EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

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

Study of molybdenum oxide by means of perturbed angular correlations and mößbauer spectroscopy

Juliana Schell[1,2]

ISOLDE Solid State Physics

João Guilherme Martins Correia[1,3], Katharina Lorenz[4], Marco Peres[4], Carlos Díaz-Guerra[5], H.P. Gunnlaugsson[1,6], Aitana Tarazaga[7], Manfred Deicher[2]

1 ISOLDE-CERN, Switzerland

2 Universität des Saarlandes, Germany

3 Centro de Ciências e Tecnologias Nucleares (C^{2}TN), Campus Tecnológico e Nuclear – CTN, Instituto Superior Técnico, Universidade de Lisboa, Portugal

4 Instituto de Plasmas e Fusão Nuclear, Campus Tecnológico e Nuclear – CTN, Instituto Superior Técnico, Universidade de Lisboa, Portugal

5 Dpto. Física de Materiales, Facultad de Ciencias Físicas, Universidad Complutense de Madrid, Spain

6 KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium

7 Johannes Keppler University, Linz, Austria

OBJECTIVES

Studying the incorporation of selected dopants in MoO_3 by ion implantation using PAC and eMS.

SAMPLE PRODUCTION AND COMPLEMENTARY CHARACTERIZATION

Crystal structures by x-ray diffraction (XRD)

Chemical analyses by x-ray fluorescence (XRF)

BY OUR COLLABORATORS:

- Dpto. Física de Materiales, Facultad de Ciencias Físicas Universidad Complutense de Madrid, Spain

+

Johannes Keppler University, Linz, Austria

Samples‘s stoichiometry and composition by Rutherford backscattering spectrometry (RBS)/channeling (RBS/C)

- Campus Tecnológico e Nuclear, Instituto Superior Técnico, Universidade de Lisboa, Portugal

MoO_x, A "UNIVERSAL" MATERIAL

Picture Source: Wikipedia

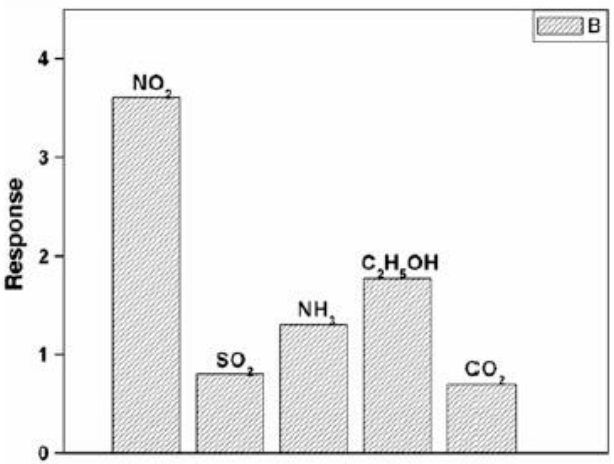
MoO_3

belongs to the family of 2D inorganic materials RT stable orthorhombic α-MoO_3 phase: (2.8 – 3.2 eV)

α-MoO_3

Solar cells, catalysis, gas sensing, lithium-ion batteries, field emission, photochromic and electrochromic devices.

Sensor response to 500 ppm of gases measured at 170°C of 10% wt MoO_3-doped SnO_2 thin films



Picture source: Metal Oxide Nano-architectures and Heterostructures for Chemical Sensors Editors: Michael A. Carpenter • Sanjay Mathur, Andrei Kolmakov, Springers, 2013

WHY PAC SPECTROSCOPY AT ISOLDE?

Atomic resolution delivers information on

- Probe's lattice location & annealing of implantation defects
- Probes-host or probes-defects interactions
- Probing electronic structure and electron polarization
- Diffusion of probe atoms (dinamic interaction)

HOW?

As a function of
- sample **stoichiometry** with different impurities/**doping**
- annealing and measuring **temperature** from 1 – 1500 K

USING?

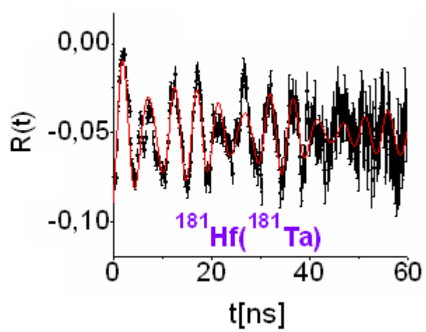
^{111}In(^{111}Cd), ^{111m}Cd(^{111}Cd), ^{117}Cd(^{117}In), ^{115}Cd(^{115}In)

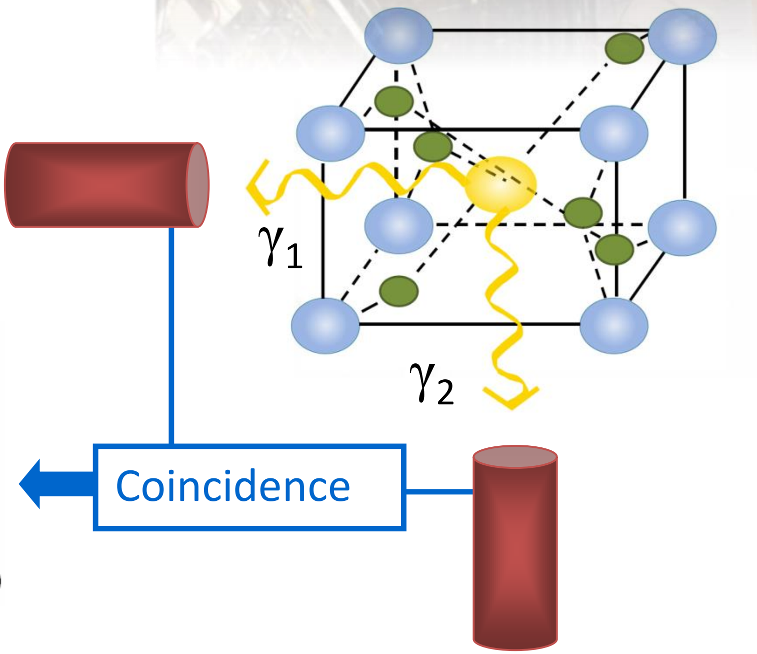
Magnetic interaction:

$$\omega_L = -g \frac{\mu_N}{\hbar} B_{hf}$$

Quadrupole interaction:

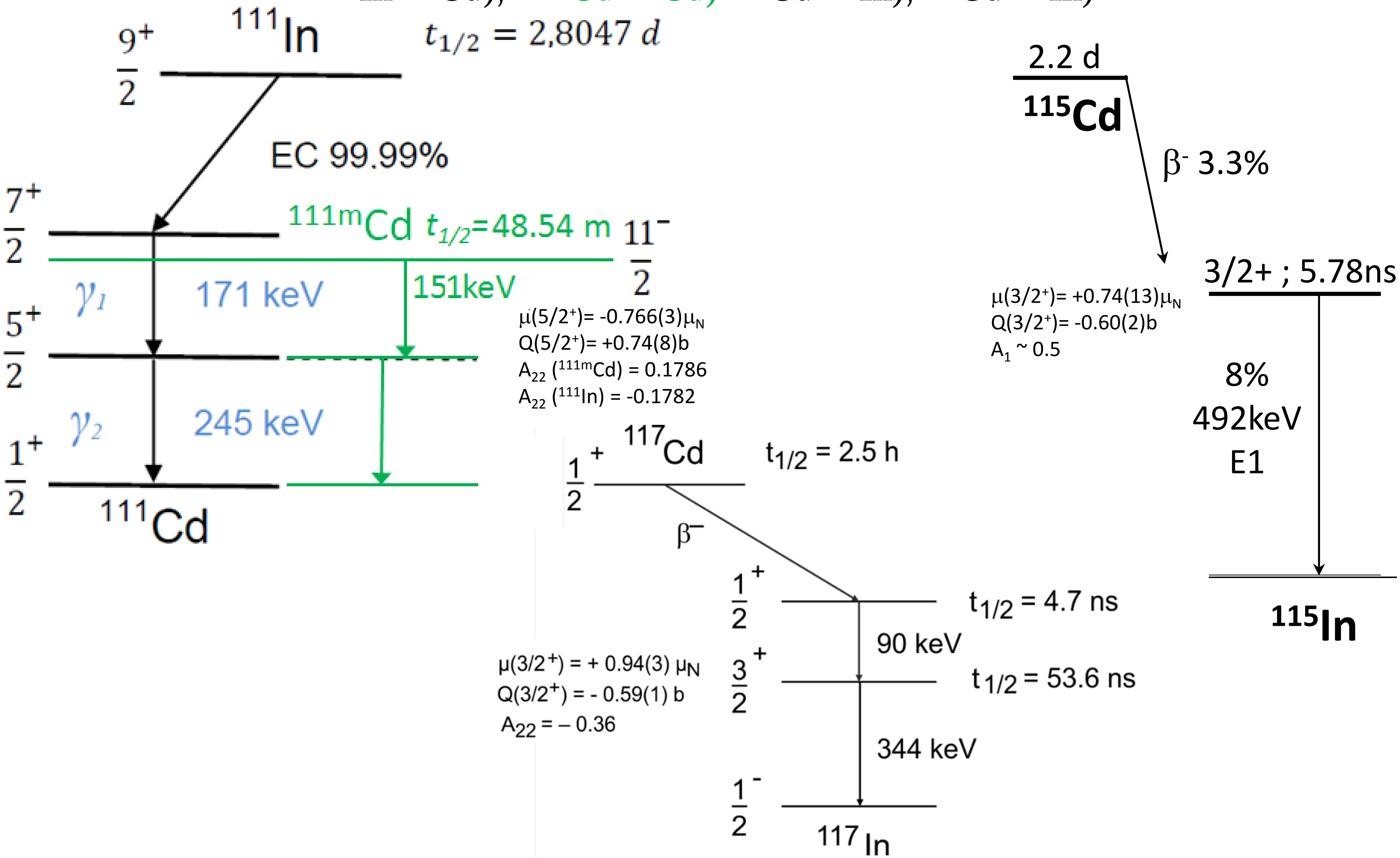
$$\omega_Q = \frac{eQV_{zz}}{4I(2I-1)\hbar}$$





WHY THESE PAC ISOTOPES?

$^{111}In(^{111}Cd)$, $^{111m}Cd(^{111}Cd)$, $^{117}Cd(^{117}In)$, $^{115}Cd(^{115}In)$



WHY *emission* MÖßBAUER SPECTROSCOPY (AT ISOLDE)?

Complement of the PAC study:

- Probe's lattice location & annealing of implantation defects
- Probes-host or probes-defects interactions
- Valence(/spin) state of probe atom (X^{n+})
- Diffusion of probe atoms (few jumps ~100 ns)
- Binding properties (Debye-Waller factors)

HOW?

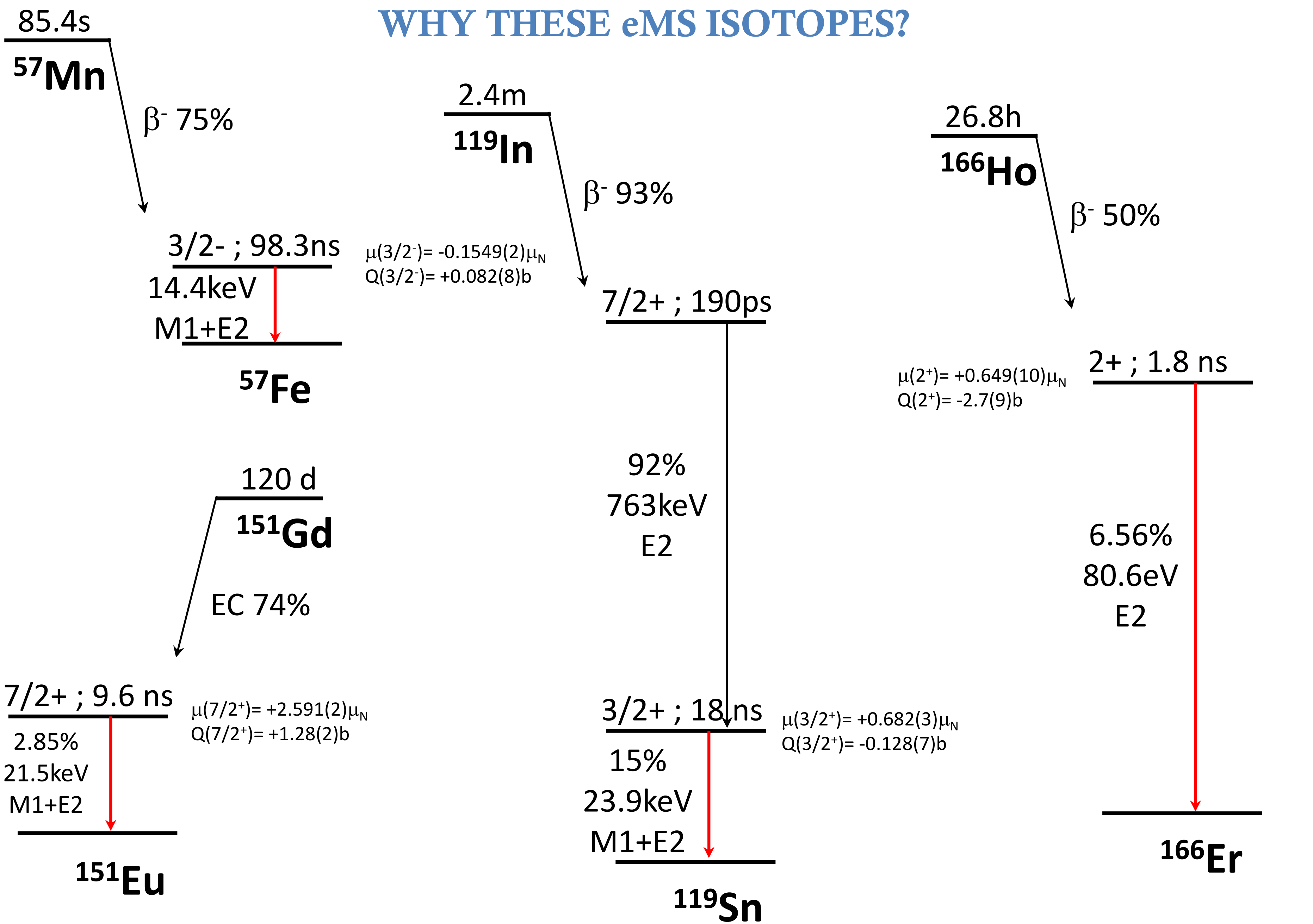
As a function of

- Sample **stoichiometry**
- Annealing and measuring **temperature**

USING?

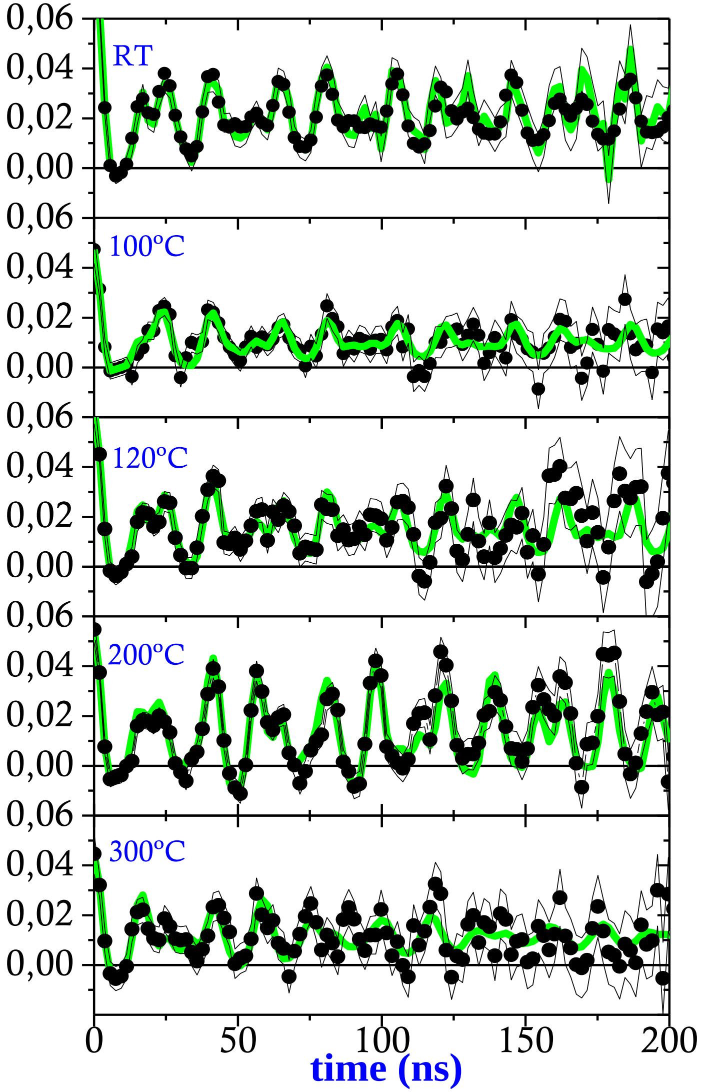
- Complementary Fe and Sn probes
- Optically active Er and Eu elements

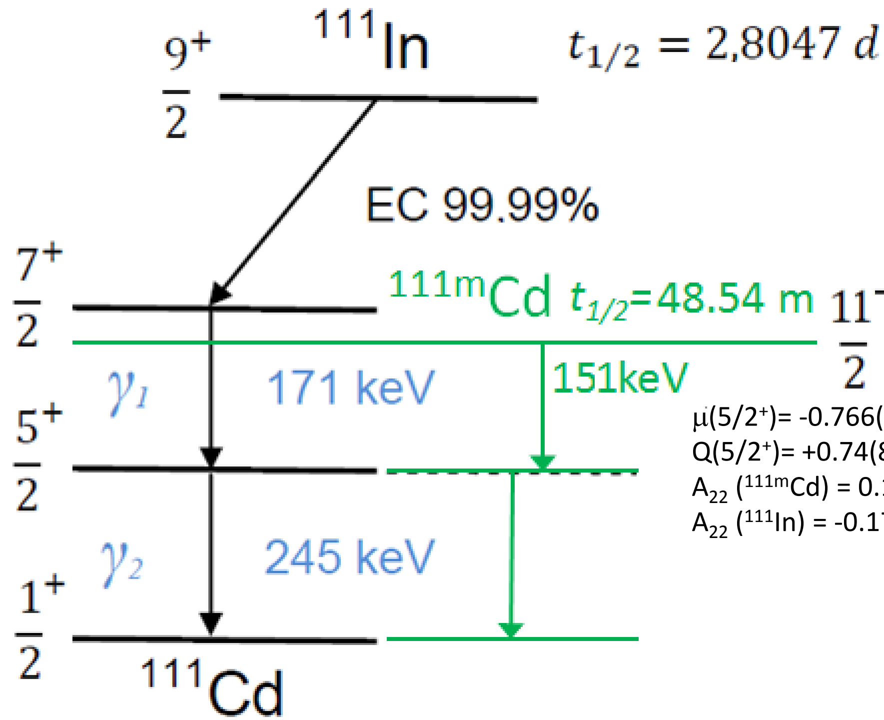
WHY THESE eMS ISOTOPES?



FEASIBILITY OF CURRENT PROPOSAL

$^{111}Cd:MoO_3$ γ-γ (151-243 keV)
PAC from decay of ^{111m}Cd





μ(5/2⁺)= -0.766(3)μ_N
Q(5/2⁺)= +0.74(8)b
A_{22} (^{111m}Cd) = 0.1786
A_{22} (^{111}In) = -0.1782

observation of a dynamic atomic rearrangement of the dopant Cd with the defect as a function of temperature

SUMMARY OF REQUESTED SHIFTS

Perturbed Angular Correlations Studies

Required isotope	Implanted beam	Probe element	Type of experiment	Approx. Intensity [at/μC]	Target / Ion source	Required atoms per sample	Comments	nº of shifts
^{111m}Cd(48m)	^{111m}Cd	^{111}Cd	γ–γ, e⁻–γ PAC	10^8	Molten Sn; plasma	2 x 10^{10}	γ–γ PAC (10K – 1200K) e-γ PAC (50K-823K)	4
^{117}Cd(2.49h)	^{117}Ag	^{117}In	γ–γ PAC	10^8	UC_x; RILIS (Ag)	5 x 10^{10}	γ–γ PAC (10K – 1200K)	1
^{115}Cd(53.46h)	^{115}Ag	^{115}In	β–γ PAC	10^8	UC_x; RILIS (Ag)	1 x 10^{11}	β–γ PAC (RT=300K)	0.5
^{111}In(2.8d)	^{111}In	^{111}Cd	γ–γ PAC	10^5	UC_x; RILIS (In)	1 x 10^{11}	γ–γ PAC (10K – 1200K)	0.5

Mossbauer Studies

Required isotope	Implanted beam	Probe element	Type of experiment	Approx. Intensity [at/μC]	Target / Ion source	Required atoms per sample	Comments	nº of shifts
^{57}Mn (1.5m)	^{57}Mn	^{57}Fe	eMS	2 x 10^8	UC_x, RILIS (Mn)	1 x 10^{12}	Measurement temperatures below 850 K	1
^{119}In (2.1m)	^{119}In	^{119}Sn	eMS	2 x 10^8	UC_x, RILIS (In)	1 x 10^{12}	Measurement temperatures below 750 K	1
^{151}Gd(120d)	^{151}Dy(17.9m) → ^{151}Tb (17.6h) → ^{151}Gd (120d)	^{151}Eu	eMS	1 x 10^8	Ta foil RILIS (Dy)	2 x 10^{12}	Measurement temperatures below 750 K	0.5
^{166}Ho(26.9h)	^{166}Ho	^{166}Er	eMS	1 x 10^9	Ta foil, RILIS (Ho)	2 x 10^{10}	Measurements done at 4K (LHe)	0.5

FUNDING AGENCIES INVOLVED

ISOLDE Solid State Physics

SPONSORED BY THE

Federal Ministry of Education and Research

BMBF

Bundesministerium für Bildung und Forschung

Erforschung kondensierter Materie mit Großgeräten

Ausbau und Unterhalt der Einrichtungen an ISOLDE/CERN

Germany, contract: 05K10TS2,

M. Deicher, J. Schell

FCT

Fundação para a Ciência e a Tecnologia

Caracterização de Materiais com Técnicas Nucleares Radioativas - sinergia e complementaridade aplicadas ao treino e desenvolvimento.

Portugal, Project: CERN-FIS-NUC-0004-2015

K. Lorenz, J.G. Correia

Fundação para a Ciência e a Tecnologia
MINISTÉRIO DA EDUCAÇÃO E CIÊNCIA

MINECO

Ministry of Economy and Competitiveness

Consolider – Ingenio Project “IMAGINE”

Spain, Project MAT2012-31959, CSD2009-0013

C. Díaz-Guerra

MINISTERIO DE ECONOMÍA Y COMPETITIVIDAD

FFG

Österreichische Forschungsförderungsgesellschaft funded projects

Competence Headquarters Program E2-Spattertech

Austria, Project: FFGP13222004

Österreichische Forschungsförderungsgesellschaft

THANK YOU FOR YOUR ATTENTION!