

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

Proposal to the ISOLDE and Neutron Time-of-Flight Committee

Investigation of doping influence on local structure and phase transitions in vanadium oxides by time-differential perturbed angular correlations at ISOLDE-CERN

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Abstract

Extending the work started with LOI144, we intend to apply radioactive ion implantation techniques to measure hyperfine interactions at implanted ions (acting as dopants) in vanadium oxides (VO_2 and V_2O_5). Along with first-principles calculations, we aim to understanding the doping effects on the local structure in the dopant neighboring and its consequence on the electric and magnetic properties of the host oxides. Vanadium oxides are particularly attractive due to its phase transitions and to the capacity of the vanadium ion to change its oxidation state, being such properties well adequate for applications on, e.g., electrochemical energy storage via the intercalation of Li-ions, catalytic and optoelectronic devices. At ISOLDE-CERN, we aim studying the incorporation of selected dopants by ion implantation, using the nuclear technique of Time-Differential Perturbed Angular Correlations (TDPAC). The objectives of this project are to study at the atomic scale the dopant probe's lattice sites and local environment, its electronic configuration, interaction with point defects and its recombination dynamics at different temperatures related to phase transitions of vanadium oxides (VO_2 and V_2O_5). With specific experiments, we aim to advance in fundamental research, which can be used to optimize manufacture procedures of devices while strengthening the collaboration between synergetic institutions.

Requested shifts: 10 shifts for 2018, (split among the different probe isotopes according to the ISOLDE schedule)

1. Introduction and motivation

The doping with other elements than the native cationic metal can enhance certain properties of oxides and turn them better materials for specific applications or make them suitable for new ones [LOU2014, OGA2010, ROB2011]. When a dopant atom replaces the cationic metal in an oxide host, even at very small concentrations, the properties of the host can be dramatically affected producing changes in electronic and transport properties, and altering phase transition temperatures. The goal of the doping is to improve the functional performance of the oxide host. It should take the possibility of defect creation into account, such as oxygen vacancies or clusters in the dopant neighbourhood. These, in their turn, may lead to the formation of mixed phase systems. Clearly, the presence of dopants may alter phase transition parameters, which is an essential aspect for technological applications. The role of the dopant and its influence in the host oxide is desirable to be understood so that a general model of the connection between dopant–oxide pairing and the functional performance must be developed. The lack of quantitative experimental data on the local neighbourhood of the dopant, which can give information about the local structure and the electronic structure in this region, has prevented the formulation of a general theoretical description of the doping phenomenon in oxides.

Time-Differential Perturbed angular correlation (TDPAC) spectroscopy allied to first-principles calculations is among the most promising candidate technique to provide valuable information about these doped systems. The group has a large experience of TDPAC studies on oxides as can be read on references [RIC2010, MUN2010, RIC2015, RIC2017, SEN2015] combining TDPAC and first-principles calculations, including results from LOI144 (Local investigation of impurities in wide band gap nanostructured oxides with radioactive probes) and collaboration with the University of Bonn [RAM2013, SCH2017a, SCH2017b, SCH2017c, SCH2017d]. We have chosen vanadium oxides due to their important properties, which are described below.

1.1. Vanadium oxides (V_2O_5 and VO_2)

The scope of already implemented and potential applications of vanadium oxides is, indeed, impressive [HEN1994, HER2001]. The properties of each particular phase may be tuned by doping to satisfy specific requirements and/or improve the functional performance. Understanding the role of dopant and doping mechanism is, therefore, a key to control these features. Vanadium oxides appear in a large number of stoichiometries with a possibility of interphase transformations under certain conditions. Since surface effects have much impact in the case of nanoparticles and thin films, stoichiometry issue is even more evident for such systems. More specifically, desorption of vanadyl-oxygen from the surface leads to oxygen diffusion and creation of vacancies in the bulk. Thus, a reduced phase clusters may be nucleating [FAN1989].

Dopant implantation and impurities in general may be another reason for oxygen ions rearranging leading to phase transformations. Obviously, distinct phases have different properties, and thus suit for different applications. In this regard, the phenomenon that gained more attention is metal-to-insulator transition (MIT), whose parameters depend significantly on oxide stoichiometry. In what follows we consider separately the peculiarities of VO_2 and V_2O_5 phases with respect to this effect.

MIT takes place at 341 K for vanadium dioxide (VO_2), the semiconductor to metal transition being accompanied by a monoclinic-rutile structural one. Its origin is not a consensus yet, and recently prevailing scenario suggests a Peierls assisted orbital selective Mott transition [WEB2012]. Various experiments revealing the role of doping and its effect on the transition temperature have been known for decades [GOO1971].

Vanadium pentoxide (V_2O_5) may be the most important compound of vanadium oxides since it is the most stable of vanadium oxides and the principal precursor to reduced oxides and vanadium alloys. Though it was believed that V_2O_5 experiences no MIT, there appeared several works where the possibility of the transition was discussed for thin films and V_2O_5 crystal surface [BLU2007, KAN2011].

The V_2O_5 crystallizes in an orthorhombic structure with layers of VO_5 of square pyramidal form sharing edges and corners (figure 1).

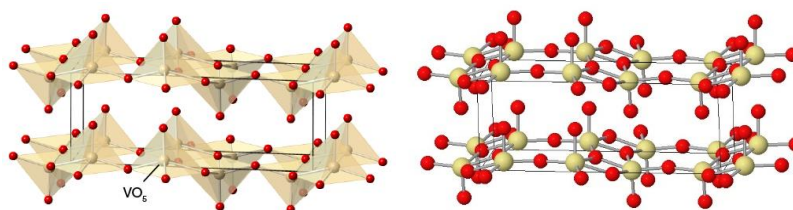


Figure 1: Structural representation of V_2O_5 . The central light spheres represent the vanadium atoms and the red spheres represent the oxygen atoms [UNILIVE].

These layers are weakly linked along the c-axis and the space between them allows the accommodation of guest ions [PAN2012]. The Sol-Gel method can be used to obtain the $\text{V}_2\text{O}_5 \cdot n\text{H}_2\text{O}$ and from this VO_2 [NIN2002, WAN2014], which presents semiconductor-metal phase transition at a critical temperature $T_c = 341$ K (68 °C), changing the structure monoclinic for the tetragonal rutile structure. Due to this transition, a drastic change in the electrical resistivity ($\Delta_{R_{\text{max}}} = 10^5 \Omega$) and optical properties occurs [WEN1994, CAV2004, HAV2005, JIN1997]. All their properties allow V_2O_5 as well as VO_2 applications in electrochemical sensors [RAJ2017] and gaseous [MAN2017], storage of electrochemical energy through the intercalation of lithium ions [WAN2005, KUB2012, PAN2012, MAW2016], catalytic devices [MON2014] and optoelectronic [KUB2012, BOO2015, GER2016].

The physics behind these multiple applications is linked to the nanoscopic phenomenology, such as oxygen vacancies, point defects and influence of different probes on the structure. Based on these questions, we aim using the TDPAC spectroscopy nuclear radioactive technique to study thin films and pellets of vanadium oxides. These techniques provides information on the atomic scale due to the detection of the local electronic charge densities (Electric Field Gradient - EFG) [FRA1965, SCH1996, JOH2017].

2. Objectives

We intend to investigate the doping mechanism in selected vanadium oxides thin films and pellets by measuring the temperature dependence of hyperfine interactions at the implanted nuclei, which are the dopants, using the TDPAC spectroscopy as well as by first-principles calculations based on density functional theory (DFT). Our goal in the present project is to provide a description of the doping effects at an atomic level on the local crystal structure and the electronic structure around the impurity and the consequences on the properties of the host oxides.

We, therefore, will use different radioactive isotopes provided by ISOLDE-CERN, which will be implanted into the oxides and used as probe nuclei to measure hyperfine interactions with TDPAC spectroscopy. The results from these measurements along with first-principles calculations, will give a comprehensive picture of interactions, electronic structure and local structure at dopant sites and it will allow understanding the physics behind the amazing properties of vanadium oxides.

The objective is to insert in the samples different probe ions having different valences and investigate the local effect of probe elements on the charge density, oxygen vacancy occurrence, and electronic structure by measuring the electric field gradient. In addition, intrinsic properties of samples such as crystal phase transition and magnetism [NAI1993, GRI2015], by measuring the magnetic hyperfine field, will be investigated too. So, $^{111}\text{In}(^{111}\text{Cd})$, $^{117}\text{Cd}(^{117}\text{In})$ and $^{181}\text{Hf}(^{181}\text{Ta})$ will be used to carry out TDPAC measurements on the implanted element with element transmutation and $^{111\text{m}}\text{Cd}(^{111}\text{Cd})$ will be used to carry out PAC measurements on the implanted element without element transmutation ($^{111\text{m}}\text{Cd}/^{111}\text{Cd}$) to compare with results obtained with $^{111}\text{In}(^{111}\text{Cd})$. The $^{119\text{m}}\text{Sn}$ (Sn) will be used to make a study from the correlation e-gamma.

Additionally, the proposed experiment series will include the probe ^{181}Hf , thus requiring the possibility of running several TDPAC instruments in parallel offered at ISOLDE-CERN during the long-shutdown. This campaign requires CERN services in terms of radioprotection and the access to the ISOLDE-CERN off-line laboratories (508/R-004 and 508/R-008) infrastructure, mainly the annealing and TDPAC laboratories, and integrated equipment.

3. Detailed description of the proposed work

3.1 Sample production, characterization and DFT simulations at home institutions

The Sol-Gel and Spin Coating methods are used to obtain pellets and thin films of the $\text{V}_2\text{O}_5\cdot n\text{H}_2\text{O}$ at IPEN hyperfine interactions laboratory (HIL-IPEN, São Paulo) [BOI2010, NIN2002, WAN2014]. The VO_2 will be obtained as described above. Additional thin film samples of V_2O_5 and VO_2 will be prepared by magnetron sputtering in the Engineering College at São Paulo University.

In order to obtain a detailed picture of the doping effect, TDPAC results will be complemented by X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), extended X-ray absorption fine structure (EXAFS) and First-principles calculations, using full-potential linearized augmented plane waves method (FP-LAPW) based on the DFT, which will be implemented in order to simulate the doping in the host oxides to interpret mainly the experimental hyperfine interactions results.

3.2 TDPAC probes to be implanted at ISOLDE-CERN (requested shifts)

$^{111}\text{In}(^{111}\text{Cd})$, $^{117}\text{Cd}(^{117}\text{In})$, $^{111\text{m}}\text{Cd}(^{111}\text{Cd})$, $^{119\text{m}}\text{Sn}$ (Sn).

After implantation, prior to the TDPAC measurements, the samples will be submitted to different temperatures of annealing: 120 °C; between 210-270 °C and 350 °C, in which the samples suffer total dehydration and present the orthorhombic phase. The obtained V_2O_5 will be subjected to an annealing at 480 °C under 1-2 Pa for 20 minutes, obtaining VO_2 . This VO_2 will be subjected to annealing above and below 68 °C, which is the semiconductor (monoclinic) - metal (tetragonal) transition temperature. This procedure will be done for thin films and $\text{V}_2\text{O}_5\cdot n\text{H}_2\text{O}$ pellets.

Only at ISOLDE-CERN it will be possible to perform this investigation using different TDPAC probes (production and addition of the isotope by implantation is only possible at ISOLDE-CERN). $^{117}\text{Cd}(^{117}\text{In})$ and $^{111}\text{In}(^{111}\text{Cd})$ can be produced in the IEA-R1 research reactor (IPEN). However for a systematic investigation, using same experimental conditions are essential. We would like to emphasize that at IPEN the addition of the isotope by ion implantation is not possible.

3.3 TDPAC measurements at ISOLDE-CERN during the long shutdown (no shifts required)

$^{181}\text{Hf}(^{181}\text{Ta})$ probe nuclei will be produced at IPEN, São Paulo, and exported to ISOLDE-CERN for measurements during the Long Shutdown.

We aim optimized experiments during the long-shutdown, exploiting the parallel use of the four 6D-TDPAC instruments present at the ISOLDE-CERN off-line laboratory 508/R-008.

4. TDPAC Spectroscopy technique and methodology justification

The TDPAC spectroscopy is based on the conservation of the angular momentum between the spin direction of the gamma emitting probe nucleus and the direction of the gamma radiation emission pattern. The hyperfine interaction consists of the coupling of the total angular momentum of the electrons with the nucleus spin. When the probe nucleus is inserted in the sample the hyperfine interaction induces a variation in the time of this emission pattern and the measurement of the time variation of this emission pattern in a plane at different angles it is possible to obtain the hyperfine electric field gradient and the magnetic hyperfine field. For all probe cores present in the sample to emit radiation in the same direction generating an anisotropic pattern, TDPAC spectroscopy uses the coincidence measurement ($W(\theta)$) between two gamma photons emitted successively in cascade. TDPAC spectroscopy is able to measure electrical, magnetic or combined electrical and magnetic hyperfine interactions.

The number of radioactive nuclei, which are necessary to perform experiments, is generally less than 10^{12} radioactive atoms, at highly diluted concentrations generally, in the range between 0.01% and ppm. This number of atoms is still enough to produce an observable modulation of the decay curve, described by the so called anisotropy ratio, $R(t)$. A fit to this curve allows identifying multiple fractions of probe atoms interacting with certain local environments [FRA1965, SCH1996, JOH2017].

Phenomena related to the observation of lattice sites, defects, orbital ordering, electronic polarization, the whole being observed as a function of a multitude of parameters like temperature, electric field, and pressure are examples of the potentiality of the TDPAC technique. Thus, TDPAC spectroscopy can be successfully used to characterize doped oxides [SEN2015, SCH2017c]. The method is complemented by first-principles calculations. This methodology has been used with success by our team [SEN2015, SCH2017c].

5. Resume of our earlier findings:

An EFG study of ^{111}Cd in vanadium oxides thin metal packets were made by [NAI1993]. ^{111}In TDPAC probe nuclei were ion-implanted at 400 keV and significant values of $\nu_Q=88.1(3)$ MHz, $\eta=0.62(2)$ and $\sigma=5.6(5)$ MHz, were obtained in vacuum under 596.85 °C during 60 minutes. The samples were prepared by pressing the commercially obtained oxide powders. However, TDPAC measurements considering the transition temperatures and

V_2O_5 hydration stages in a systematic investigation, using the same experimental conditions are essential to know more details of the behavior and properties of this material.

Our initial early TDPAC measurements performed at ISOLDE-CERN during the test experiments resulted in promising spectra for V_2O_5 sample after annealing at 630 °C under pressure of $2 \cdot 10^{-4}$ mbar for 10 minutes [Figure 2] using ^{111m}Cd as radioactive probe. This sample will be submitted to complementary characterisation at the participating home institutions to check its structural conditions and the vanadium oxide phase present. However, systematic measurements using different radioisotopes as probes under different temperatures are necessary.

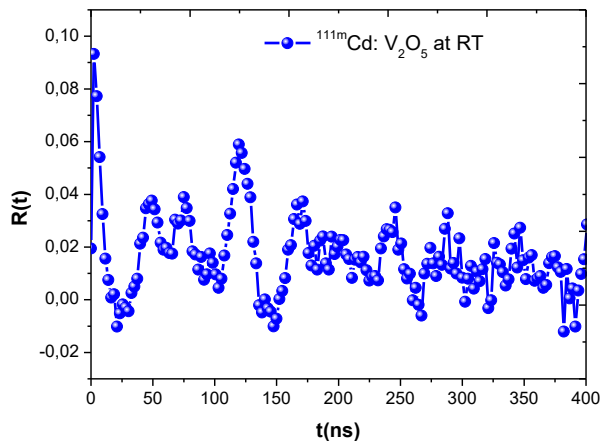


Figure 2: TDPAC spectrum recently obtained at ISOLDE-CERN for V_2O_5 samples using ^{111m}Cd as probe, synthesized by the Sol-Gel method at HIL-IPEN, proving a viability of the technique for this type of material.

Our collaboration includes the expertise of both material and nuclear applied physicists using this technique at ISOLDE-CERN [JOH2017].

6. Summary of requested shifts:

We estimate the total number of ISOLDE-CERN beam time needed to accomplish the above- described tasks to be 10 shifts, distributed according to table I:

Table I: Beam time request for TDPAC studies

Time-Differential Perturbed Angular Correlations Studies								
Required isotope	Implanted beam	Probe element	Type of experiment	Approx. Intensity [at/ μ C]	Target / Ion source	Required atoms per sample	Comments	n° of shifts
^{111m}Cd (48m)	^{111}Cd	^{111}Cd	γ - γ TDPAC	10^8	Sn target; VD5 ion source	2×10^{10}		4
^{117}Cd (2.49h)	^{117}Cd	^{117}In	γ - γ TDPAC	10^8	UC target; RILIS (Ag) ion source	5×10^{10}		2
^{111}In (2.8d)	^{111}In	^{111}Cd	γ - γ TDPAC	10^8	UC target; surface or RILIS ion source	1×10^{11}		2
^{119m}Sn (293d)	^{119m}Sn	^{119}Sn	e- γ TDPAC	10^8	UC target; surface or RILIS ion source	5×10^{10}		2
TOTAL of requested shifts								10

7. References:

- [BLU2007] R. P. Blum et al. Phys. Rev. Lett., 99, 226103 (2007). <http://10.1103/PhysRevLett.99.226103>
- [BOI2010] A. B. Cezar, Thesis, UFPR (2010). <http://acervodigital.ufpr.br/handle/1884/25571?show=full>
- [BOO2015] W. Boonmeemaka, C. Fongsamut, P. Ngaotrakanwiiwata, Energy Procedia 79, 903 (2015). <http://10.1016/j.egypro.2015.11.585>
- [CAV2004] A. Cavalleri, Th. Dekorsy, H. H. Chong, J. C. Kieffer, R.W. Schoenlein, Phys. Rev. B 70, 161102(R) (2004). <http://10.1103/PhysRevB.70.161102>
- [FAN1989] H. J. Fan and L.D. Marks, Ultramicroscopy, 31, 357—364 (1989). [http://10.1016/0304-3991\(89\)90334-3](http://10.1016/0304-3991(89)90334-3).
- [FRA1965] H. Frauenfelder, R.M. Steffen, 1965, Alpha, Beta and Gamma Ray Spectroscopy, ed. K. Siegbahn (Amsterdam: North Holland).
- [GER2016] L. G. Gerlinga, G. Masmitjaa, C. Voza, P. Ortega, J. Puigdollersa, R. Alcubilla, Energy Procedia 92, 633 – 637 (2016). <http://10.1016/j.egypro.2016.07.029>
- [GOO1971] J. B. Goodenough, J. of Sol. St. Chem., 3, 490 (1971). [http://10.1016/0022-4596\(71\)90091-0](http://10.1016/0022-4596(71)90091-0)
- [GRI2015] D. Grieger, M. Fabrizio, Phys. Rev. B 92, 075121 (2015). <https://doi.org/10.1103/PhysRevB.92.075121>
- [HAV2005] M. W. Haverkort, Z. Hu, A. Tanaka, W. Reichelt et al., Phys. Rev. Lett. 95, 196404 (2005). <https://doi.org/10.1103/PhysRevLett.95.196404>
- [HEN1994] V. E. Henrich and P. A. Cox., Cambridge University Press, Cambridge (1994). <http://10.1002/adma.19950070122>
- [HER2001] K. Hermann and M. Witko. The Chemical Physics of Solid Surfaces: Oxide Surfaces. Elsevier, New York (2001).
- [JIN1997] P. Jin, K. Yoshimura, and S. Tanemura, J. V. Sci. Technol. A, 15, 1113 (1997). <http://dx.doi.org/10.1116/1.580439>
- [JOH2017] K. Johnston et. al., J. Phys. G: Nucl. Part. Phys. 44, 104001 (25pp) (2017). <https://doi.org/10.1088/1361-6471/aa81ac>
- [KAN2011] M. Kang et al. Appl. Phys. Lett., 98, 131907 (2011). <http://10.1063/1.3571557>
- [KUB2012] S. Kubuki, H. Masuda, K. Akiyama, Z. Omonnay, E. Kuzmann, T. Nishida, Hyp. Inter. (2012). <http://10.1007/s10751-012-0657-9>
- [LOU2014] S. D. Lounis, E. L. Runnerstrom, A. Bergerud, D. Nordlund, and D. J. Milliron, J. Am. Chem. Soc., 136, 7110, 136 (2014). <http://10.1021/ja502541z>
- [MAN2017] A. A. Manea, M. P. Suryawanshic, J.H. Kimc, A.V. Moholkara, Appl. S. Sci. 403, 540 (2017). <http://dx.doi.org/10.1016/j.apsusc.2017.01.220>
- [MAW2016] W. Ma, C. Zhang, C. Liu, X. Nan, H. Fu, G. Cao, Appl. Mater. Inter., 8, 19542 (2016). <http://10.1021/acsami.6b06359>
- [MON2014] O. Monfort, T. Roch, L. Satrapinsky, M. Gregor, T. Plecenik et. al., Appl. S. Sci., 322 21 (2014). <http://dx.doi.org/10.1016/j.apsusc.2014.10.009>
- [MUN2010] E. L. Muñoz, D. Richard, A. W. Carbonari, L. A. Errico, M. Rentería, Hyperfine Interact. 197, 199 (2010). <https://doi.org/10.1007/s10751-010-0207-2>

- [NIN2002] Y. Ningyi, L. Jinhua, L. Chenglu, *Ap. Surf. Sc.*, 191, 1-4; 176 (2002). [http://10.1016/S0169-4332\(02\)00180-0](http://10.1016/S0169-4332(02)00180-0)
- [OGA2010] S. B. Ogale, *Adv. Mater.* 22, 3125 (2010). <http://10.1002/adma.200903891>
- [PAN2012] A. Pan, H. B. Wu, L. Yu, T. Zhu, X. W. Lou, *ACS Appl. Mater. Interfaces* 4, 3874 (2012). <http://dx.doi.org/10.1021/am3012593>
- [RAJ2016] S. Raja, G. Subramania, D. Bheeman, R. Rajamani, C. Belland, *Optik*, 127, 461 (2016). <http://dx.doi.org/10.1016/j.ijleo.2015.08.045>
- [RAJ2017] K. Rajesh, J. Santhanalakshmi, *Mat. Chem. and Phys.* 199, 497 (2017). <http://dx.doi.org/10.1016/j.matchemphys.2017.07.022>
- [RAM2013] J. M. Ramos, T. Martucci, A.W. Carbonari, M.S. Costa et al., *Hyperf. Interact.* 221, 129 (2013). <https://doi.org/10.1007/s10751-012-0704-6>
- [RIC2010] D. Richard, et al., *Phys. Rev. B* 82, 035206 (2010). <http://10.1016/j.physb.2011.12.045>
- [RIC2015] D. Richard, L.A. Errico, M. Rentería, *Comp. Mater. Sci.* 102, 119 (2015). <http://10.1016/j.commatsci.2015.02.023>
- [RIC2017] D. Richard, M. Rentería, A. W. Carbonari, *Semicond. Sci. Technol.* 32, 085010 (2017). <http://10.1088/1361-6641/aa7a74>
- [ROB2011] J. Robertson and S. J. Clark, *Phys. Rev. B*, 83, 075205 (2011). <https://doi.org/10.1103/PhysRevB.83.075205>
- [SCH1996] G. Schatz and A. Weidinger, 1996, *Nuclear Condensed Matter Physics: Nuclear Methods and Applications* (Chichester; New York: John Wiley).
- [SCH2017a] J. Schell, D. C. Lupascu, J. G. M. Correia et al., *Hyperf. Interact.* 238, 2 (2017). <http://10.1063/1.4980168>
- [SCH2017b] J. Schell, D. C. Lupascu, A. W. Carbonari et al., *J. Appl. Phys.* 121, 145302 (2017). <http://dx.doi.org/10.1063/1.4980168>
- [SCH2017c] J. Schell, D. C. Lupascu, A. W. Carbonari et al., *J. Appl. Phys.* 121, 195303 (2017). <http://dx.doi.org/10.1063/1.4983669>
- [SCH2017d] J. Schell, D. C. Lupascu, A. W. Carbonari et al., *AIP ADVANCES* 7, 055304 (2017). <http://dx.doi.org/10.1063/1.4983270>
- [SEN2015] C. Sena, M.S. Costa, E.L. Muñoz, G.A. Cabrera-Pasca et al., *J. Magn. Magn. Mater.* 387, 165 (2015). <https://doi.org/10.1016/j.jmmm.2015.03.092>
- [UNILIVE] University of Liverpool, Chem. Tube 3D. <http://www.chemtube3d.com/solidstate/SS-V2O5.htm>
- [WAN2005] Y. Wang, H. Shang, T. Chou, G. Cao, *J. Phys. Chem. B*, 109 (22), 11361 (2005). <http://10.1021/jp051275>
- [WAN2014] Y. Wanga, L. Pana, Y. Lia, A.I. Gavrilyuk, *Applied Surface Science*, 314, 384 (2014). <http://dx.doi.org/10.1016/j.apsusc.2014.06.167>
- [WEB2012] C. Weber et al., *Phys. Rev. Lett.*, 108, 256402 (2012). <http://10.1103/PhysRevLett.108.256402>
- [WEN1994] R. M. Wentzcovitch, W. W. Schulz, P.B. Allen, *Phys. Rev. Lett.* 23, 72(21):3389 (1994). <http://10.1103/PhysRevLett.72.3389>

Appendix

DESCRIPTION OF THE PROPOSED EXPERIMENT

The experimental setup comprises: *(name the fixed-ISOLDE installations, as well as flexible elements of the experiment)*

Part of the Choose an item.	Availability	Design and manufacturing
SSP-GLM chamber, SSP-GHM chamber	<input checked="" type="checkbox"/> Existing	<input checked="" type="checkbox"/> To be used without any modification
Existing equipment on the solid state labs in building 508-r-002, r-004 and r-008 - 6 detector PAC standard setups - annealing furnaces - glove boxes art 1 of experiment/ equipment]	X Existing	<input type="checkbox"/> To be used without any modification <input type="checkbox"/> To be modified
	<input type="checkbox"/> New	<input type="checkbox"/> Standard equipment supplied by a manufacturer <input type="checkbox"/> CERN/collaboration responsible for the design and/or manufacturing
[Part 2 experiment/ equipment]	<input type="checkbox"/> Existing	<input type="checkbox"/> To be used without any modification <input type="checkbox"/> To be modified
	<input type="checkbox"/> New	<input type="checkbox"/> Standard equipment supplied by a manufacturer <input type="checkbox"/> CERN/collaboration responsible for the design and/or manufacturing
[insert lines if needed]		

HAZARDS GENERATED BY THE EXPERIMENT

(if using fixed installation) Hazards named in the document relevant for the fixed SSP-GLM chamber and building 508-r-002, r-004 and r-008 installations. Every experiment has its one written procedure file discussed with Radio Protection services, before every beam time.

Additional hazards:

Hazards	SSP-GLM	Building 508	[Part 3 of the experiment/ equipment]
	Thermodynamic and fluidic		
Pressure	vacuum[Bar], [volume][l]	Vacuum	
Vacuum	10-6 mbar at SSP chamber 10 during collections	10-5mbar	
Temperature	[temperature] [K]	Ambient – 630 °C	
Heat transfer			
Thermal properties of materials			
Cryogenic fluid	[fluid], [pressure][Bar], [volume][l]		
Electrical and electromagnetic			
Electricity	[voltage] [V], [current][A]		
Static electricity			
Magnetic field	[magnetic field] [T]		
Batteries	<input type="checkbox"/>		
Capacitors	<input type="checkbox"/>		
Ionizing radiation			
Target material	[material]		

Beam particle type (e, p, ions, etc)	^{111m}Cd , ^{111}Cd , ^{117}In , ^{119}Sn		
Beam intensity			
Beam energy	50KeV		
Cooling liquids	[liquid]		
Gases	[gas]		
Calibration sources:	<input type="checkbox"/>		
• Open source	<input type="checkbox"/>		
• Sealed source	<input type="checkbox"/> [ISO standard]		
• Isotope			
• Activity			
Use of activated material:			
• Description	<input type="checkbox"/> Removal from chamber, transport to TDPAC laboratory 508/R-002 in standard Pb castle shielding. Placed in PAC machine at 508/R-008 for measurement.		
• Dose rate on contact and in 10 cm distance	Max. 0.3 $\mu\text{Sv/h}$ (Nucleonica gamma dose rate)		
• Isotope	^{111m}Cd , ^{111}Cd , ^{117}In , ^{119}Sn		
• Activity	Max 6 MBq per sample		
Non-ionizing radiation			
Laser			
UV light			
Microwaves (300MHz-30 GHz)			
Radiofrequency (1-300MHz)			
Chemical			
Toxic	[chemical agent], [quantity]	$\text{V}_2\text{O}_5\text{nH}_2\text{O}$, V_2O_5 , VO_2	
Harmful	[chemical agent], [quantity]	$\text{V}_2\text{O}_5\text{nH}_2\text{O}$, V_2O_5 , VO_2	
CMR (carcinogens, mutagens and substances toxic to reproduction)	[chemical agent], [quantity]		
Corrosive	[chemical agent], [quantity]		
Irritant	[chemical agent], [quantity]		
Flammable	[chemical agent], [quantity]		
Oxidizing	[chemical agent], [quantity]		
Explosiveness	[chemical agent], [quantity]		
Asphyxiant	[chemical agent], [quantity]		
Dangerous for the environment	[chemical agent], [quantity]	$\text{V}_2\text{O}_5\text{nH}_2\text{O}$, V_2O_5 , VO_2	
Mechanical			
Physical impact or mechanical energy (moving parts)	[location]		
Mechanical properties (Sharp, rough, slippery)	[location]		
Vibration	[location]		
Vehicles and Means of Transport	[location]		
Noise			
Frequency	[frequency],[Hz]		
Intensity			
Physical			
Confined spaces	[location]		
High workplaces	[location]		
Access to high workplaces	[location]		
Obstructions in	[location]		

passageways			
Manual handling	SSP protocol		
Poor ergonomics	[location]		

0.1 Hazard identification

3.2 Average electrical power requirements (excluding fixed ISOLDE-installation mentioned above):
(make a rough estimate of the total power consumption of the additional equipment used in the experiment)