NEUTRON SPECTROSCOPY OF FAST HYDROGEN DIFFUSION IN BCC TRANSITION METALS*

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ABSTRACT

Quasielastic neutron scattering reveals microscopic details of both the time and space development of the H-diffusion process on an atomic scale. After outlining the method on the example of PdH_x, new results on the jump geometry in bcc metals are surveyed. In particular, the anomalous diffusion behavior of H in Nb, Ta, and V at elevated temperature is emphasized, where correlated jump processes are important. The influence of impurities on the H-diffusion process is demonstrated by experiments performed on NbH_x doped with nitrogen impurities, which act as trapping centers for the diffusing hydrogen. The results are discussed in terms of a two-state random walk model which includes multiple trapping and detrapping processes. The concentration and temperature dependence of the capture and escape rates of traps are obtained.

INTRODUCTION

H dissolved in transition metals exhibits a
large number of anomalous properties which are
mainly related to the smallness of the H atom
(1,2,3). The time scale of motion e.g. is ex-
tremely short. The characteristic frequencies
of the localized modes of H in Ta, Nb or V are
in the order of 10^{-14} sec; the jump frequencies
for H diffusion at elevated temperatures are be-
tween 10^{12} and 10^{13} sec $^{-1}$ which is comparable
to the correlation times for diffusion in
liquids and more than ten orders of magnitudes
larger than e.g. the jump frequencies for N or
O in Nb.

For the investigation of the fast H-diffusion in
these metals quasielastic neutron scattering
(QNS) is a unique tool which reveals microscopic
details of both the space and the time develop-
ment of the diffusive process on an atomic
scale. This paper surveys three diffusion exper-
iments which demonstrate the capabilities of the
method. In the second chapter we outline the
method on the 'classic' example of H diffusion
in Pd(4) where the H interstial sites form a
Bravais sublattice and jumps occur only between
nearest neighbor sites. In chapter 3 we deal
with H-diffusion in bcc metals. Here a compli-
cated non Bravais H-sublattice and severe devia-
tions from a simple nearest neighbor jump model
have made an understanding more difficult. New
results on the jump geometry and with special em-
phasis to the anomalous behavior at elevated tem-
peratures, where correlated jump processes are
important, are reviewed (5,6). The influence of
impurities or defects which are present in each
real system on the H diffusion is treated in
chapter 4. Their trapping capability has been
concluded firstly from thermodynamic data (7).
Resistivity (8), internal friction (9) and
Gorsky effect (10) experiments reveal further ev-
idence for the trapping process. The contribu-
tion of neutron scattering to the understanding
of H-trapping at impurities in metals is
outlined on the example of H diffusion in Nb
doped with nitrogen impurities (11).

APPLICATION OF QUASIELASTIC NEUTRON SCATTERING TO THE INVESTIGATION OF H-DIFFUSION IN METALS - BASIC CONCEPT

In the case of hydrogen which scatters predomi-
nantly incoherent a QNS-experiment reveals infor-
mation on the behavior of single protons in
space and time (12). Following the concept of
van Hove (13) the observed double differential
cross section $\partial^2\sigma/\partial\omega\partial\Omega$ is proportional to the
Fourier transform of the self-correlation func-
tion $G_s(r,t)$ of the proton

$$\frac{\partial^2 \sigma}{\partial\omega\partial\Omega} \sim S_{inc}(\vec{Q},\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt$$

$$\int_{-\infty}^{+\infty} d^3r \; e^{i(\vec{Q}\vec{r}-\omega t)} \; G_s(\vec{r},t) \tag{1}$$

where $S_{inc}(\vec{Q},\Omega)$ is the so-called incoherent scattering law, $\vec{Q} = \hbar\vec{K}_f - \hbar\vec{K}_i$ is the momentum transfer and $\hbar\omega = E_f - E_i$ is the energy transfer at the sample. In the classical limit $G_s(\vec{r},t)$ can be interpreted as the conditional probability to find a proton at a time t at a site $\vec{r}$ if it has been at $\vec{r} = 0$ for $t=0$. The results of QNS experiments on H-diffusion are commonly interpreted in terms of the Chudley-Elliott model (CE) (14) which introduces the following assumptions:

(i) the jump time from site to site is small compared to the mean rest time of hydrogen on its interstitial site.

(ii) there is no correlation between vibration and jump processes.

Under these circumstances the self-correlation function can be obtained by solving a master equation:

$$\frac{\partial}{\partial t} G_s(\vec{r},t) = \frac{1}{z\tau} \sum_{i=1}^{z} (G_s(\vec{r}+\vec{S}_i,t) - G_s(\vec{r},t)) \tag{2}$$

where $\vec{S}_i$ are the jump vectors to the accessible neighboring sites, z is the number of these sites and τ the mean rest time at a certain site. Eq. (2) can be integrated by a Fourier transformation yielding in the case of Bravais lattices:

$$\frac{\partial}{\partial t} G_s(\vec{Q},t) = -\frac{1}{z\tau} \sum_{i=1}^{z} (1-e^{i\vec{Q}\vec{S}_i}) G_s(\vec{Q},t) \tag{3}$$

$$= \frac{1}{\tau} f(\vec{Q}) \; G_s(\vec{Q},t)$$

$$G_s(\vec{Q},t) = e^{-\frac{t}{\tau}f(\vec{Q})} \tag{4}$$

$G_s(Q,t)$ fulfills already the appropriate initial condition. Finally, Fourier transformation with respect to the time yields

$$\text{Sinc}(\vec{Q},\omega) = \frac{1}{\pi} \frac{f(\vec{Q})/t}{[\frac{f(\vec{Q})}{\tau}]^2 + \omega^2} \quad (5)$$

The intensity of the quasielastic line can be described by a the Debye-Waller – or form factor $\exp - 1/3Q^2 \langle u^2 \rangle$, where $\langle u^2 \rangle$ is the mean-square displacement of the proton at its site. Using the diffusion of H in Pd as an example we outline briefly what kind of information can be obtained from an investigation of the $\vec{Q}$ and ω-dependence of the quasielastic scattering law. Fig. 1 shows the two possible interstitial sites for hydrogen in fcc Pd together with the jump vectors to nearest-neighbor sites.

For equal diffusion coefficients the mean rest time for octahedral jumps is twice as large as for tetrahedral jumps. For both models the functions $f(\vec{Q})$ can be easily calculated yielding:

$$f_o(\vec{Q}) = \frac{1}{6}\{6 - \cos\frac{a}{2}(Q_x+Q_y) - \cos\frac{a}{2}(Q_x-Q_y)$$

$$- \cos\frac{a}{2}(Q_x+Q_z) - \cos\frac{a}{2}(Q_x-Q_z)$$

$$(6)$$

$$- \cos\frac{a}{2}(Q_y+Q_z) - \cos\frac{a}{2}(Q_y-Q_z)\}$$

$$f_t(\vec{Q}) = \frac{1}{3}\{3 - \cos\frac{a}{2}Q_x - \cos\frac{a}{2}Q_y - \cos\frac{a}{2}Q_z\} \quad (7)$$

For small momentum transfers $\hbar\vec{Q}$ the width $\Gamma(\vec{Q})=\tau^{-1} f(\vec{Q})$ of the Lorentzian is independent of the jump model $\Gamma(\vec{Q}) = \hbar D Q^2$. It reveals the macroscopic diffusion coefficient measured over microscopic distances. The $\vec{Q}$ dependence of line width at large $\vec{Q}$'s is determined by the geometrical details of the jump mechanism. For fcc-Pd Fig. 2 shows the theoretical $\vec{Q}$ dependence of line width for the models in question. The experimental points (4) are clearly in favor for H jumps between nearest-neighbor octahedral sites. With respect to the high barrier and the large spacing between the interstitial sites this result is quite reasonable.

RECENT RESULTS ON H-DIFFUSION IN THE BCC METALS
Ta, Nb and V

For the bcc metals with their complicated hydrogen sublattice (6 sites per unit cell) (Fig. 3), the situation is much more complicated. Besides the complication due to the

non-Bravais-E-sublattice, there is experimental
evidence that the diffusion process itself is
not as simple as for the fcc metals. Already
earlier results on V (15) Ta (16) and Nb (17)
showed systematic deviations from the predic-
tions of a simple nearest-neighbor jump model.
Also, anomalies in the intensity of the
quasielastic line have been reported (15,18).
These anomalies have been attributed to the oc-
currence of further neighbor jumps and/or to
jumps between different types of institial sites
(15,16) and to the influence of a finite time of
flight (19) but no conclusive picture has been
reached.

Very recently, Lottner et al. (5,6) have
reexamined the problem for Ta, Nb, and V.
Quasielastic neutron scat-ering experiments
where performed at $NbH_{0.02}$, $TaH_{0.13}$ and $VH_{0.07}$
single crystals at temperatures between 290 and
760 K for Q values between 0.3 and 2.5 $\mathring{A}^{-1}$.
The data were analyzed in terms of 4 different
models always assuming that H jumps occur be-
tween tetrahedral sites.

Model (1): Hydrogen jumps occur only between
nearest neighbor sites with jump vectors in
(110) direction and a jump rate $1/\tau_1$.

Model (2): In extension to model (1) also jumps
to second nearest neighbors are included. They
occur in (100) direction across the cube face
center with a jump rate $1/\tau_2$.

Model (3): Assumes that in addition to near-
est-neighbor jumps correlated double jumps are
possible. The corresponding jump rate is $1/\tau_2$.

Model (4): Generalizes model (3). It considers
the H alternatively in a mobile "state" (life
time τ_1), where it can perform repeated jumps to
nearest neighbors with a jump rate $1/\tau_1$, and in
an immobile self-trapped "state" (life time τ_t).
The exchange between both "states" is described
by transition rates given by the inverse life
times. This concept is formal identical to the
treatment of H diffusion in the presence of
trapping impurities (20) which will be discussed
later on.

Model (1) includes 2 independent parameters, the
jump rate $1/\tau_1$ and the quasielastic intensity
I(Q), models (2) and (3) have 3 parameters and
finally (4) is a four-parameter model. While at
room temperature model (1) explains the experi-
mental data sufficiently well, at higher tempera-
tures a decrease of $1/\tau_1$, with increasing Q has
been found. This decrease can be understood
qualitatively as an increase of the effective
jump length. Fig. 4 presents results obtained
by an analysis of the high temperature data with
the models (2) to (4). The jump rates calcu-

lated by a simultaneous fit of the spectra measured at different Q values for one crystal orientation ϕ are plotted vs ϕ. For a correct description of the data the obtained jump rates should not depend on the crystal direction. Fig. 4 makes it clear that the extension of model (1) to jumps to next-nearest neighbors does not solve the problem whereas the assumption of correlated jumps leads to a satisfactory agreement between theory and experiment. Similarly, also for H in Ta and V, the simple jump model (1) fails to explain the data at elevated temperatures, whereas model (3) seems to lead to an adequate description of the experimental results also for Ta and V. Model (4) has not been used for the data analysis for Ta and V. However, the large ratio τ_1/τ_2 found for the contribution of double jumps makes the application of model (4) desirable.

The authors do not specify the physical origin of the occurrence of correlated jumps. Here the relation between the jump rate and lattice relaxation time τ_r, the time the lattice needs to dissipate the energy necessary to produce the jump, may be important. For the case of electronic small polaron hopping Emin has shown (21,22) that for times short compared to τ_r the energy required for a successive jump is only 1/3 of the activation energy in the relaxed lattice. However, the involved electronic hopping rates were in the order of 10^{+14} s^{-1}. In view of the much smaller jump rates of the proton 10^{+12} - 10^{+13} s^{-1} on the one hand and the differences in the coupling to the lattice on the other hand, it is not clear, whether this concept is applicable. Quantitative calculations are necessary.

The Q dependence of the quasielastic intensity evaluated from this experiment follows a normal Debye-Waller factor (DWF) behavior with mean-square amplitudes for the H-motion of $1/3 \langle u^2 \rangle$ = 0.02 -0.04 Å^2 which is near to the value expected from harmonic calculations (5). For V an anomalous decrease of the intensity has been observed at larger Q values and high temperature (T = 763 K) which was attributed to non-negligible jump times (5,6). The normal DWF evaluated for Nb and Ta even at high temperatures is in contrast to earlier reports of an anomalous behavior, which was mainly caused by errors in the integration of the quasielastic spectrum neglecting wing contributions. The observation of a normal DWF shows that the proton is well localized at its interstitial site contrary to earlier speculations about an extended proton wave function (23).

THE INFLUENCE OF IMPURITIES ON H-DIFFUSION
IN METALS

Numerous investigations have demonstrated that
the physical properties of H dissolved in bcc-
transition metals are strongly changed by the
presence of small amounts of impurities.
Thermodynamic data like equilibrium H pressure
(7,24) or H solubility (25) are sensitive to in-
terstitial impurities or cold working. Resistiv-
ity experiments on Nb-H doped with N (8) yield
a reduced residual H-resistivity at temperatures
well above the phase boundary to the β-phase.
Furthermore, Gorsky-effect measurements in
NbN_xH_y samples (10) showed a strong decrease of
the H-diffusion coefficient in particular at
lower temperatures. Finally, in the presence of
O- and N-impurities in the Nb-H system
additional relaxation peaks in internal friction
experiments are observed (9). All these
features are naturally explained in terms of H
trapping at the impurities. In their vicinity
they lower the ground state energy for the H.
This increases the enthalpie of solution and
changes thereby the equilibrium properties of
the system. Trapping implies the formation of
impurity hydrogen pairs. They are assumed to
scatter conduction electrons with a smaller prob-
ability than the two single scattering centers
and they give rise to relaxation processes in in-
ternal fraction experiments. Such trapping
processes also slow down the long range
diffusion. The significance of the trapping
processes will increase with increasing ratio of
binding energy and thermal energy kT.

On a microsopic level, the influence of intersti-
tial impurities on the H-diffusion process was
studied recently by quasielastic neutron
scattering on Nb-H samples doped with nitrogen
impurities (11). For low concentrations of
trapping impurities, where trapping regions and
regions of undisturbed host material are
present, relatively simple arguments can be
given, in order to explain what kind of informa-
tion can be obtained from a quasielastic neutron
scattering experiment. For small momentum
transfers, the scattering process averages over
large volumes in space (of the order $(2\pi/Q)^3$).
Therefore, a long section of the diffusive path
of the proton will be probed by the neutron wave
packet. This path consists out of periods of
undisturbed diffusion as well as of portions
where the proton is trapped. Under these
circumstances, the scattering law is expected to
be a single Lorentzian whose width is given by
the effective or macroscopic H-diffusion
coefficient D_{eff} in the system. At large Q's,
however, the average occurs over short distances
and the scattering law depends on the single dif-
fusive step. In this case, the scattering law

contains information about the mean trapping
time and on the fraction of protons being
trapped.

Quantitatively, the scattering law has been cal-
culated in terms of a phenomenological two-state
random walk model (RWM) thereby approximating
the complicated structure of the trapping region
around the impurity by a single escape rate
$1/\tau_o$. This approach was confirmed later using
the average T-matrix approximation in the limit
of dilute concentration of traps (26). We
survey briefly the RWM approach. Here it is
assumed that the proton diffuses in a crystal
with randomly distributed traps. The proton
diffuses e.g. through the undisturbed parts of
the lattice for an average time τ_1 exhibiting
jumps with the jump rate of the undisturbed
lattice $1/\tau$. Thereafter, it is trapped at the
impurity for an average time τ_o. Thus $1/\tau_1$ is
the trapping rate and $1/\tau_o$ the escape rate. The
self-correlation function is easily calculated
using the self-correlation functions of the
proton in the undisturbed lattice and in the
trapped state. The mathematical procedure is
outlined in detail in Ref. (11). The result for
the incoherent scattering law is a superposition
of two Lorentzians with widths Λ_1 and Λ_2 and
weights R_1 and R_2. $\Lambda(\vec{Q})$ is the line width in
the undisturbed lattice.

$$S_{inc}(\vec{Q},\omega) = R_1 \frac{\Lambda_1/\pi}{\Lambda_1^2+\omega^2} + (1-R_1) \frac{\Lambda_2}{\Lambda_2^2+\omega^2} \qquad (8)$$

$$W = \{(\tau_o^{-1} + \tau_1^{-1} + \Lambda(\vec{Q}))^2 - 4\Lambda(\vec{Q})/\tau_o\}^{\frac{1}{2}}$$

$$\Lambda_{1/2} = \frac{1}{2}(\tau_o^{-1} + \tau_1^{-1} + \Lambda(Q)) \pm \frac{1}{2} W \qquad (9)$$

$$R_1 = \frac{1}{2} + \frac{1}{2}(\Lambda(\vec{Q}) \frac{\tau_1-\tau_o}{\tau_1+\tau_o} - \tau_1^{-1} - \tau_o^{-1})/W \qquad (10)$$

The typical properties of the scattering law are
shown in Fig. 5, where the widths Λ_1 and Λ_2 of
the two components are plotted together with
their weights vs. DQ^2. Included also is $\Lambda(\vec{Q})$
of the undisturbed lattice. For the sake of
simplicity the calculations are made for a
simple cubic lattice. Using the average T-
matrix approach, explicit expressions for $1/\tau_1$
and $1/\tau_o$ were found (26). The leading term of
the escape rate $1/\tau_o$ is independent of the trap
concentration whereas the trapping rate $1/\tau_1$ is
proportional to the concentration as expected.

Quasielastic neutron scattering experiments were carried out on Nb samples doped with N and H. The N-concentrations were $C_N^1 = 0.7\%$ and $C_N^2 = 0.4\%$. The corresponding H concentrations were $C_H^1 = 0.4\%$ and $C_H^2 = 0.3\%$. The experiments have been performed in a temperature range $180 \le T \le 373$ K for $0.1 \le Q$ 1.9 $\mathring{A}^{-1}$, using the high-resolution back-scattering spectrometer at the ILL Grenoble. The experimental spectra for $Q \le 0.9$ $\mathring{A}^{-1}$ (see below) were fitted with the scattering law of the RWM, τ_0 and τ_1 being the only disposable parameters. The result is presented in Fig. 6. Compared to typical jump rates τ^{-1} of 10^{+11} jump/sec τ_0 and τ_1 are two orders of magnitude smaller. At higher temperatures $\tau_1 > \tau_0$ holds; the protons are mainly in undisturbed regions. At lower temperatures, we have $\tau_1 < \tau_0$, the protons are predominantly trapped. τ_0 as a local property of the traps does not depend on the N-concentration justifying the assumption of well-separated trapping and undisturbed regions in the lattice. From the activation energy of $1/\tau_0$ (166 meV) a binding energy of approximately 100 meV for the N-H pair can be deduced. The capture rate $1/\tau_1$ depends on the N-concentration. The ratio of $1/\tau_1$ for the two N-concentrations of 1.8 ± 0.2 compared to the ratio of N-concentrations of 1.9 ± 0.2 is in agreement with theory (26). According to the average T-matrix approximation as well as to results of simple reaction theory for trapping (27) which yields

$$1/\tau_1 = 4\pi R_t D c_t \qquad (11)$$

where R_t is the trapping radius and C_t is the trap concentration, the activation energy for $1/\tau_1$ should agree with the activation energy for the self-diffusion coefficient D. The resulting higher values (94 meV) can be explained by the assumption that the nitrogen impurities are saturated as soon as they have trapped a single hydrogen (see also Ref. 8). After correction for saturation effects Eq. (12) allows the evaluation of the trapping radius R_t. Values in the order of 5 $\mathring{A}$ result which are in good agreement with calculations using anisotropic continuum theory. Furthermore, the mean-free path between two trapping events can be calculated. It decreases with increasing temperature demonstrating the saturation effects of the traps. Its absolute value is slightly larger than the mean distance between the nitrogen impurities. Summarizing, the simple two-state RWM represents the experimental results below Q = 0.9 $\mathring{A}^{-1}$ very well. It has been shown that it is also applicable to muon diffusion in the presence of traps (28). Also problems of chemical reactions implying hydrogen atoms might be treated with such a model.

At large Q-values, where only the narrow component in the spectrum is observed, a direct determination of the escape rate $1/\tau_0$ should be possible. However, already the small activation energy of the line width $\Gamma(T)$ at $Q = 1.9 \text{ Å}^{-1}$ of 115 meV (11) compared to the expected value of 170 meV shows that the connection between $\Gamma(T)$ and the escape process is more intricate than expected. Here the detailed structure of the trapping region around the nitrogen interstitial influences the scattering law. For a detailed discussion we refer to the literature (29,30).

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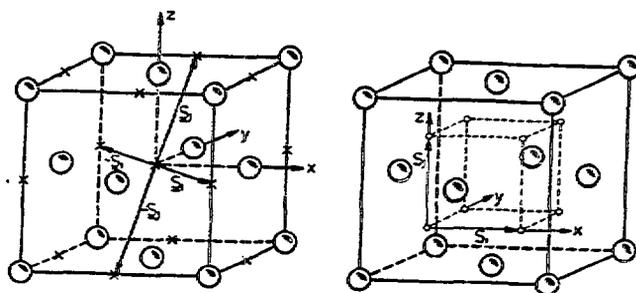30. K. W. Kehr, D. Richter, K. Schroeder, IAEA - Report SM 219/24, Vienna (1978).

Fig. 1. Possible H-interstitial sites in fcc-Pd,
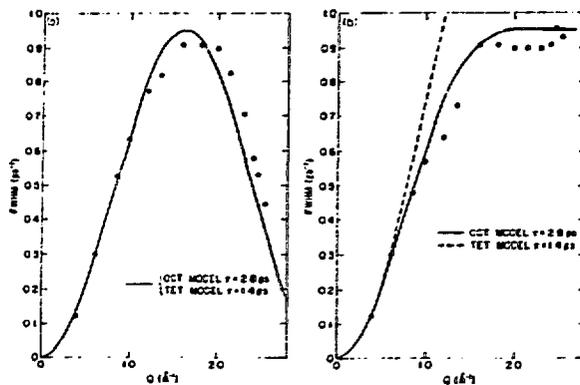O Pd atoms, x octahedral sites, O tetrahedral
sites, Si H jump vectors.

Fig. 2. Experimental results for the quasielastic
line width in PdH$_x$ for a (100) (left) and a (110)
direction; solid line: octahedral jump model,
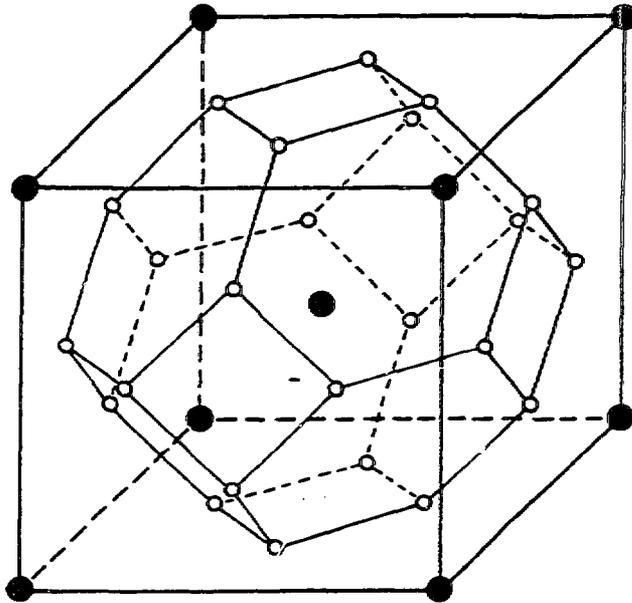dashed line tetrahedral jump model (4).

Fig. 3. Hydrogen sublattice for tetrahedral
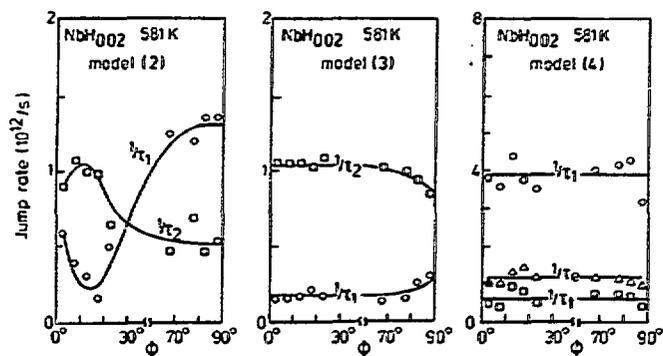interstitial sites in bcc models.

Fig. 4. Jump rates as a function of sample
orientation ϕ obtained by a simultaneous
fit of the scattering law for the models (2),
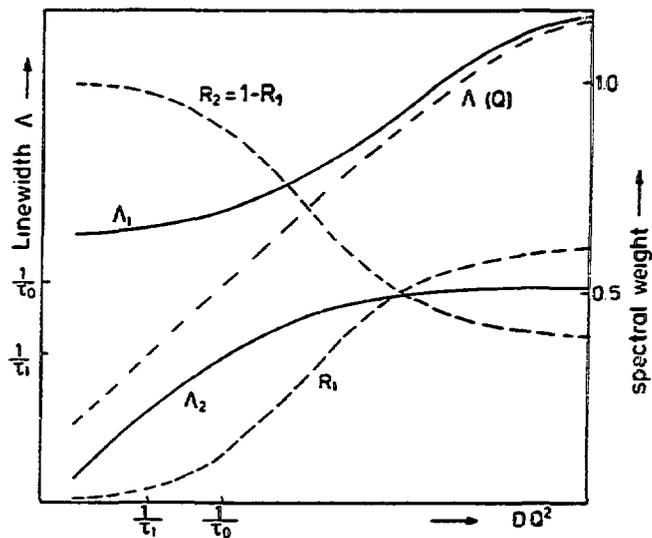(3), (4) to the QNS result at 581 K (6).

Fig. 5. Line width of the two components Λ_1 and Λ_2 (solid lines) and their spectral weights (dashed lines) R_1, R_2 in the scattering law for the RWM description of diffusion in the presence of traps. Dashed dotted Line: line width for an estimated lattice (11).
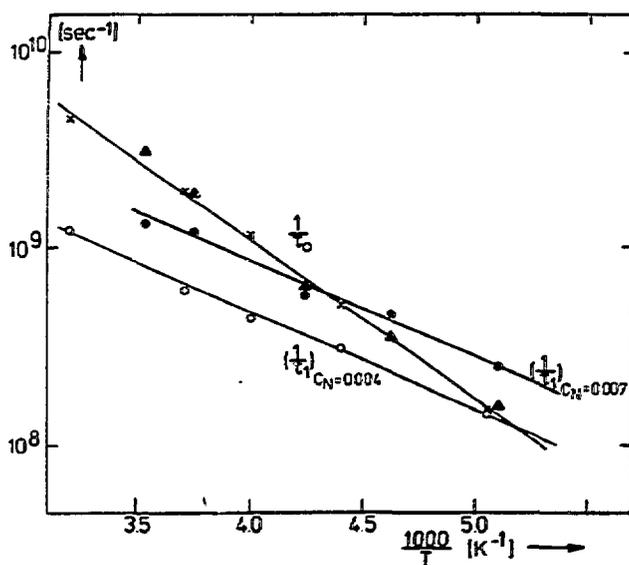
Fig. 6. Escape rate $1/\tau_0$ and trapping rate $1/\tau_1$ as a function of inverse temperature and nitrogen temperature. For $1/\tau_0$: Δ: $C_N = 0.7\%$, $x = C_N = 0.4\%$ (11).