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STRUCTURAL TRANSFORMATION OF NANO – MERCURY OXIDE UNDER HIGH PRESSURE

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ABSTRACT:

Nanostructured orthorhombic mercury oxide is prepared by sonochemical reaction. The influence of pressure on the structural properties are investigated by Energy Dispersive X-ray Diffraction upto 15 GPa. For the increasing pressure no transition is observed. The volume fraction decreases monotonically as the pressure increases. It has been observed that the particle size reduction enhances the first order transition pressure and the stability of the phase has increased.

Keywords*: High Pressure, phase transition, nanocrystalline, EDXRD.*

Introduction: The systematic high-pressure studies of II – VI semiconductors have revealed several new structures and phase transitions(1), leading to new insights in the structural systematic of these materials as well as prompting computational studies of the structural behaviour using first principle methods(2). Among II – VI semiconductors, mercury oxide is the most unusual one in terms of its ambient – pressure structural properties. In fact mercury oxide has attracted attention because of its low – pressure chain like structure with linear O-Hg-O units(3).

Under ambient conditions, HgO crystallizes in a orthorhombic structure (space group Pnma) with cell constants a = 6.61Å, b= 5.52 and c=3.52 as reported(4-6) and it undergoes phase transition at 14 GPa from an orthorhombic to a tetragonal cell. A recent study by San Miguel (7) using EXAFS and EDXRD reported two transitions of mercury oxide at 2 and 5 GPa. Subsequently EDX / Raman study found no transition of mercury oxide below 10 GPa but crystallization mercury from mercury oxide is observed(3). The influence of pressure on bulk HgO was studied by many researchers for pressures upto 35 GPa(8-11) and reported three transitions at 2GPa, 5GPa, 13GPa respectively and at 28 GPa it undergoes electronic to metallic transition.

As per literature the thermodynamic conversion efficiency of a material can be improved by reducing the crystallite size to a nanometric dimension(<100nm). From structural point of view, nanostructured materials have two components one crystalline,made of crystallites of nanometric dimensions with the same structure as the bulk counterparts and another interfacial made of different types of defects (grain boundaries, interphase boundaries

and dislocation etc). The nanosized semiconductor exhibit particle size dependence of electrical and optical properties, making them potential candidates for application [12]. The issue of the effects of crystallite size on structural stability in these nanocrystals is of considerable interest from fundamental point of view and also with respect to the applicability of these materials. Pressure act as a tool to study the structural stability of these materials.

In this paper, the effect of high pressure on nanocrystalline mercury oxide phase stability is investigated by EDXRD and the results obtained are reported and discussed. (Vasanthy and Jeganathan 2007, Vasanthy et.al., 2008, Raajasubramanian et.al., 2011, Jeganathan et.al., 2012, 2014, Sridhar et.al., 2012, Gunaselvi et.al., 2014, Premalatha et.al., 2015, Seshadri et.al., 2015, Shakila et.al., 2015, Ashok et.al., 2016, Satheesh Kumar et.al., 2016).

2. Experimental Procedure

Nanocrystalline mercury oxide prepared by sonochemical reaction and characterized by XRD, TEM etc[13] with particle size15nm is loaded in to a Mao- Bell type diamond – anvil cell. The high pressure powder X-ray diffraction experiments are performed using the Mao-Bell Diamond anvil cell which is mounted on the Rigaku 12 kW Rotating anode X-ray generator with energy dispersive X-ray diffraction system as explained [13]. The face diameter of the diamond anvil is 600 μm. The samples are placed in between the diamonds with the help of a stainless steel plate of grade T 301 which acts as gasket and the sample hole diameter is 300 μm along with methanol-ethanol (4:1) pressure transmitting medium. The pressure is applied slowly. The experiment is carried out at room temperature. The sample is pressurized to various pressures up to 15 GPa. The detector angle is fixed to $2\theta = 16°$.

3. Results and Discussion

According to literature, the bulk HgO undergoes a structural transition from orthorhombic to a phase that has been tentatively characterized as a slight tetragonal distortion of the NaCl structure with space group I4/mmm or a very close variant of NaCl structure at 14 GPa and the second transition is expected to be at 26 GPa.

The nanocrystalline mercury oxide crystallizes as that of bulk HgO with the same crystal structure and the sequence of phase transition as that of bulk is expected. At ambient pressure a X-ray diffraction pattern of mercury oxide is collected and indexed in an orthorhombic structure with lattice constant a = 6.621Å, b= 5.577Å and c=3.55Å of space group Pnma. This result is in good agreement with the results reported by Zhou et al for bulk mercury oxide. Fig. 1 shows the EDXRD pattern of the nanostructured mercury oxide upto the highest pressure of 15 GPa. It has been found that nano – HgO doesn't undergo any structural transition upto the working pressure range. As per literature in most cases the nanocrystalline materials shows an enhanced transition pressure or reduced transition pressure when compared with bulk materials. In this case the first order transition is not obtained. With increasing pressure all the diffraction peaks shifts towards the lower 2θ

values and the peaks are all well separated. This confirms that the interatomic distance decreases and the lattice constant decreases with the increase in pressure.

Due to the application of pressure the volume decreases monotonically and calculated as 131.13Å3. The volume as function of pressure V(P) was obtained by fitting to Birch-Murnaghan equation of state. Figure 2 shows the pressure – volume change of nano – HgO. The bulk modulus (Bo) is calculated as 41.89 (4) GPa and the compressibility of the nano – HgO is found to be 2.3% at 4 GPa.

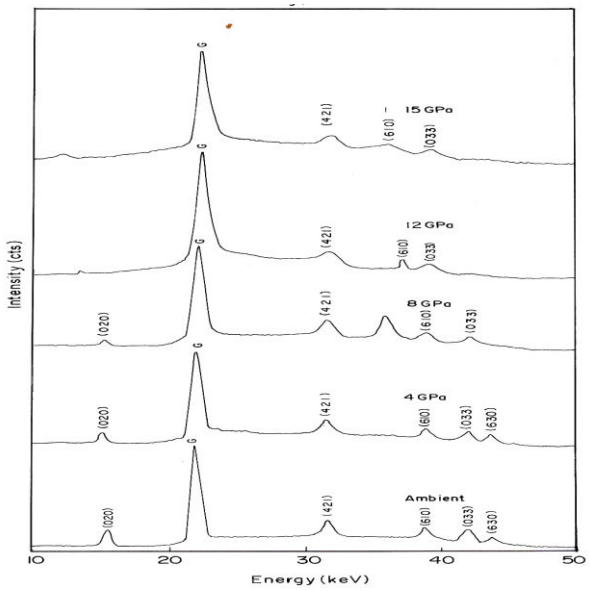

Fig 1. EDXRD pattern of nano HgO at high pressure.

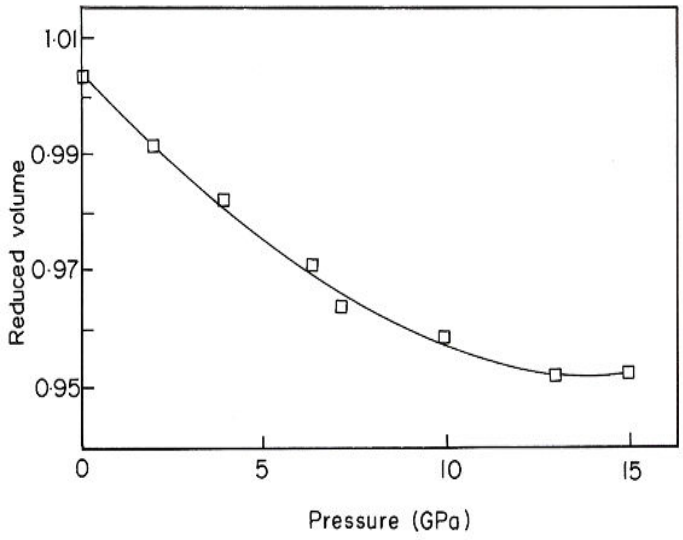

Fig 2. Pressure Vs Volume graph of nano – HgO.

From the above results it is evident that there is discrepancy in the transition pressure for both bulk and nano crystalline materials. The driving force for the phase transformation is the thermodynamical reduction of Gibbs free energy from the initial phase to the final phase. Moreoverfor bulk materials the internal energy is contributed by each and every crystallite separately whereas for nano crystalline materials the internal energy consists of contribution from the core as well as from the surface. Also the surface to volume ratio of nanocrystalline materials is more than that of bulk materials. These factors produce a difference between the transition pressures of both bulk and nanocrystal. This provides information about the surface tension and surface energy difference of the nano materials. In most cases the volume collapse and surface energy difference at the transition pressure is considered to be dominating force leading to the observed enhancement of transition pressure for nanocrystals. (Manikandan et.al., 2016, Sethuraman et.al., 2016, Senthil Thambi et.al., 2016, Ashok et.al., 2018, Senthilkumar et.al., 2018).

4. Conclusion: The nanocrystalline mercury oxide by sonochemical method is subjected to high pressure and no structural phase transformation is observed. The reduction of particle size has enhanced the transition pressure which in turn increases the surface energy. Due to the application of pressure the volume is reduced and the compressibility has enhanced. The volume collapse, internal energy and surface to volume ratio plays a vital role in enhancing the transition pressure.

Refrences:

1. M.I. Mc Mahon and R.J. Nelmes, Phys. Status Solidi B 198, 389 (1996), and references therein.
2. See, e.g., X. Chen, X. Hua, J. Hu, J.M. Langlois and W.A. Goddard III, Phys. Rev. B 53, 1377 (1996);A. Mujica, R.J. Needs and A. Munoz, Phys. Status Solidi B 198, 461(1996);R. Ahuja, P. James, O. Eriksson, J.M. Wills and B. Johansson, ibid 199, 75 (1997)
3. Jinyuan Yan, Bin Chen, Selva Raju, Jason Knight and B.K. Godwal, High Pressure Research 31(4), 555(2011)
4. T. Zhou, U. Schwarz, M. Hanfland, Z. Liu, K. Syassen and M. Cardona, Phy. Rev B 57 (1), 153(1998)
5. K. Aurivillius, Acta. Chem. Scand, 10, 852 (1956).
6. E.A. DeCampsa, M. Duranda, Y. Marquetonam and B. Ayraultb, Opt Commun.4(5), 358(1972).
7. A.S. Miguel, A.G. Penedo, J.P. Itie, A. Polian and P. Bordet, Proceedings of the Joint XVAIRAPT &XXXIII EHPRG International Conference, Varsovie (September 11-15), 1995, 438-440.
8. V.V. Shchennikov, Phys. Solid state 35, 401 (1993).

9. I.M. Tsidil'kowski, V.V. Shchennikov and N.G. Gluzman, Sov. Phys. Semicond. 19, 901 (1985).
10. V.I. Voronin and V.V. Shchennikov, Sov. Phys. Crystallogr. 34, 293 (1989).
11. A. San Miguel, A. Gonzalez Penedo, J.P. Itie, A. Polian and P. Bordet, High Pressure Science and Technology, edited by W.A. Trzeciakowski (World Scientific, Singapore, 1996) p 438.
12. J.Z. Jiang, Journal of Mat. Sci 39, 5103(2004).
13. K. M. Freny Joy, "HighPressureStudies on Nanocrystalline Aurivillius Oxides, Lead and Mercury Chalcogenides", Chapter 5, 138 – 146 (2006).
14. Vasanthy M and M. Jeganathan. 2007. Ambient air quality in terms of NOx in and around Ariyalur, Perambalur DT, Tamil Nadu. Jr. of Industrial pollution Control., 23(1):141-144.
15. Vasanthy. M ,A.Geetha, M. Jeganathan,and A.Anitha. 2007. A study on drinking water quality in Ariyalur area. J.Nature Environment and Pollution Technology. 8(1):253-256.
16. Ramanathan R ,M. Jeganathan, and T. Jeyakavitha. 2006. Impact of cement dust on azadirachtain dicaleaves – ameasure of air pollution in and Around Ariyalur. J. Industrial Pollution Control. 22 (2): 273-276.
17. Vasanthy M and M. Jeganathan. 2007. Ambient air quality in terms of NOx in and around Ariyalur, Perambalur DT, Tamil Nadu. Pollution Research., 27(1):165-167.
18. Vasanthy M and M. Jeganathan. 2008.Monitoring of air quality in terms of respirable particulate matter – A case study. Jr. of Industrial pollution Control.,24(1):53 - 55.
19. Vasanthy M, A.Geetha, M. Jeganathan, and M. Buvaneswari. 2008. Phytoremediation of aqueous dye solution using blue devil (Eichhornia crassipes). J. Current Science. 9 (2): 903-906.
20. Raajasubramanian D, P. Sundaramoorthy, L. Baskaran, K. Sankar Ganesh, AL.A. Chidambaram and M. Jeganathan. 2011. Effect of cement dust pollution on germination and growth of groundnut (*Arachis hypogaea* L.). IRMJ-Ecology. International Multidisciplinary Research Journal 2011, 1/1:25-30 : ISSN: 2231-6302: Available Online: http://irjs.info/.
21. Raajasubramanian D, P. Sundaramoorthy, L. Baskaran, K. Sankar Ganesh, AL.A. Chidambaram and M. Jeganathan. 2011. Cement dust pollution on growth and yield attributes of groundnut. (*Arachis hypogaea* L.). IRMJ-Ecology. International Multidisciplinary Research Journal 2011, 1/1:31-36.ISSN: 2231-6302. Available Online: http://irjs.info/
22. Jeganathan M, K. Sridhar and J.Abbas Mohaideen. 2012. Analysis of meterological conditions of Ariyalur and construction of wind roses for the period of 5 years from January 2002. J.Ecotoxicol.Environ.Monit., 22(4): 375-384.
23. Sridhar K, J.Abbas Mohaideen M. Jeganathan and P Jayakumar. 2012. Monitoring of air quality in terms of respirable particulate matter at Ariyalur, Tamilnadu. J.Ecotoxicol.Environ.Monit., 22(5): 401-406.
24. Jeganathan M, K Maharajan C Sivasubramaniyan and A Manisekar. 2014. Impact of cement dust pollution on floral morphology and chlorophyll of *healianthus annus* plant – a case study. J.Ecotoxicol.Environ.Monit., 24(1): 29-34.
25. Jeganathan M, C Sivasubramaniyan A Manisekar and M Vasanthy. 2014. Determination of cement kiln exhaust on air quality of ariyalur in terms of suspended particulate matter – a case study. IJPBA. 5(3): 1235-1243. ISSN:0976-3333.

26. Jeganathan M, S Gunaselvi K C Pazhani and M Vasanthy. 2014. Impact of cement dust pollution on floral morphology and chlorophyll of *healianthus annus.*plant a case study. IJPBA. 5(3): 1231-1234. ISSN:0976-3333.
27. Gunaselvi S, K C Pazhani and M. Jeganathan. 2014. Energy conservation and environmental management on uncertainty reduction in pollution by combustion of swirl burners. J. Ecotoxicol. Environ.Monit., 24(1): 1-11.
28. Jeganathan M, G Nageswari and M Vasanthy. 2014. A Survey of traditional medicinal plant of Ariyalur District in Tamilnadu. IJPBA. 5(3): 1244-1248. ISSN:0976-3333.
29. Premalatha P, C. Sivasubramanian, P Satheeshkumar, M. Jeganathan and M. Balakumari.2015. Effect of cement dust pollution on certain physical and biochemical parameters of castor plant (*ricinus communis*). IAJMR.1(2): 181-185.ISSN: 2454-1370.
30. Premalatha P, C. Sivasubramanian, P Satheeshkumar, M. Jeganathan and M. Balakumari.2015. Estimation of physico-chemical parameters on silver beach marine water of cuddalore district. Life Science Archives. 1(2): 196-199.ISSN: 2454-1354.
31. Seshadri V, C. Sivasubramanian P. Satheeshkumar M. Jeganathan and Balakumari.2015. Comparative macronutrient, micronutrient and biochemical constituents analysis of *arachis hypogaea.* IAJMR.1(2): 186-190.ISSN: 2454-1370.
32. Seshadri V, C. Sivasubramanian P. Satheeshkumar M. Jeganathan and Balakumari.2015. A detailed study on the effect of air pollution on certain physical and bio chemical parameters of *mangifera indica* plant.Life Science Archives. 1(2): 200-203.ISSN: 2454-1354.
33. Shakila N, C. Sivasubramanian, P. Satheeshkumar, M. Jeganathan and Balakumari.2015. Effect of municipal sewage water on soil chemical composition- A executive summary. IAJMR.1(2): 191-195.ISSN: 2454-1370.
34. Shakila N, C. Sivasubramanian, P. Satheeshkumar, M. Jeganathan and Balakumari.2015. Bacterial enumeration in surface and bottom waters of two different fresh water aquatic eco systems in Ariyalur, Tamillnadu. Life Science Archives. 1(2): 204-207.ISSN: 2454-1354.
35. Ashok J, S. Senthamil kumar, P. Satheesh kumar and M. Jeganathan. 2016. Analysis of meteorological conditions of ariyalur district. Life Science Archives. 2(3): 579-585.ISSN: 2454-1354. DOI: 10.21276/lsa.2016.2.3.9.
36. Ashok J, S. Senthamil Kumar, P. Satheesh Kumar and M. Jeganathan. 2016. Analysis of meteorological conditions of cuddalore district. IAJMR.2 (3): 603-608.ISSN: 2454-1370. DOI: 10.21276/iajmr.2016.2.3.3.
37. Satheesh Kumar P, C. Sivasubramanian, M. Jeganathan and J. Ashok. 2016. South Indian vernacular architecture -A executive summary. IAJMR.2 (4): 655-661.ISSN: 2454-1370. DOI: 10.21276/iajmr.2016.2.3.3.
38. Satheesh Kumar P, C. Sivasubramanian, M. Jeganathan and J. Ashok. 2016. Green buildings - A review. Life Science Archives. 2(3): 586-590.ISSN: 2454-1354. DOI: 10.21276/lsa.2016.2.3.9.
39. Satheesh Kumar P, C. Sivasubramanian, M. Jeganathan and J. Ashok. 2016. Indoor outdoor green plantation in buildings - A case study. IAJMR.2 (3): 649-654.ISSN: 2454-1370. DOI: 10.21276/iajmr.2016.2.3.3.
40. Manikandan R, M. Jeganathan, P. Satheesh Kumar and J. Ashok. 2016. Assessment of ground water quality in Cuddalore district, Tamilnadu, India. Life Science Archives. 2(4): 628-636.ISSN: 2454-1354. DOI: 10.21276/lsa.2016.2.3.9.

41. Manikandan R, M. Jeganathan, P. Satheesh Kumar and J. Ashok. 2016. A study on water quality assessment of Ariyalur district, Tamilnadu, India. IAJMR.2 (4): 687-692.ISSN: 2454-1370. DOI: 10.21276/iajmr.2016.2.3.3.
42. Sethuraman G, M. Jeganathan, P. Satheesh Kumar and J. Ashok. 2016. Assessment of air quality in Ariyalur, Tamilnadu, India. Life Science Archives. 2(4): 637-640.ISSN: 2454-1354. DOI: 10.21276/lsa.2016.2.3.9.
43. Sethuraman G, M. Jeganathan, P. Satheesh Kumar and J. Ashok. 2016. A study on air quality assessment of Neyveli, Tamilnadu, India. IAJMR.2 (4): 693-697.ISSN: 2454-1370. DOI: 10.21276/iajmr.2016.2.3.3.
44. Senthil Thambi J, C. Sivasubramanian and M. Jeganathan. 2018. Ambient Air quality monitoring in terms of (Nitrogen di oxide in and around Ariyalur District, Tamilnadu, India. IAJMR.4 (3): 1414-1417.ISSN: 2454-1370. DOI: 10.22192/iajmr.2018.4.3.2.
45. Senthil Thambi J, C. Sivasubramanian and M. Jeganathan. 2018. Study of Air pollution due to vehicle emission in Ariyalur District, Tamilnadu, India. Life Science Archives. 4(4): 1409-1416.ISSN: 2454-1354. DOI: 10.22192/lsa.2018.4.4.3.
46. Ashok J, S.Senthamil kumar, P.Satheesh kumar and M.Jeganathan. 2018. Estimation of Cement kiln exhaust on Air quality of Ariyalur in terms of suspended particulate matter - A Case Study. International Journal Of Civil Engineering And Technology. 9 (12): Scopus Indexed Journal ISSN: 0976 – 6316.
47. Ashok J, S.Senthamil kumar, P.Satheesh kumar and M.Jeganathan.2018. Air quality assessment of Neyveli in Cuddalore District, Tamilnadu, India. International Journal Of Civil Engineering And Technology. 9 (12): Scopus Indexed Journal ISSN: 0976 – 6316.
48. Senthilkumar M, N. Nagarajan, M. Jeganathan and M. Santhiya. 2018. Survey of Medicinal Plants diversity on Bodha Hills in Salem District, Tamil Nadu, India. Indo – Asian Journal Of Multidisciplinary Research (IAJMR) ISSN: 2454-1370.
49. Senthilkumar M, N. Nagarajan, M. Jeganathan and M. Santhiya. 2018. Survey of Traditional Medicinal Plants in and around Ariyalur in TamilNadu, India. Life Science Archives (LSA) ISSN: 2454-1354. DOI: 10.22192/lsa.2018.4.6.5.
50. Malarvannan J, C. Sivasubramanian, R. Sivasankar, M. Jeganathan and M. Balakumari. 2016. Shading of building as a preventive measure for passive cooling and energy conservation – A case study. Indo – Asian Journal of Multidisciplinary Research (IAJMR): ISSN: 2454-1370. Volume – 2; Issue - 6; Year – 2016; Page: 906 – 910. DOI: 10.21276.iajmr.2016.2.6.10.
51. Malarvannan J, C. Sivasubramanian, R. Sivasankar, M. Jeganathan and M. Balakumari. 2016. Assessment of water resource consumption in building construction in tamilnadu, India. Life Science Archives (LSA) ISSN: 2454-1354 Volume – 2; Issue - 6; Year – 2016; Page: 827 – 831 DOI: 10.21276/lsa.2016.2.6.7.
52. Sivasankar R, C. Sivasubramanian, J. Malarvannan, M. Jeganathan and M. Balakumari. 2016. A Study on water conservation aspects of green buildings. Life Science Archives (LSA),ISSN: 2454-1354. Volume – 2; Issue - 6; Year – 2016; Page: 832 – 836, DOI: 10.21276/lsa.2016.2.6.8.
53. Ashok J , S. Senthamil Kumar , P. Satheesh Kumar and M. Jeganathan. 2016. Analysis and design of heat resistant in building structures. Life Science Archives (LSA), ISSN: 2454-1354. Volume – 2; Issue - 6; Year – 2016; Page: 842 – 847. DOI: 10.21276/lsa.2016.2.6.10.