_3	0.13	0.12	0.27	0.27
CuO	0.02	0.02	0.03	0.07
ZnO	0.02	0.02	0.03	0.03
SUM	**100.00**	**100.00**	**100.00**	**100.00**

Case studies from international publications

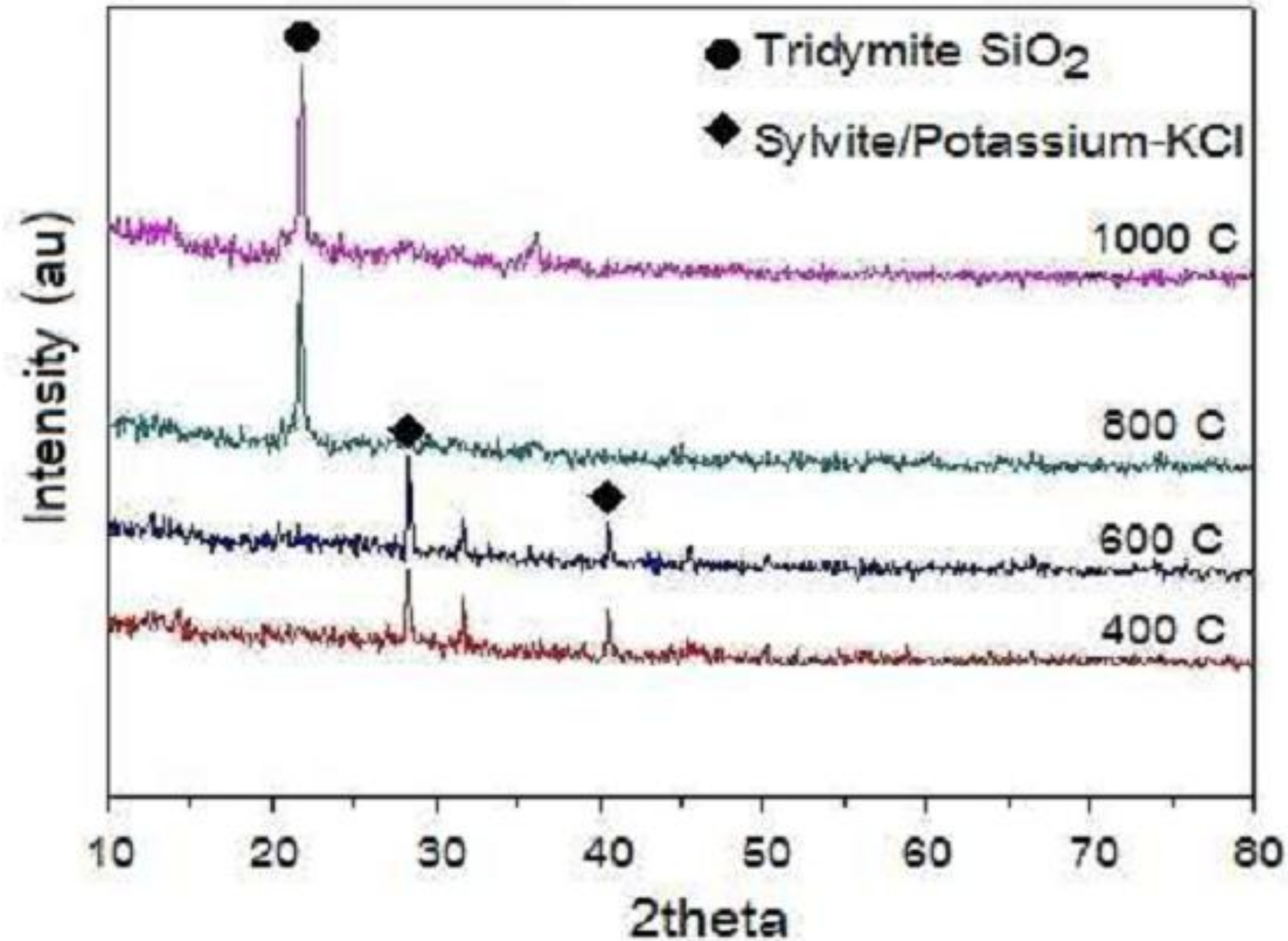

Fig. 13 XRD pattern of RSA at different burning temperature

Case studies from international publications

Case 9

Advanced Materials Research Vols. 93-94 (2010) pp 455-458

doi:10.4028/www.scientific.net/AMR.93-94.455

Effect of Nd^{3+} concentration on the Physical and Absorption Properties of Soda-Lime-Silicate Glasses

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Case studies from international publications

- Composition: $25Na_2O$ - $10CaO$ - $(65\text{-}x)SiO_2$ - xNd_2O_3 where x = 0.00, 1.00, 2.00, 3.00, 4.00 and 5.00 mol%

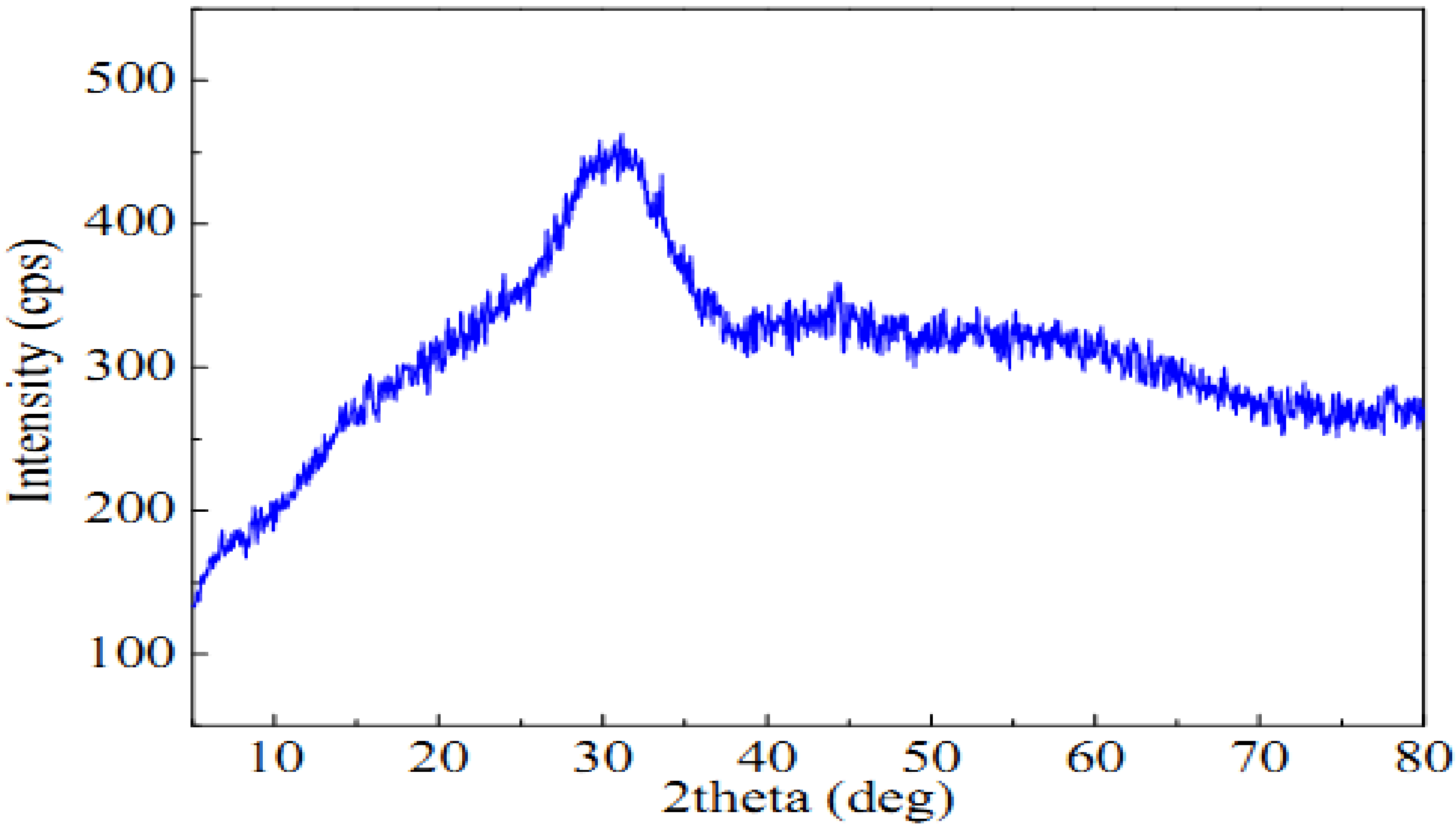

Fig. 14 XRD spectrum of the $25Na_2O$ - $10CaO$ - $65SiO_2$ - Nd_2O_3 glass

Case 10

Available online at www.sciencedirect.com

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Procedia Engineering 32 (2012) 787 – 792

Procedia Engineering

www.elsevier.com/locate/procedia

I-SEEC2011

Physical and optical properties of the SLS glass doped with low Cr_2O_3 concentrations

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Elsevier use only: Received 30 September 2011; Revised 10 November 2011; Accepted 25 November 2011.

Case studies from international publications

Table 4 Chemical composition of glass samples

Glass ID	Cr_2O_3 (*mol%*)	Glass composition (*mol%*)
S65Cr0	0	$65SiO_2$-$25Na_2O$-10CaO
S65Cr1	0.01	$64.99SiO_2$-$25Na_2O$-10CaO-$0.01Cr_2O_3$
S65Cr2	0.02	$64.98SiO_2$-$25Na_2O$-10CaO-$0.02Cr_2O_3$
S65Cr3	0.03	$64.97SiO_2$-$25Na_2O$-10CaO-$0.03Cr_2O_3$
S65Cr4	0.04	$64.96SiO_2$-$25Na_2O$-10CaO-$0.04Cr_2O_3$
S65Cr5	0.05	$64.95SiO_2$-$25Na_2O$-10CaO-$0.05Cr_2O_3$

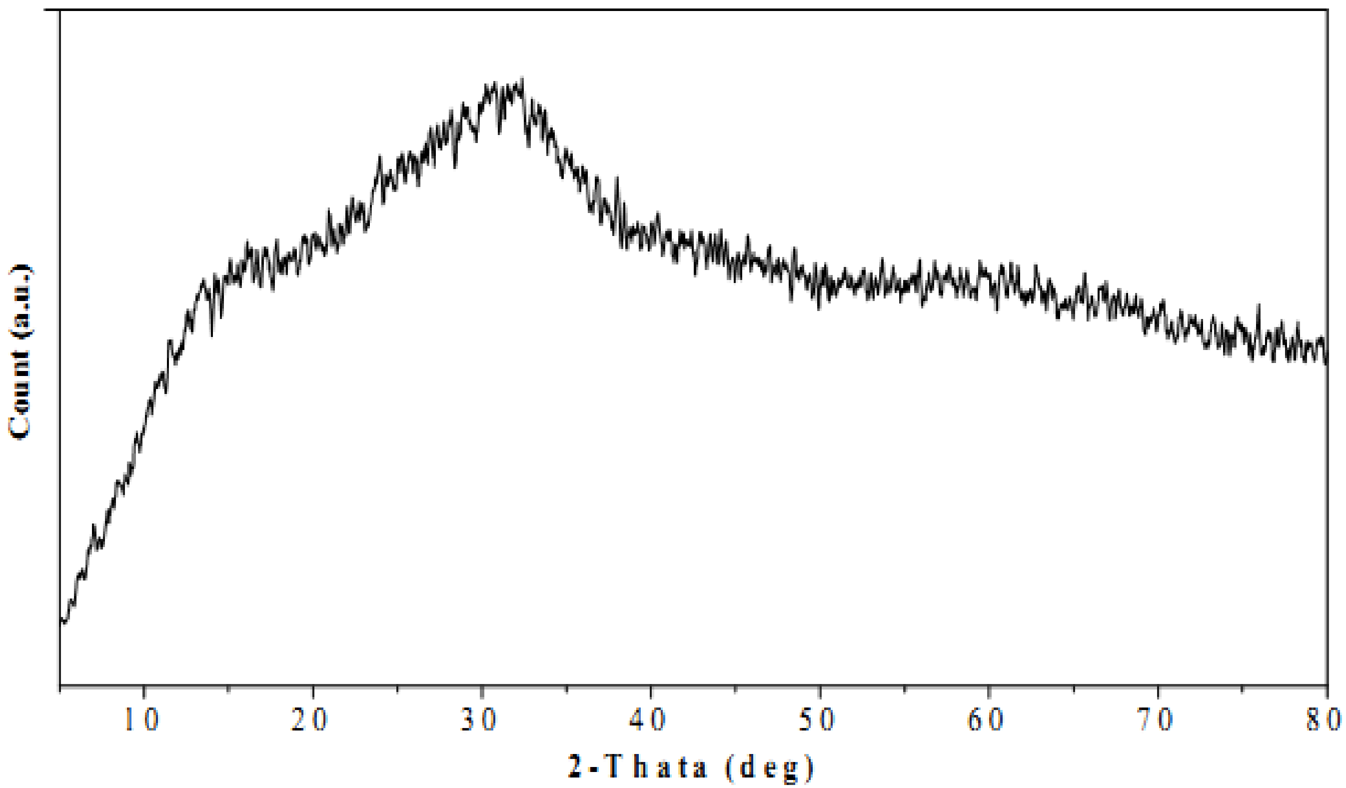

Fig. 15 XRD pattern of 0.05 mol% Cr_2O_3-doped soda lime silicate glass

Case studies from international publications

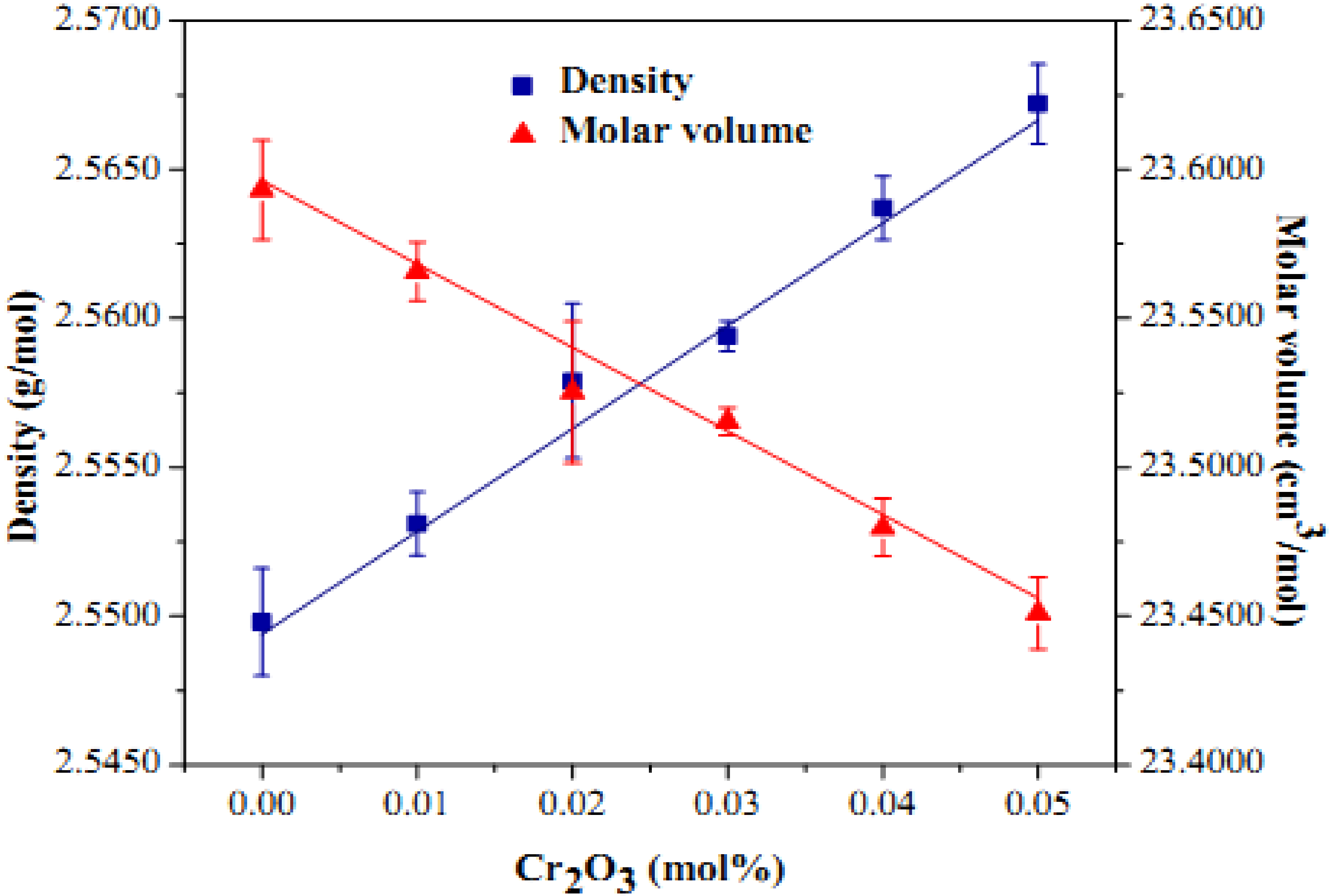

Fig. 16 The density and molar volume of glass samples as a function of Cr_2O_3 content

Next week

Course Outine:

Week 4: Optical properties, advanced measurement/calculation analysis

- Refractive index
- Dispersion
- Scattering
- Absorption

Case studies from international publications