

EUROPEAN ORGANIZATION FOR NUCLEAR RESEARCH

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

Direct Measurement of Self-Diffusion Jump Rates in an Intermetallic Compound

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Direct Measurement of Self Diffusion Jump Rates...

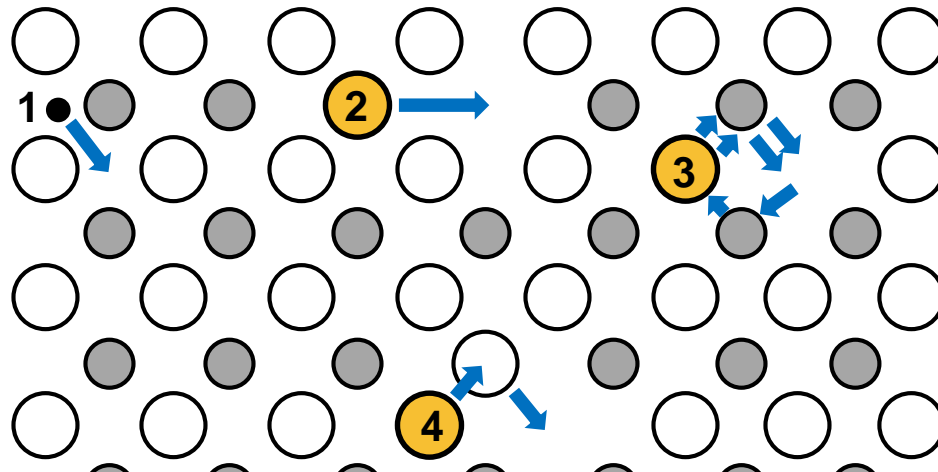
Outline

- Background
- Project description
- Why ISOLDE?
- Project feasibility
- Requested beam shifts
- Future prospects

Direct Measurement of Self Diffusion Jump Rates...

Background/Motivation

- Diffusion is of fundamental importance in **solid state reactions** → affects processing and selection of materials
- Need to understand in detail how atoms move through solids to engineer new materials



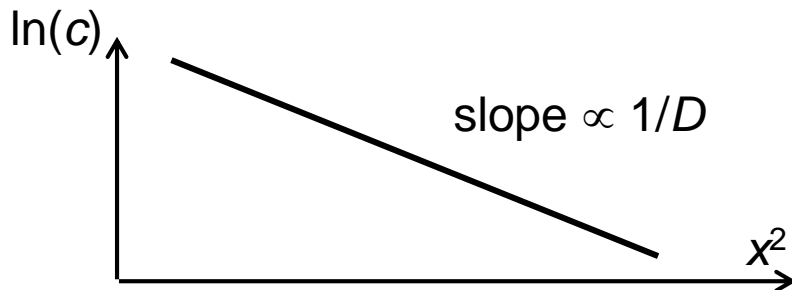
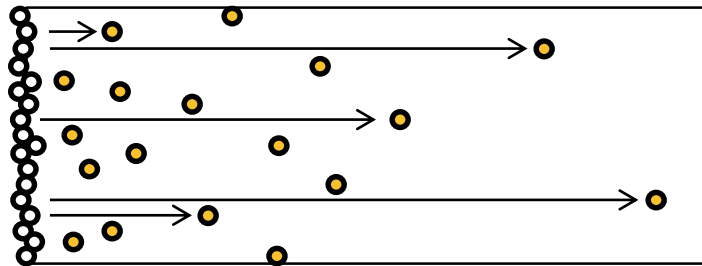
Tracers undergo **correlated** random walks in vacancy-mediated diffusion mechanisms (2-4)

- **Intermetallic compounds** interesting because atoms can move through the “wrong” sublattice

Direct Measurement of Self Diffusion Jump Rates...

Background/Motivation

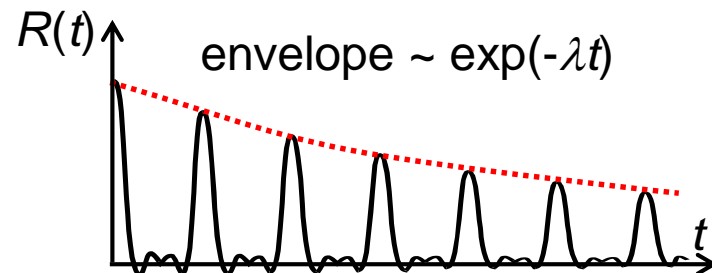
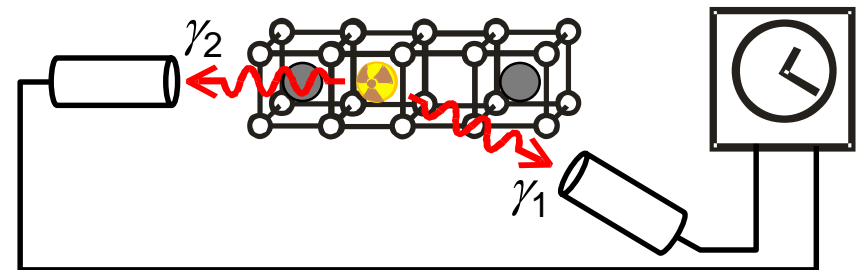
Microscopic techniques
(concentration profiling)



$$D = g \cdot a^2 \cdot f \cdot w$$

to find $f =$ correlation factor, which gives diffusion mechanism

Nuclear techniques
(PAC)



$$\lambda = g' \cdot P_{\Delta efg} \cdot w$$

Direct Measurement of Self Diffusion Jump Rates...

Project description

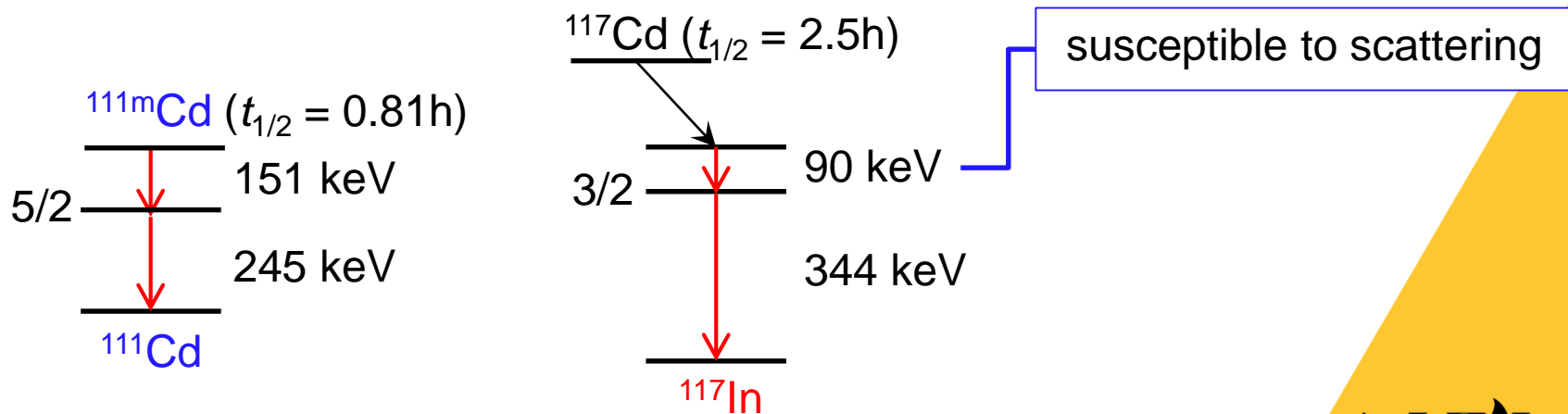
- **Goal:** first-time measurement of absolute jump rate of a tracer diffusing via a vacancy mechanism
- **Objective:** measure Cd jump rate at different temperatures and compositions in NbCd_3
- Sample preparation & characterization
 - Alloy formation at NKU
 - Compound formation verified using x-ray diffraction at NKU
- Implantation, anneals, and measurement using $^{111\text{m}}\text{Cd}$ PAC at ISOLDE

Direct Measurement of Self Diffusion Jump Rates...

Why ^{111m}Cd PAC at ISOLDE?

- Compound(s) with the $L1_2$ crystal structure are ideal
- Need isotope that substitutes for the non-cubic sublattice and is a host element to study self-diffusion
- Candidate experiments:

$^{111m}\text{Cd}/\text{Cd}$ in NbCd_3 or $^{117}\text{Cd}/\text{In}$ in $R\text{In}_3$ (R =rare earth)



- Isotopes, sample handling, and measurement facilities only available at ISOLDE

Direct Measurement of Self Diffusion Jump Rates...

Project feasibility

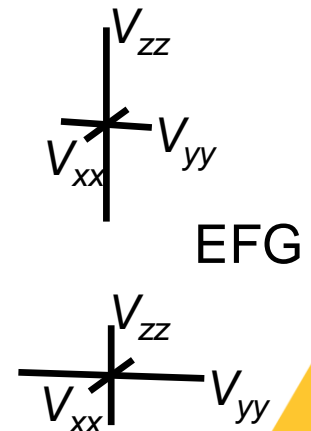
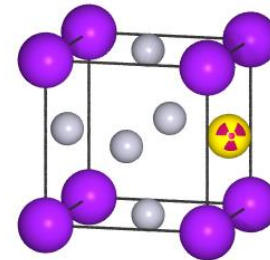
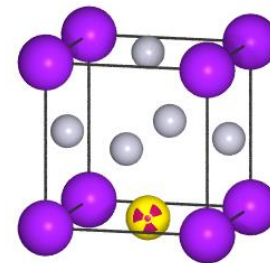
$^{111}\text{In}/\text{Cd}$ PAC used previously to measure Cd-motion-induced damping in 22 compounds with $L1_2$ structure

Indides: LaIn_3 , CeIn_3 , PrIn_3 , GdIn_3 ,
 TbIn_3 , DyIn_3 , HoIn_3 , ErIn_3 ,
 TmIn_3 , LuIn_3

Stannides: LaSn_3 , CeSn_3 , SmSn_3 , GdSn_3

Gallides: DyGa_3 , ErGa_3 , LuGa_3

Other: ErAl_3 , PrPd_3 , NdPd_3 , EuPd_3 ,
 SmPd_3

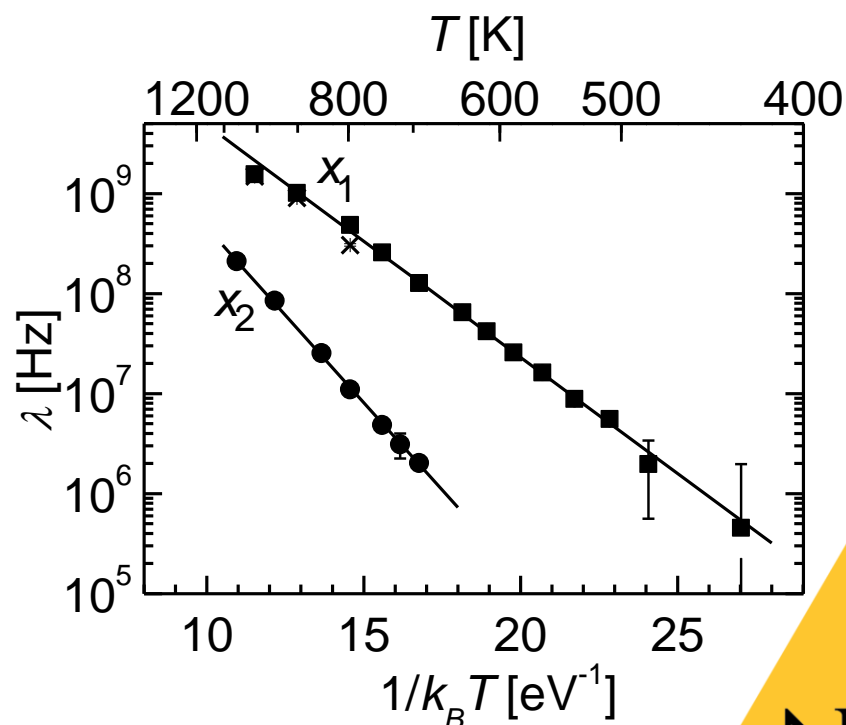
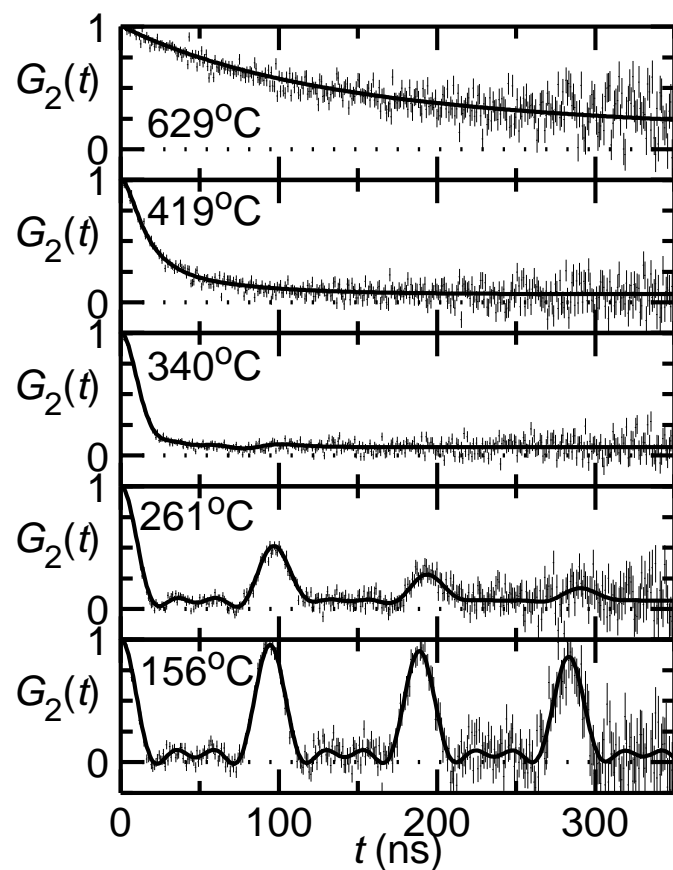


- Collins, Jiang, Bevington, Selim, Zacate. *PRL* **102**, 155901 (2009)
- Jiang, Zacate, Collins. *Def & Diff Forum* **289-292**, 725 (2009)
- Wang, Collins. *Hyperfine Interact* **221**, 85 (2013)
- Lockwood, Norman, Newhouse, Collins. *Def & Diff Forum* **311**, 159 (2011)

Direct Measurement of Self Diffusion Jump Rates...

Project feasibility

Representative results: $^{111}\text{In}/\text{Cd}$ PAC in $\text{La}_{1-4x}\text{In}_{3+4x}$



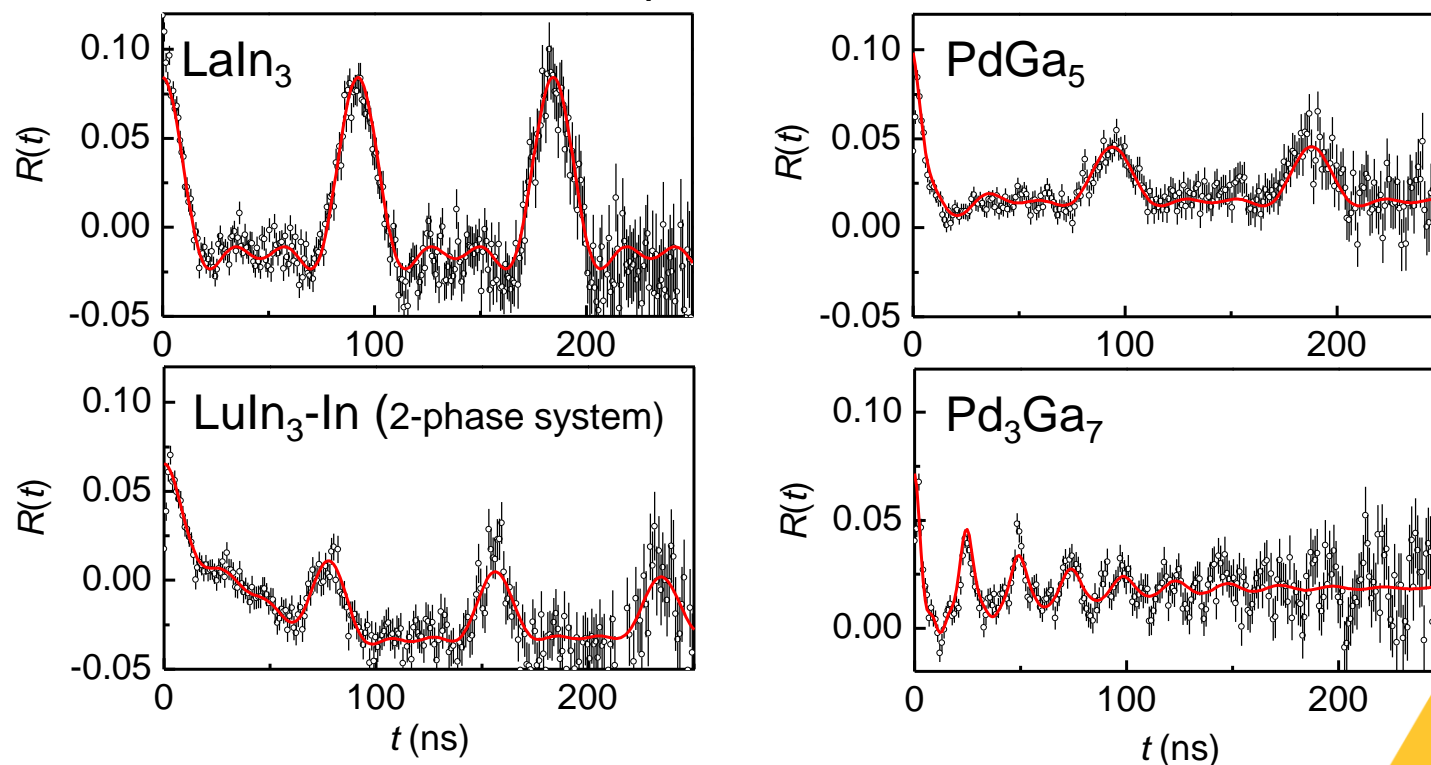
Zacate, Favrot, Collins,
PRL **92**, 225901 (2004)

Direct Measurement of Self Diffusion Jump Rates...

Project feasibility

Previous ^{111m}Cd PAC measurements in intermetallic compounds show successful removal of implantation damage (experiment IS-514).

Room temperature measurements



Direct Measurement of Self Diffusion Jump Rates...

Beam time request

Parent Isotope	$t_{1/2}$	Target	Ion source	Yield (ions/ μC)	No. of shifts
$^{111\text{m}}\text{Cd}$	48 min	Sn (molten)	VADIS	10^8	12 (2017 & 2018)

Additional notes

- Activity to be implanted into samples in the solid state collection chamber on the GLM.
- Beam times can be shared with other experiments using the $^{111\text{m}}\text{Cd}$ isotope.
- Should not interfere with experiments utilizing higher mass isotopes on the central beam line.

Summary and Future Prospects

- This project will provide a measurement of tracer jump rates for a tracer diffusing via a vacancy mechanism for the first time.
 - A follow-up measurement of vacancy concentration will allow determination of vacancy jump rates.
- This project creates framework for a more comprehensive application of PAC using short-lived isotopes to identify diffusion mechanisms in other crystal structures.
 - Concentration profiling in conjunction with PAC
 - Use of PAC to observe transient defect configurations formed near PAC tracers during diffusion.