Muon diffusion in hcp metals

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Studies of muon motion in elementary metals were done very early, and motional narrowing studies in the metals Cu, Nb, Al etc were easily done since they possess large nuclear moments. In several cases the intrinsic muon diffusion is however too fast to be seen directly by this method, and in addition many metals have too small nuclear moments. With the improved MUSR facilities with very low background like ISIS, more metals could be studied and attempts to systematics could be made, at least among the f.c.c metals. The present study contains results from measurements on h.c.p metals with large nuclear moments like Sc and La, but also some challenging measurements on h.c.p. metals with very low depolarization rates like Y, Hf, Zr and others.

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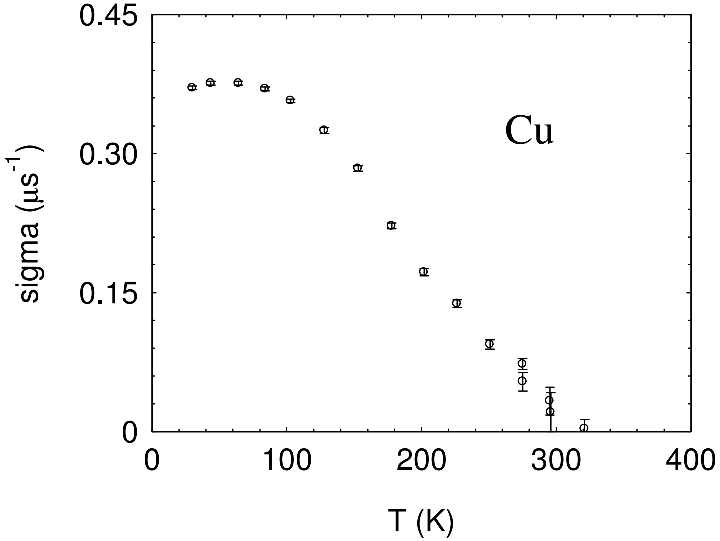
Studies of muon diffusion by motional narrowing technique.
Introduction and background:

~ 35 years ago:

Depolarization and motional narrowing in metals with <u>large</u> nuclear moments were studied. e.g. the fcc metals Cu and Al. The diffusion mechanisms for light particles in metals were investigated.

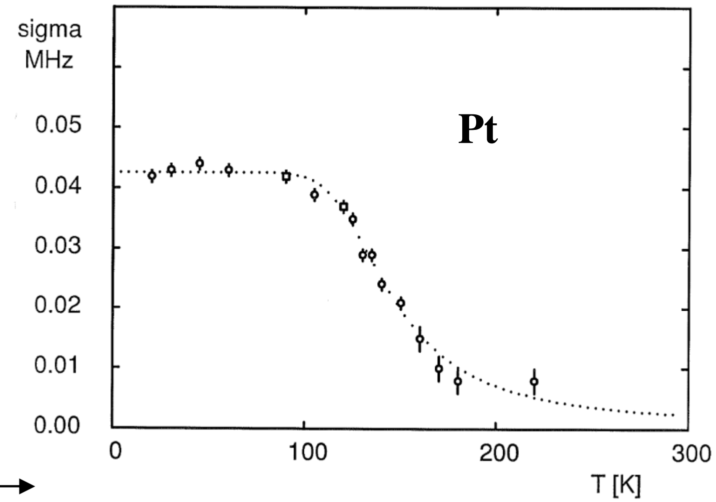
In Al, and in the bcc metals Nb and, V diffusion appaers fast and strongly influenced by trapping at impurities.

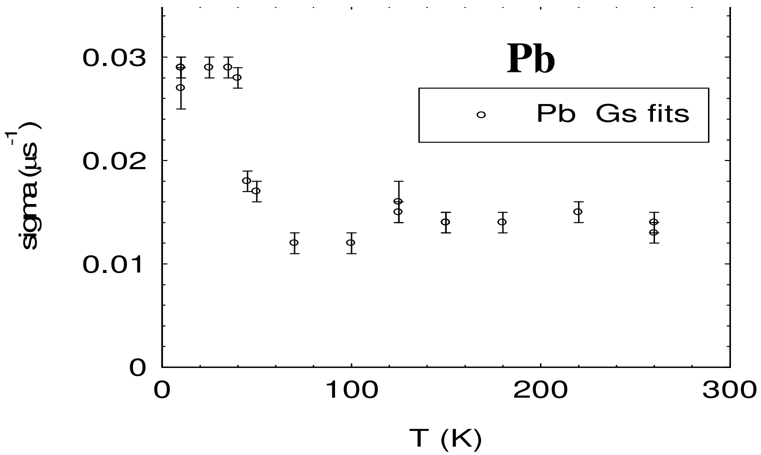


For display purposes the presented linewidth parameter is from fits to $A(t) = A(0) \exp(-\sigma^2/t^2)$.
For static muons this parameter σ is approximately the K-T Δ

~ 25 years ago.

MUSR at ISIS starts and it is possible to study lower relaxation rates. The diffusion studies in metals were extended to fcc metals Pt, Pb, Pd ("challenging studies") and others like bcc Li, Na, Mo.





~ 5 Years ago. Hcp ?

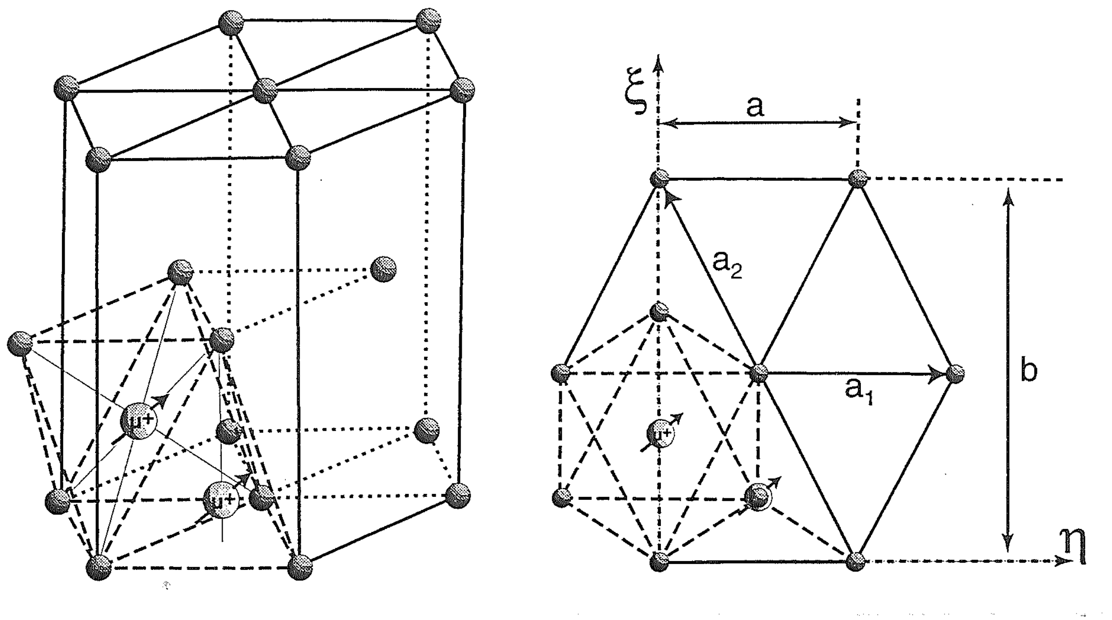
Which hcp metals are possible to study ?

Examples of static depolarization rate (μs-1) for muons in ZF, tetrahedral sites

Be 0.25 Sc 0.42 Ti 0.04 Y 0.02 Zr 0.03
Ru 0.05 La 0.17 Hf 0.03

Motivation: General interest to know if the muons is likely to be stationary while we observe the properties of its surroundings

Hcp structure and interstitial sites



Hydrogen normally in tetrahedral sites.
Muon data from magnetic metals (Gd, Co) indicate octahedral sites.

The calculated dipolar widths for muons is ~ 20% lower in octahedral sites

Comparing muon mobility to hydrogen in metals ?

Activation energy (eV) for H diffusion

fcc

Cu 0.38

Ni 0.40

Al 0.22

Pt 0.34

Pd 0.13 (T< 220 K)

Muons apperar fast moving in pure Al and Pd

bcc

Nb 0.068 (T<220 K)

V 0.045

Ta 0.040

Fe 0.105

Muons appear fast in Nb,V, Fe

Hydrogen in hcp

Activation energy (eV)

Hf 0.46

Zr 0.46

Lu 0.57

Y 0.60

Sc 0.54

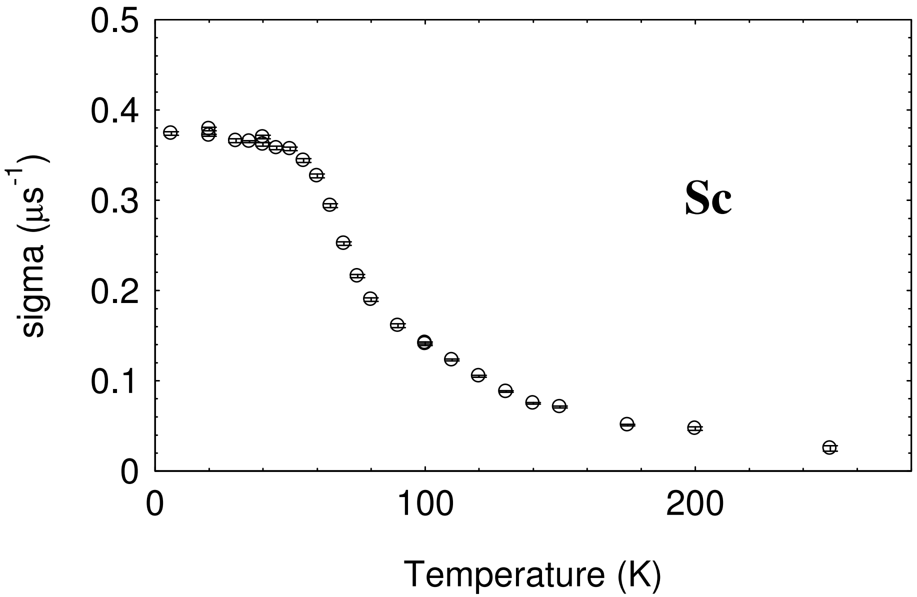
Be 0.40 (th.)

In general higher Ea than in fcc. Do we expect muons to be slow ?.

Hcp results from ISIS:

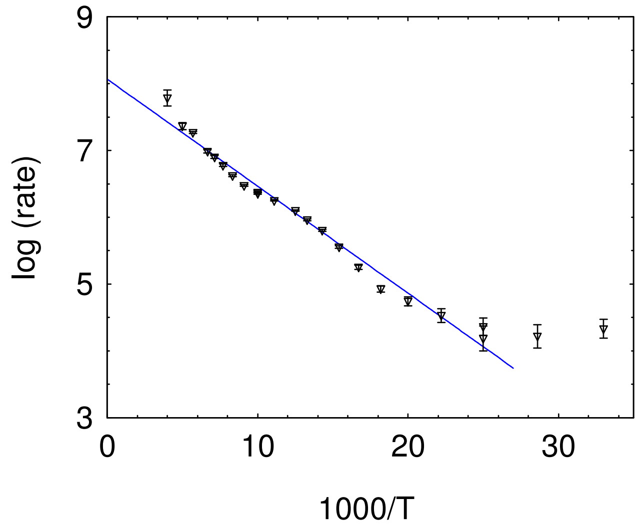
Scandium. ZF- μSR:

Sc poly initial depolarization rate 05.01



Sample = Sc polycr. 99.9 %

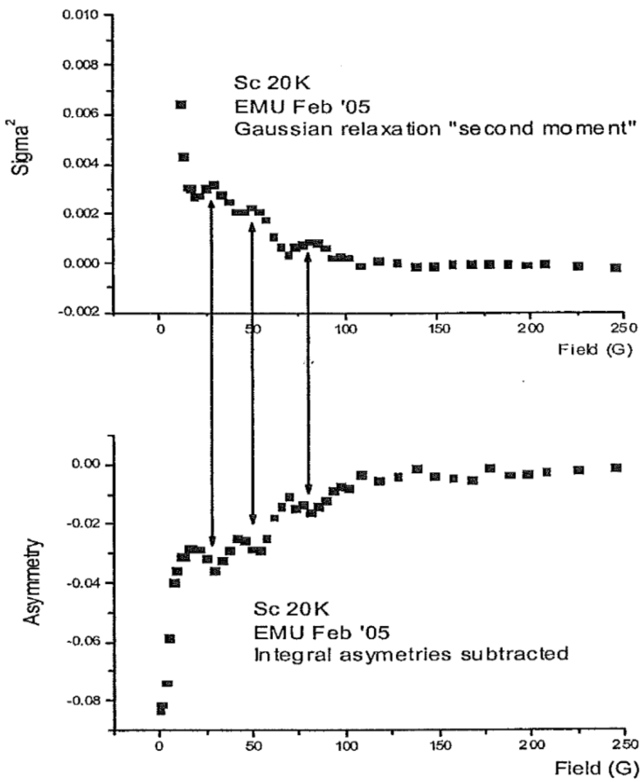
Sc. Ea = 32 meV



Diffusion activation energy 32 meV agrees well with single crystal data from Gygax et al PRB 61 168 (2000)

Level-crossing resonances in Sc.

Size of EFG in agreement with Gygax data.

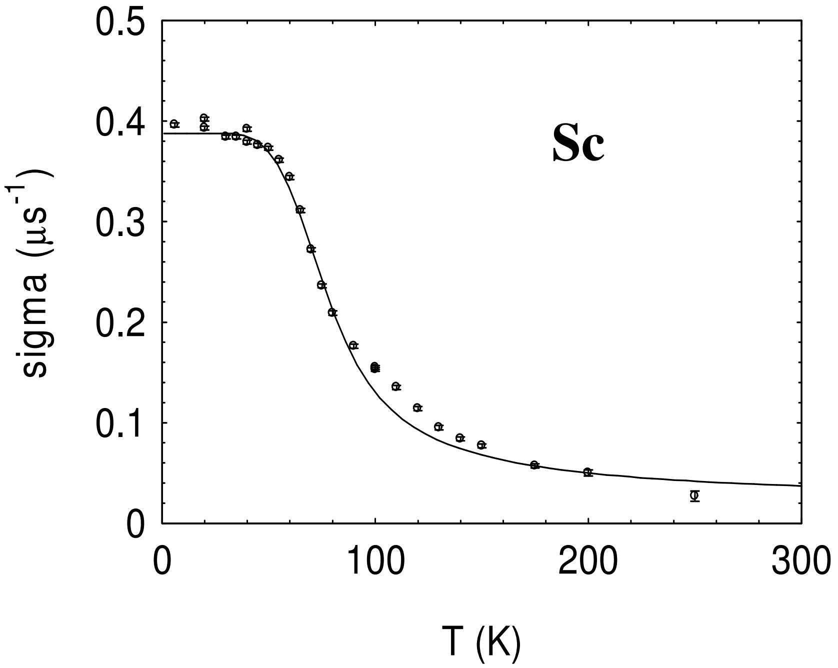


Sc and Y

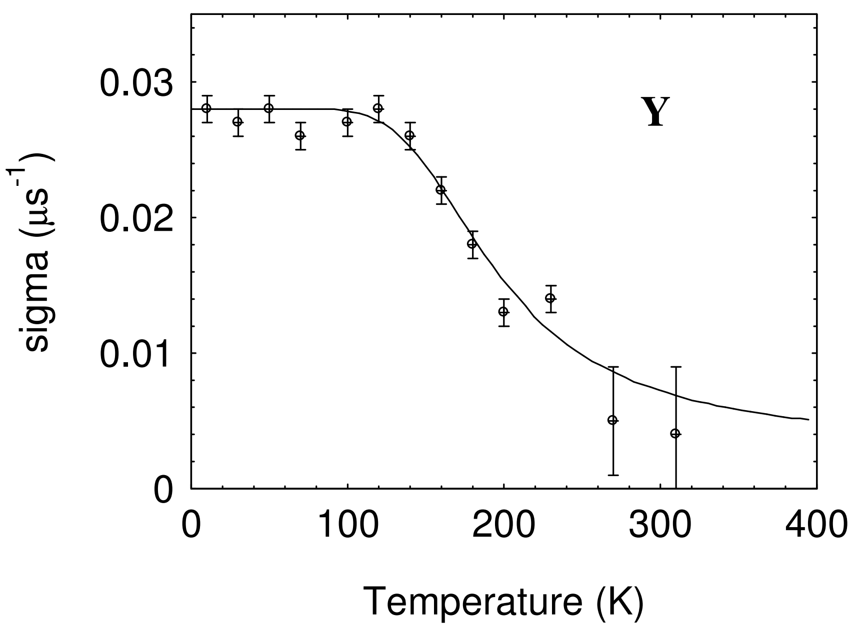
Interstitial hydrogen is normally found in tetrahedral sites in hcp metals. In Sc and Y hydrogen can also locally tunnel between two adjacent sites. The Gygax data on Sc supports a similar view for muons in Sc

The diffusion of muons appear quite different in the two metals

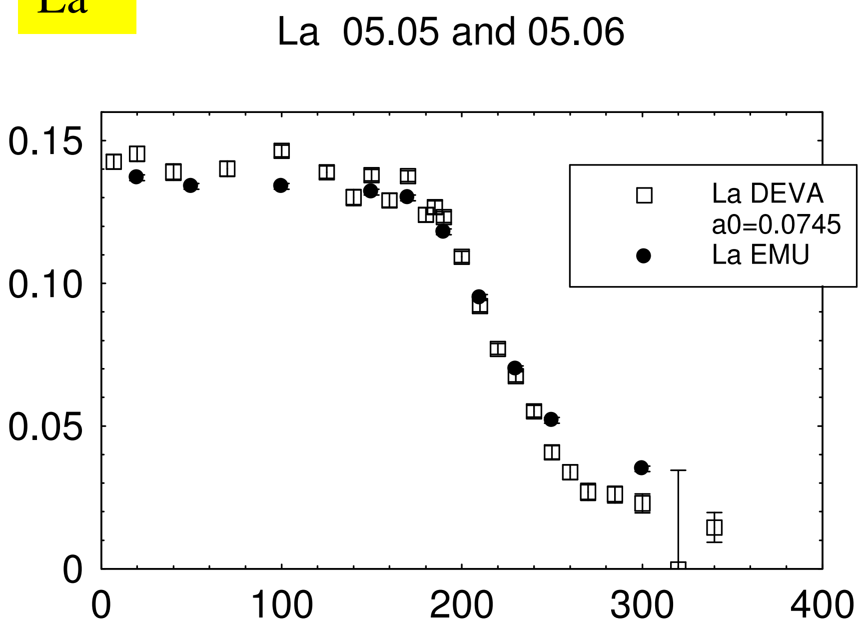
Sc Ea = 32 meV



Y metal 05-23 calc Ea=85 meV / 8.0

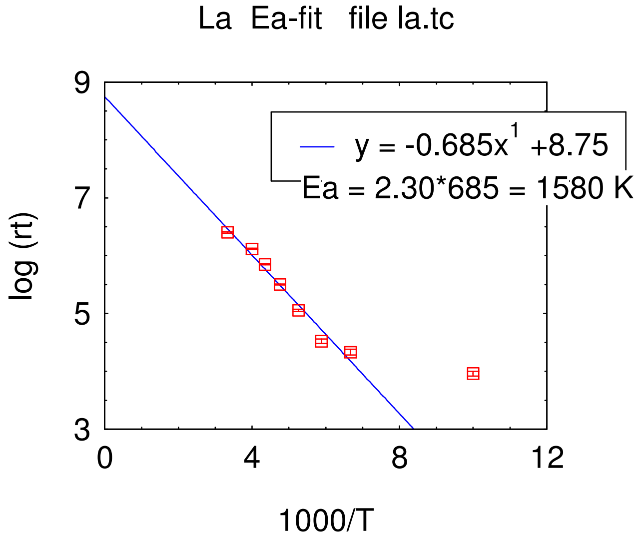


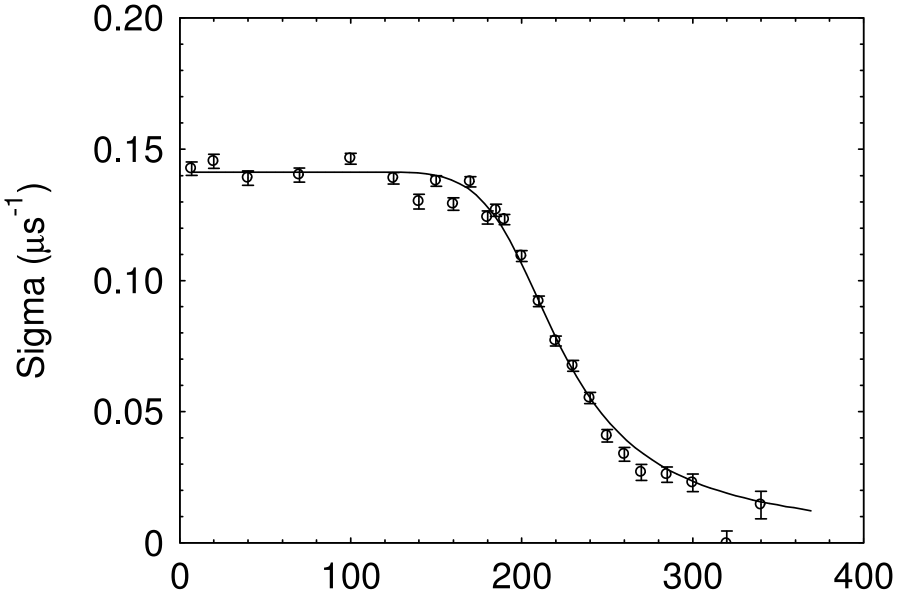
La



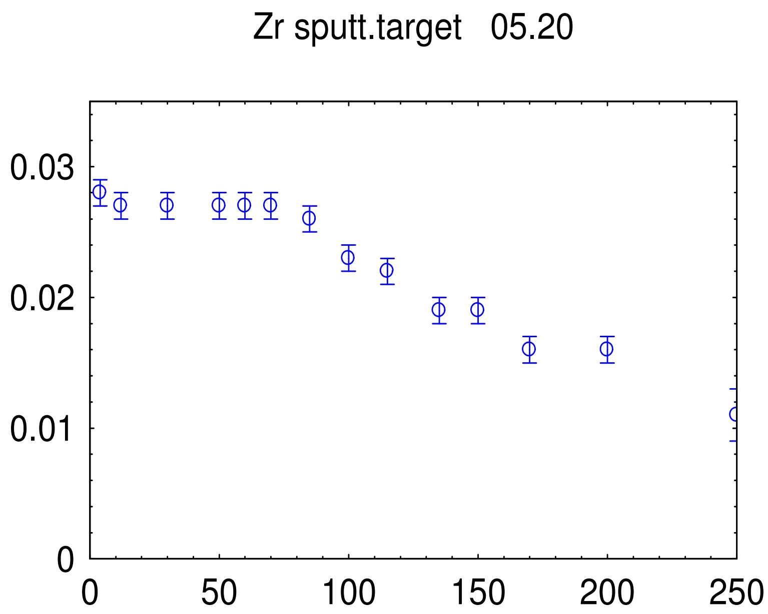
Sample = La polycrystal 99.9 %. Results from two sets of measurements

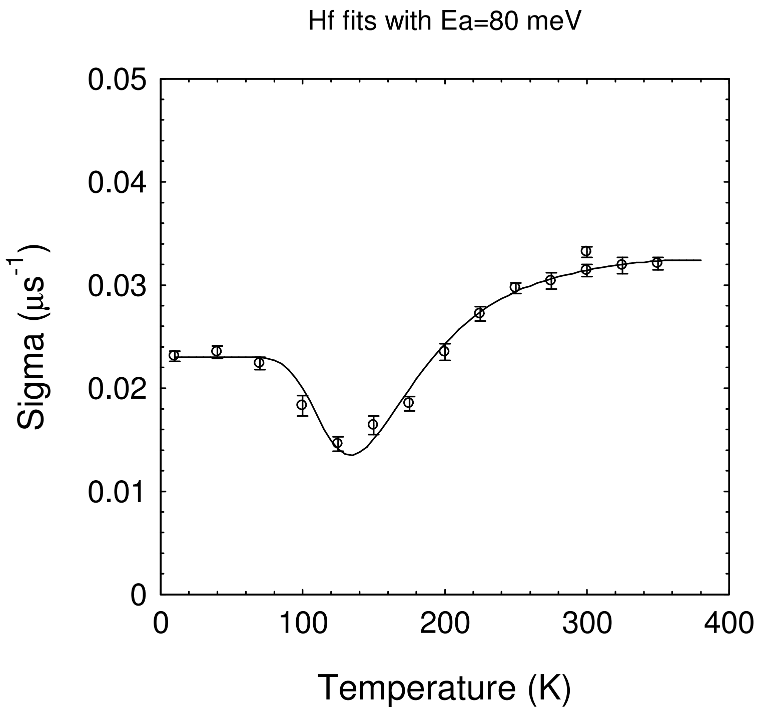
Fits with static width and activation energy as free parameters. Fitted Ea = 135 meV.





Metals with small nuclear moments. Zr, Hf …



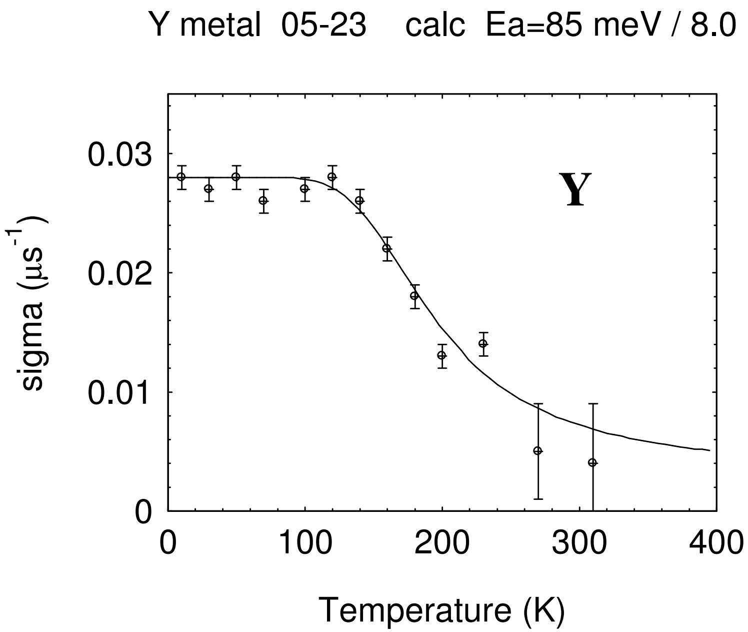


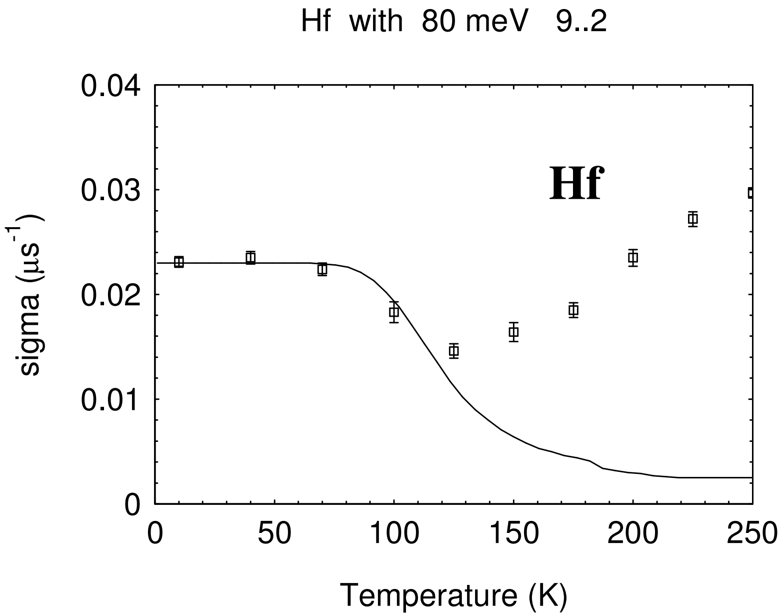
Zirconium motional narrowing above T = 100 K. This region is not well fitted by a single activation energy.
Sample purity nominally 99.9 %
. .

Hafnium is a very clear example of trapping. The two-state fit model has an eacape energy Ea = 80 meV followed by trapping to a deeper site.

Sample nominally 99.9 % except the main impurity Zr (3 %)

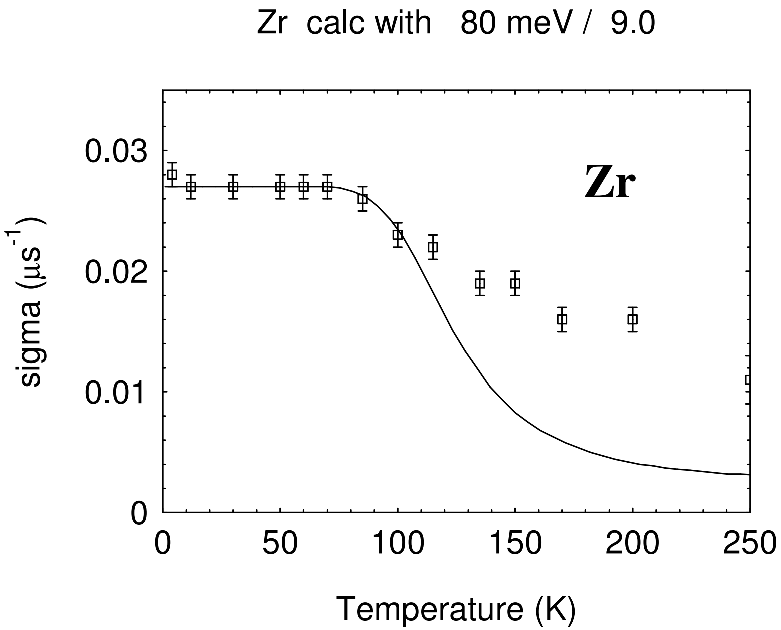
Hf Zr Y comparison





The trapping in Hf could be due to the Zr inpurities (3 %) in the sample

Similarly the Zr sample may be affected by the presence of impurities.



A look at some other hcp metals

Older muon experiments:

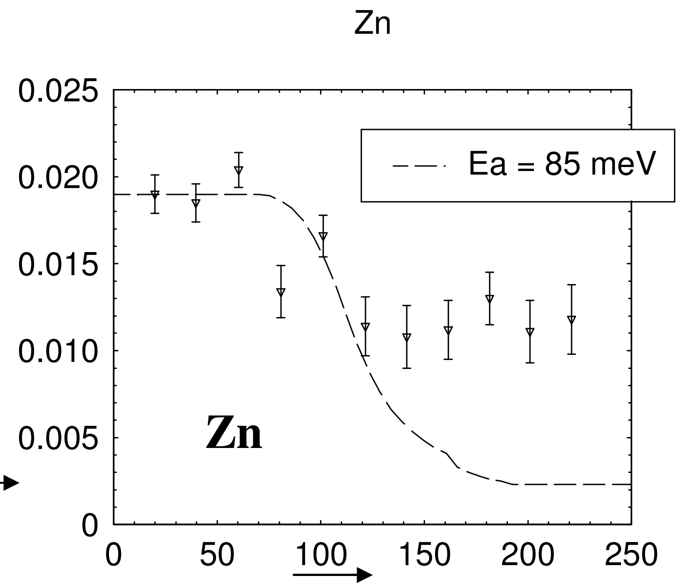
Be (Metz et al 1979) Ea = 95 meV

Zn (Gygax et al 1983) Ea = 85 meV

Dy (AFM) (Barsov et al 1986) Ea = 34 meV

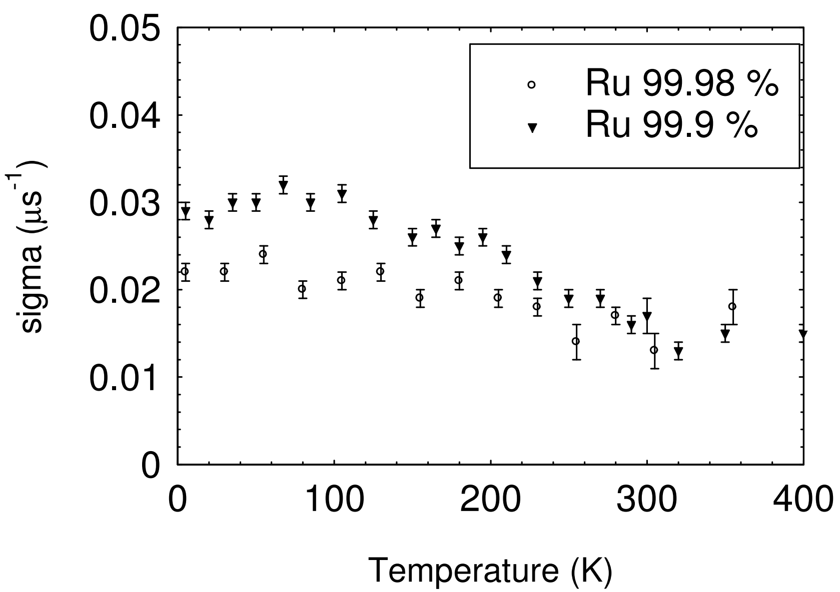
Zn A peak in Knight shift data around 300 K suggests diffusion + trapping. The diffusion interval T = 100 -270 K was fitted with Ea = 85 (10) meV (Gygax et al PRL 51 1983.

An ISIS measurement on Zn suggests mobility starting around 100 K, and is compatible with Ea = 85 meV

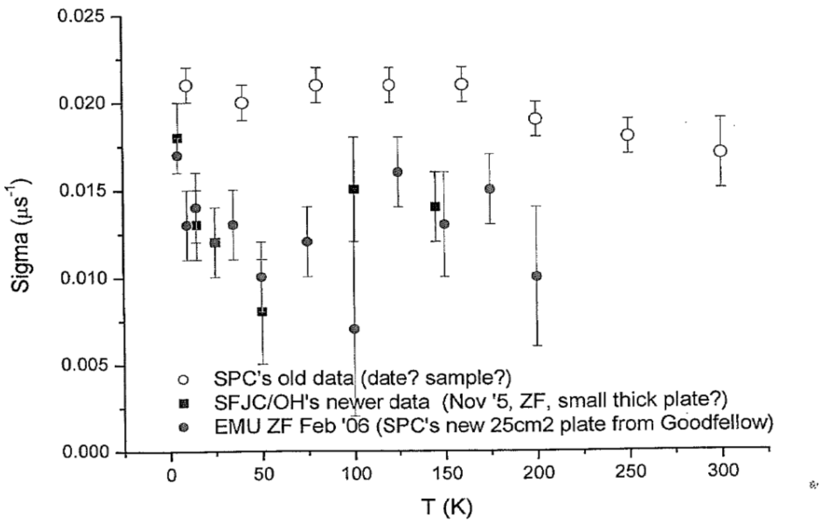


Two hcp metals where diffusion and trapping at defects dominates

Ruthenium

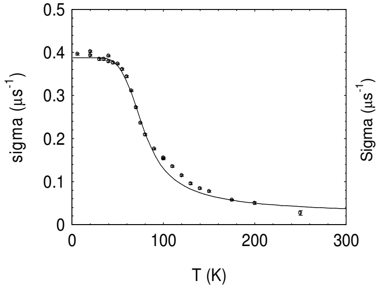


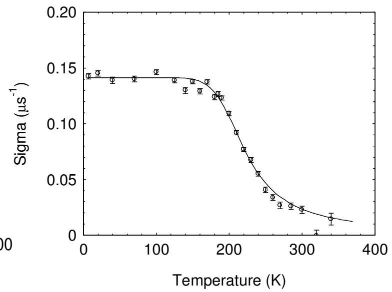
Ruthenium with expected static width 0.045 μs-1 Results from two different samples

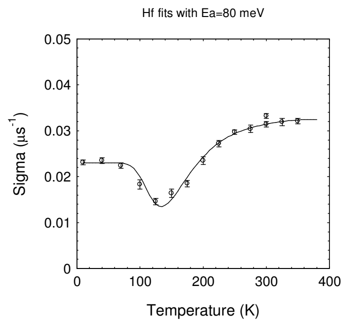


Titanium shows clear evidence of trapping at impurities. The low static width (0.02 μs^{-1}) is lower than expected, and makes detailed analysis difficult.

SUMMARY







This study of muon diffusion in hcp metals aims mainly at the question if the muons are likely to be stationary in the lattice during their lifteime, and in what temperature range muon motion is likely to set in.

In hcp metals and also in some of the fcc metals a typical range of diffusion to set in is 50-150 K with activation energies 50-100 meV. The prefactors for the diffusion are typically 10^8 - 10^9 s^{-1} In both types of structures there are exceptions (Al, Pd, Ru, Ti) where motion and localization to a large extent appearas to be affected by trapping at defects.

The measurement of the very low depolarization rates in some of these metals has been possible due to the development of modern MUSR facilities like ISIS