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Nuclear spin relaxation and diffusion of hydrogen in the A15 compound Nb_3AlH_x

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Abstract

The theory of nuclear spin relaxation is developed for a random walk model of H diffusing between sites that form a non-Bravais lattice structure, including multiple rates of jumps between sites in a unit cell. The results are applied to H diffusing by first and second nearest neighbour jumps between interstitial d sites in the A15 compound Nb_3AlH_x . The random walk model is exact for H–metal dipolar relaxation in the low H concentration limit and provides a good approximation at arbitrary concentrations when average site-blocking of jumps is included. This model can show the high temperature $1/\sqrt{\omega}$ frequency dependence of the relaxation rates for one-dimensional diffusion possible in this structure for nearest neighbour jumps along the crystal axes. The low and high H concentration proton-relaxation data for Nb_3AlH_x , as a function of temperature and resonance frequency, are fitted well at high temperatures using a simple set of H jump parameters. The theory provides a more rigorous approach and enables a more complete analysis than the simple Bloembergen–Purcell–Pound model used in previous work.

1. Introduction

The diffusion of H in the cubic A15-type structure Nb_3AlH_x has been studied by nuclear magnetic resonance (NMR) [1] and by quasielastic neutron scattering (QENS) [2]. Nb_3Al is an example of intermetallic A_3B compounds with the A15 structure that can absorb large amounts of H, and the aim of the NMR and QENS studies was to understand the H diffusion mechanism in these compounds.

It was deduced [1, 2] that the H occupy tetrahedral interstitial d sites formed by four Nb atoms, and that there are two coexisting processes of jumps between these sites. The faster jump is to one of the two nearest neighbour d sites and the slower jump is to one of the eight second nearest neighbour d sites. The structure is described in detail in [2]. The nearest neighbour jumps correspond to one-dimensional diffusion along the crystal axes. Both types of jumps together result in three-dimensional diffusion.

It has been known for many years that nuclear spin-relaxation rates show characteristic behaviour as a function of frequency (or magnetic field strength) at high temperatures for one-, two- and three-dimensional translational diffusion [3]. The relaxation rates are proportional to $1/\sqrt{\omega}$ for diffusion in one dimension, show a $\log 1/\omega$ dependence for diffusion in two dimensions, and are independent of frequency for diffusion in three dimensions. The H-relaxation rates for Nb_3AlH_x , and other similar materials with the A15 structure, might therefore show frequency dependent effects at high temperatures similar to the $1/\sqrt{\omega}$ behaviour if the jumps along the crystal axes dominate to produce quasi-one-dimensional diffusion.

The commonly used simple Bloembergen–Purcell–Pound (BPP) model [4] was used in [1] to analyse the proton spin–lattice relaxation rate data for Nb_3AlH_x . The BPP model assumes a correlation function that depends only on the mean time before the first jump of a diffusing spin occurs. This model cannot therefore show any of the dimensional effects of diffusion on the frequency dependence of the high-temperature relaxation rates. The BPP model also cannot distinguish between jumps to nearest or second nearest neighbours. A better model is therefore desirable for analysing H-relaxation data for A15 compounds.

At low H concentrations the H will undergo a random walk on the interstitial d sites. This random walk model is called the Chudley–Elliott model in calculating the dynamic structure factor relevant to QENS [5]. The d sites form a non-Bravais lattice structure and the generalization of the Chudley–Elliott model to a random walk on a non-Bravais lattice has been used in analysing the Nb_3AlH_x QENS data [2]. An aim of this paper is to use this same random walk model to calculate the nuclear spin-relaxation rates for H diffusion between the interstitial d sites in the A15 A_3B structure. This model can then provide a rigorous theory for analysing both the QENS and H-relaxation rates in the low H concentration limit, including H jumps to both first and second nearest neighbour d sites. The random walk model has been developed previously for calculating nuclear spin-relaxation rates due to diffusion on Bravais lattices [6]. It is extended here to diffusion on a non-Bravais lattice structure, including multiple jumps in a unit cell.

At higher H concentrations there are spatial and temporal correlations between diffusing H due to site-blocking effects and a rigorous analysis of diffusion, and its application to QENS and spin-relaxation rates, is not then possible. The random walk theory can, however, provide an approximate theory at higher concentrations by simply including a concentration dependent factor $(1 - c)$ into the jump rates where c is the probability of a target site for a jump being occupied. This application of the random walk theory then takes account of the site-blocking effects in an average way. The detailed correlations between diffusing H will become significant at very high H concentrations. For example, if almost all d sites were occupied by H in Nb_3AlH_x (corresponding to $x = 3$), the few H jumps that could occur would be a result of jumps to the few vacant sites. Successive jumps of a particular H would then be highly correlated and the random walk model with average site blocking effects would be less satisfactory.

The nuclear spin-relaxation theory for the random walk model is described in the following section. The theory is then applied in section 3 to fitting the proton-relaxation data for Nb_3AlH_x for both the low concentration $x = 0.13$ case and the higher concentration $x = 2.75$ case.

2. Nuclear spin-relaxation theory

Nuclear spin-relaxation rates due to diffusion modulated dipolar interactions are linear combinations of spectral density functions $J^{(p)}(\omega)$ defined by [7]

$$J^{(p)}(\omega) = \int_{-\infty}^{\infty} G^{(p)}(t) \exp(i\omega t) dt, \quad (1)$$

where the dipolar correlation functions $G^{(p)}(t)$ are

$$G^{(p)}(t) = d_p^2 \sum_{\alpha, \beta} u_p(\mathbf{r}_\alpha) u_p^*(\mathbf{r}_\beta) P(\mathbf{r}_\alpha, \mathbf{r}_\beta, t). \quad (2)$$

In these expressions $u_p(\mathbf{r}) = Y_{2p}(\Omega)/r^3$, $\mathbf{r}_\alpha = (r_\alpha, \Omega_\alpha)$, Y_{2p} are spherical harmonics relative to the magnetic field direction as the z axis, $P(\mathbf{r}_\alpha, \mathbf{r}_\beta, t)$ is the probability of a pair of spins being separated by \mathbf{r}_α at time zero and these same spins then being separated by \mathbf{r}_β at time t , and $d_0^2 = 16\pi/5$, $d_1^2 = 8\pi/15$ and $d_2^2 = 32\pi/15$.

The dipolar contribution to proton relaxation in Nb_3AlH_x has contributions from both H–metal and H–H dipolar couplings, but the H–metal interactions are dominant (even at large H concentrations) so only this contribution will be considered. For fixed metal nuclei interacting with diffusing H, the random walk expression for $P(\mathbf{r}_\alpha, \mathbf{r}_\beta, t)$ provides an exact method of calculating the relaxation rates in the low concentration limit. The random walk theory could also be applied to the case of proton relaxation due to H–H dipolar coupling, but it is not then an exact solution in the limit of low H concentration. This is because the dipolar coupling involves a pair of spins and the diffusion of each of the spins are not then independent random walks. These correlations between a pair of diffusing spins can be taken into account in the low concentration limit and this theory has been applied to diffusion on cubic Bravais lattices [6, 8].

The nuclear spin–lattice relaxation rate R_1 of diffusing H due to dipolar interaction with fixed metal nuclei is [6]

$$R_1 = \gamma_I^2 \gamma_S^2 \hbar^2 S(S+1) \left[\frac{1}{12} J^{(0)}(\omega_I - \omega_S) + \frac{3}{2} J^{(1)}(\omega_I) + \frac{3}{4} J^{(0)}(\omega_I + \omega_S) \right], \quad (3)$$

where γ_I and γ_S are the gyromagnetic ratios for the proton and metal nucleus, respectively, S is the spin quantum number of the metal nucleus, and $\omega_I = \gamma_I B$ and $\omega_S = \gamma_S B$, where B is the applied magnetic field. Relaxation of H due to interaction with Nb and Al in Nb_3AlH_x is the sum of the above expression for each metal. The H–Nb interactions are the dominant contribution.

A difficulty in evaluating the spectral density functions $J^{(p)}(\omega)$ from (1) and (2) is that the lattice summations in (2) are very slowly convergent. An efficient computational method that overcomes this difficulty is a reciprocal space formalism [6, 8], which has been used for some models of diffusion on Bravais lattices. The generalization of this theory to H–metal interactions for H diffusion on non-Bravais lattice structures gives the result

$$J^{(p)}(\omega) = \frac{d_p^2}{6} \sum_{\mathbf{m}, \mathbf{j}, \mathbf{j}'} \frac{1}{N} \sum_{\mathbf{q}} T_{\mathbf{m}-\mathbf{j}}^{(p)}(\mathbf{q}) T_{\mathbf{m}-\mathbf{j}'}^{(p)*}(\mathbf{q}) P_{\mathbf{j}\mathbf{j}'}(\mathbf{q}, \omega) e^{-i\mathbf{q}\cdot(\mathbf{j}'-\mathbf{j})}, \quad (4)$$

where \mathbf{j} are the vectors of sites in a unit cell that the H can occupy, \mathbf{m} are the vectors of sites in a unit cell occupied by a particular metal, $T_{\mathbf{d}}^{(p)}(\mathbf{q})$ are the lattice sums

$$T_{\mathbf{d}}^{(p)}(\mathbf{q}) = \sum_{\mathbf{l}} u_p(\mathbf{l} + \mathbf{d}) e^{i\mathbf{q}\cdot(\mathbf{l}+\mathbf{d})}, \quad (5)$$

where \mathbf{l} are cubic lattice vectors, and $P_{\mathbf{j}\mathbf{j}'}(\mathbf{q}, \omega)$ is the Fourier transform

$$P_{\mathbf{j}\mathbf{j}'}(\mathbf{q}, \omega) = \sum_{\mathbf{l}} P_{\mathbf{j}\mathbf{j}'}(\mathbf{l}, \omega) e^{-i\mathbf{q}\cdot\mathbf{l}}. \quad (6)$$

$P_{\mathbf{j}\mathbf{j}'}(\mathbf{l}, \omega)$ is the temporal Fourier transform (1) of the probability $P_{\mathbf{j}\mathbf{j}'}(\mathbf{l}, t)$ that a single H on the structure diffuses from a site \mathbf{j} in a unit cell at the origin to a \mathbf{j}' site in a unit cell at \mathbf{l} in a time t . The \mathbf{q} summation in (4) is over the first Brillouin zone and N is the number of sites in the lattice. The factor $1/6$ in (4) occurs because there are six d sites per cubic unit cell.

A planewise summation method gives a rapidly convergent form for the lattice sums $T_{\mathbf{d}}^{(p)}(\mathbf{q})$ with the spherical harmonics relative to the crystal axes [6]. The spectral density

functions and relaxation rates for a single crystal will depend on the direction of the magnetic field relative to the crystal axes and will have an orientation dependence characteristic of the crystal symmetry [9]. For relaxation measurements on powdered samples of Nb_3AlH_x the average of the relaxation rate over all magnetic field directions is required. This results in terms of the form $T_d^{(p)}(\mathbf{q})T_d^{(p)*}(\mathbf{q})$ in (4) being replaced by $\sum_{p=-2}^2 T_d^{(p)}(\mathbf{q})T_d^{(p)*}(\mathbf{q})/5$ [9].

The expressions (3) and (4) can be used to calculate the spectral density functions and relaxation rates rigorously in the low H concentration limit. The expression for $P_{jj'}(\mathbf{q}, \omega)$ can be found by solving the master equation for jumps of H between the sites in a unit cell (see, for example, [2, 5, 10]). The spatial Fourier transform of the master equation gives

$$\frac{\partial}{\partial t}\mathbf{P} = -\mathbf{\Lambda}\mathbf{P}, \quad (7)$$

where \mathbf{P} is a matrix with elements $P_{jj'}(\mathbf{q}, t)$. The matrix $\mathbf{\Lambda}$ is given by

$$\Lambda_{jj'}(\mathbf{q}) = \delta_{jj'} \sum_{l''} \Gamma_{l''j'',0j} - \sum_l e^{-i\mathbf{q}\cdot\mathbf{l}} \Gamma_{lj,0j'}, \quad (8)$$

where $\Gamma_{l''j'',0j}$ is the jump rate of H from site j in the unit cell at the origin to site j'' in the unit cell at l'' . Solving (7) and taking the temporal Fourier transform gives

$$P_{jj'}(\mathbf{q}, \omega) = \sum_{j''} X_{jj''}(\mathbf{q}) \frac{2\lambda_{j''}(\mathbf{q})}{\omega^2 + \lambda_{j''}^2(\mathbf{q})} X_{j''j'}^{-1}(\mathbf{q}), \quad (9)$$

where $\lambda_j(\mathbf{q})$ are the eigenvalues of $\mathbf{\Lambda}(\mathbf{q})$ and $X_{jj''}(\mathbf{q})$ are the corresponding normalized eigenvectors. For H jumps between interstitial d sites in the cubic A15 structure, the jump model includes a jump rate Γ_1 to each of the two nearest neighbour d sites, and a jump rate Γ_2 to each of the eight second nearest neighbour sites. Theoretical relaxation rates may then be calculated numerically from equations (3)–(5) and (9) from these jump rates.

The above theory can calculate the relaxation rates rigorously in the low H concentration limit and, in particular, can include effects from one-dimensional diffusion of H along the crystal axes. At general H concentrations, the theory can also provide an approximation by including an average site-blocking factor in the jump rates. The jump rates are assumed to be of Arrhenius form $\Gamma_1 = \Gamma_0(1 - x/3) \exp(-E_1/kT)$ and $\Gamma_2 = \Gamma_0(1 - x/3) \exp(-E_2/kT)$, where the prefactors are assumed the same for both types of jumps, the effect of site-blocking by other H is included, and E_1 and E_2 are the activation energies for jumps to nearest and second nearest neighbours, respectively.

3. Application to Nb_3AlH_x

Proton spin–lattice relaxation rates R_1 in Nb_3AlH_x have been measured as a function of temperature and resonance frequency for $x = 0.13, 1.77$ and 2.75 [1]. The random walk theory developed in the previous section is used here to analyse the low concentration $x = 0.13$ data and the high concentration $x = 2.75$ data.

The experimental dipolar contributions to the proton spin–lattice relaxation rates R_1 [1] are shown for $x = 0.13$ in figure 1 and for $x = 2.75$ in figure 2. The first fit made was to the low concentration data in figure 1 using the random walk model with $\Gamma_2 = 0$ so that only jumps Γ_1 along the crystal axes can occur. The activation energy E_1 was determined by fitting the low-temperature slopes in figure 1 and the value of the prefactor Γ_0 adjusted to fit the values of $1000/T$ at which the maxima occur. A scaling factor f multiplying the calculated relaxation rates was also used to fit the magnitude of the maximum relaxation rates for both frequencies. The dashed curves in figure 1 show the fit for $E_1 = 0.19$ eV, $\Gamma_0 = 2.7 \times 10^{11} \text{ s}^{-1}$ and $f = 0.65$. At high temperatures these curves show the $1/\sqrt{\omega}$ frequency dependence

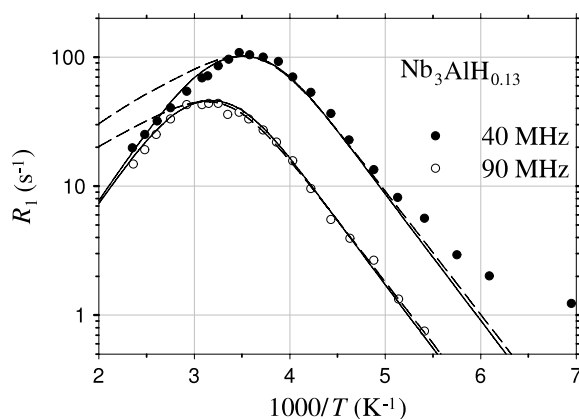


Figure 1. Temperature dependence of the dipolar part of the proton spin–lattice relaxation rate in $\text{Nb}_3\text{AlH}_{0.13}$ at 40 and 90 MHz. Symbols are experimental data. The curves are a fit to the data using the random walk theory. The dashed curves are a fit assuming only nearest neighbour jumps. The solid curves are a fit including both first and second nearest neighbour jumps.

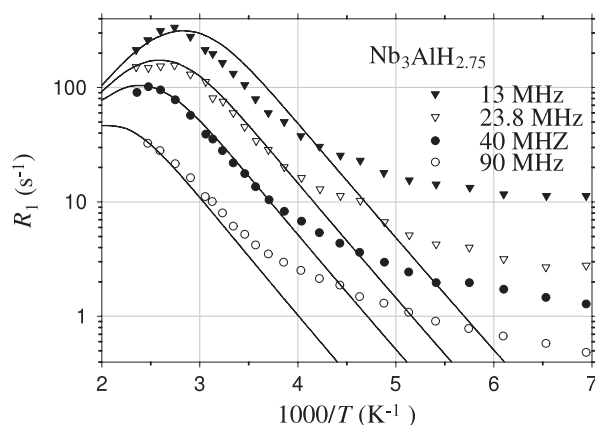


Figure 2. Temperature dependence of the dipolar part of the proton spin–lattice relaxation rate in $\text{Nb}_3\text{AlH}_{2.75}$ at 13, 23.8, 40 and 90 MHz. Symbols are experimental data. The curves are a fit to the data using similar jump rate parameters to those in figure 1 as described in the text.

expected for one-dimensional diffusion [3]. This behaviour is not observed experimentally which indicates that the H jumps Γ_2 to second nearest neighbour sites also occur and produce three-dimensional diffusion. A further fit was then made retaining the above values of Γ_0 and E_1 , but also including the effect of the second nearest neighbour jumps Γ_2 . The result is shown by the solid curves in figure 1 for which $E_2 = 0.25$ eV and $f = 0.55$. It can be seen that the inclusion of the jumps Γ_2 in the data has a major effect at high temperatures but has little effect at low temperatures. The energy E_2 was chosen to provide a good fit to the high-temperature data. The fit provided by this procedure is excellent except for the 40 MHz data at low temperatures.

The relaxation rates for the high H concentration data in figure 2 were then calculated using the above values of the energies E_1 and E_2 and just varying Γ_0 to fit the positions of the relaxation maxima and f to fit the magnitudes of the relaxation maxima. The results shown in figure 2 are for $\Gamma_0 = 1.9 \times 10^{11} \text{ s}^{-1}$ and $f = 0.64$. The values of the lattice parameters used

are $a = 5.190 \text{ \AA}$ for $x = 0.13$ and 5.358 \AA for $x = 2.75$ [1]. Other fits were also undertaken that kept Γ_0 and one of E_1 and E_2 fixed and varied the other energy. Fits of similar quality to that shown in figure 2 were obtained for increases in either E_1 or E_2 of 0.02 eV . The fits to the $x = 2.75$ data cannot therefore distinguish between the above small changes to E_1 , E_2 and Γ_0 .

The theoretical fits to the relaxation data in figures 1 and 2 are quite good in the vicinity of the high-temperature maxima, except for the 13 MHz data. The low frequency 13 MHz relaxation may, however, be complicated by cross-relaxation between the proton and quadrupolar Nb spins [1]. The fits in this temperature range are therefore consistent with a random walk diffusion model with parameters $E_1 = 0.19 \text{ eV}$, $E_2 = 0.25 \text{ eV}$ and $\Gamma_0 = 2.7 \times 10^{11} \text{ s}^{-1}$ at low concentrations and only small increase in these parameters at $x = 2.75$. The substantial shift in the position of the maxima for the 40 and 90 MHz data with increasing H concentration is mainly due to a reduction in the jump frequencies due to average site-blocking effects, with a possible smaller effect due to a concentration dependence of the prefactor frequency Γ_0 . The overall quality of the fits is similar to that obtained in [1] where the approximate BPP model was used with activation energies and a distribution of activation energies that were strongly concentration dependent. The random walk model, however, is more rigorous and has used a simpler model with fewer adjustable parameters.

The QENS data for Nb_3AlH_x with $x = 0.13$ were analysed in [2] using the same random walk model for H diffusion that has been used in the present relaxation theory. The result obtained for the nearest neighbour jumps Γ_1 ($1/(2\tau_1)$ in the notation of [2]) was an activation energy of $E_1 = 0.194 \pm 0.017 \text{ eV}$ and a prefactor $\Gamma_0 = (5.7 \pm 3.0) \times 10^{11} \text{ s}^{-1}$. These parameters are in excellent agreement with those deduced from the fits in figures 1 and 2. For $x = 1.77$ the QENS analysis gave $E_1 = 0.163 \pm 0.016 \text{ eV}$ and a prefactor $\Gamma_0 = (3.3 \pm 1.7) \times 10^{11} \text{ s}^{-1}$. The QENS analysis was not able to deduce any information regarding the jump rate Γ_2 . The analysis of the proton-relaxation rates using the simple BPP theory gave $E_1 = 0.21 \text{ eV}$ for $x = 0.13$, and 0.30 eV for $x = 2.75$ together with a distribution of activation energies [1]. An estimate was made of the jump rate Γ_2 from the $x = 1.77$ spin relaxation data by assuming that the maximum relaxation rate occurs when $\omega/\Gamma = 0.92$ for the BPP model and that the relevant jump frequency Γ was Γ_2 [2]. The random walk model provides a much more rigorous method for analysing the relaxation data and can deduce both of the jump frequencies Γ_1 and Γ_2 .

The jump rate Γ_1 that produces one-dimensional diffusion and the jump rate Γ_2 that produces three-dimensional diffusion have activation energies with similar magnitude. The expression for the diffusivity D for these jumps between the interstitial d sites in the A15 structure can be obtained in the low concentration limit from the matrix Λ given by equation (8) [10]. The diffusivity is isotropic and the result is

$$D = \frac{a^2}{12}(\Gamma_1 + 6\Gamma_2). \quad (10)$$

The temperature dependence of D for H in Nb_3AlH_x is shown in figure 3 for the jump rates obtained from the fits to the relaxation data, together with the contributions from each jump frequency. There is a small curvature in the Arrhenius plot.

The relaxation data in figure 2 show strong deviations from the theoretical curves for $T < 270 \text{ K}$. This feature is also present at lower temperatures for the 40 MHz data in figure 1. It was suggested in [1] that this behaviour was due to the two frequency scales of jumps between H to first and second nearest neighbours. This cannot be the case, however, because both of these jumps have been included in the present theory and the deviations remain. Another possibility for this behaviour is that it is due to H occupation of interstitial i sites formed by one Al and three Nb atoms [11]. Some H occupation of additional sites to the d sites is expected in A15 compounds because a number of such hydrides with $x > 3$ have been prepared and all d sites are filled with $x = 3$. The i sites form closely based pairs and H jumps between

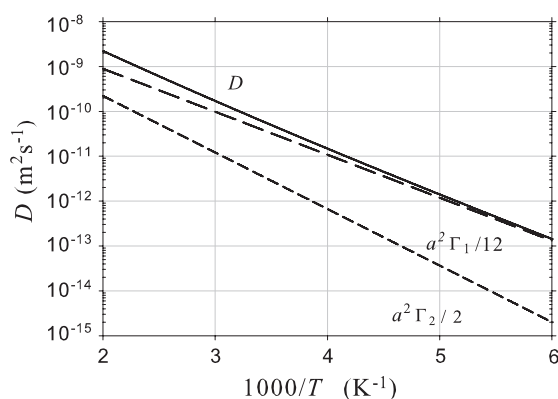


Figure 3. Temperature dependence of the diffusivity D of H in Nb_3AlH_x in the low concentration limit. The dashed curves are the contributions from each jump frequency.

these that are more rapid than those between d sites would produce enhanced relaxation rates at temperatures below those of the main peaks in figures 1 and 2. Modelling of this contribution to the relaxation would, however, have the complications of additional jump parameters and temperature dependent occupation probabilities of d and i sites. Another possible effect that can enhance H jump rates, diffusion and spin relaxation at low temperatures is quantum diffusion (see, for example, [12, 13]).

The scaling factors $f = 0.55$ for the $x = 0.13$ data and $f = 0.64$ for the $x = 2.75$ data show that the theoretical model overestimates the magnitude of the relaxation rates. This behaviour has been observed in a number of metal–hydrogen systems and has been interpreted in terms of a fraction of the H atoms not participating in the jump mechanism that produces the maximum in the relaxation rate (see, for example, [2]). This fraction of H could relax at the same rate due to proton flip-flops that establish a common spin temperature. Only a single exponential would then be observed in the relaxation, as is the case for Nb_3AlH_x . The detailed explanation for the anomalous fraction of H is unknown. The effect might be related to H occupation of additional interstitial sites as mentioned above. A reduction in the magnitude of the relaxation rate could also be caused by the local expansion of neighbouring metal sites about a H interstitial. An increase in the H–metal distance is amplified by the r^{-6} dependence of the dipolar interactions. This expansion could therefore be significant at low H concentrations but is unlikely to be important at high concentrations where most d sites are occupied.

The diffusion model discussed here involving two jump rates will produce two maxima in the temperature dependent relaxation rate for each resonance frequency ω if the jump rates are significantly different. The two maxima will occur at temperatures for which each jump rate is $\sim\omega$. Under these circumstances the BPP model could provide an estimate of the jump rate parameters by fitting each maximum separately. In Nb_3AlH_x the jump rates Γ_1 and Γ_2 are similar at temperatures for which the relaxation maxima occur so that only a single maximum is observed. It is not then possible to attribute the maximum to a single jump rate nor deduce information about both jump rates from the BPP model.

4. Conclusions

The development of the random walk model for nuclear spin relaxation theory has enabled a more accurate and complete analysis of the high-temperature relaxation data for Nb_3AlH_x than

is possible with the approximate BPP model. The random walk model provides a rigorous analysis of the relaxation rates at low concentrations. It has shown that a one-dimensional diffusion model of H in Nb_3AlH_x is not consistent with the experimental data. Good fits of both the low and high H concentration data were obtained with a simple model of H jumps to first and second nearest neighbour sites with only a small concentration dependence of the jump rate parameters. Concentration dependent distributions of jump rates, as used in [1] with the BPP model, were not necessary to fit the data.

The extension of the random walk theory of nuclear spin relaxation to multiple jump diffusion models and diffusion on non-Bravais lattice structures is also applicable to H diffusion in other intermetallic compounds. It provides a much more rigorous basis than the BPP model for analysing nuclear spin relaxation rates at both low and high H concentrations than the BPP model.

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