INSTYTUT FIZYKI JĄDROWEJ
im. H. Niewodniczańskiego
w Krakowie

MATERIAŁY XXX OGÓLNOPOLSKIEGO SEMINARIUM

NA TEMAT
MAGNETYCZNEGO REZONANSU JĄDROWEGO
I JEGO ZASTOSOWAŃ

1 - 3 grudnia 1997

KRAKÓW 1998

MAGIC ECHOES AND MOLECULAR JUMPS IN POTENTIAL WELLS WITH NONEQUIVALENT SITES

Mikołaj Siergiejew

Institute of Physics, University of Szczecin,ul. Wielkopolska 15, 70-451, Szczecin,Poland

Introduction

The influence of a thermal motions of a nuclei in solids on the magic pulse sequence of Fenzke et al [1]

$$(\tau - 90^0_{\bar{X}} - 2\tau - 90^0_X)^N - 90^0_Y - 6N\tau$$

was considered in [2,3] for the case of the molecular reorientations between the equivalent potential wells. It was shown that the mobility of the molecular groups leads to the appearance of the minimum on the temperature dependence of the magic echo amplitude.

At the last time the molecular reorientations between two or more unequal potential wells have been of interest to reseaches in the field of solid molecular dynamics [4-7]. In this report we consider the effect of the molecular jumps between nonequivalent sites on the magic echo amplitude. Our main goal is to investigate how the results obtained in [2,3] are changed when molecular group reorients in asymmetrical potential wells.

Results and discussion

For the magic pulse sequence of Fenzke et al [1] and for the correlation function of (3) from [4] we obtained the following expression for the amplitude of magic echo at $t=6N\tau$

$$V(6N\tau) = \exp(-\frac{6N\tau}{T_{2e}}), \tag{1}$$

where

$$T_{2e}^{-1} = \sum_{i=1}^{n} \left(T_{2e}^{-1}\right)_i, \tag{2}$$

and

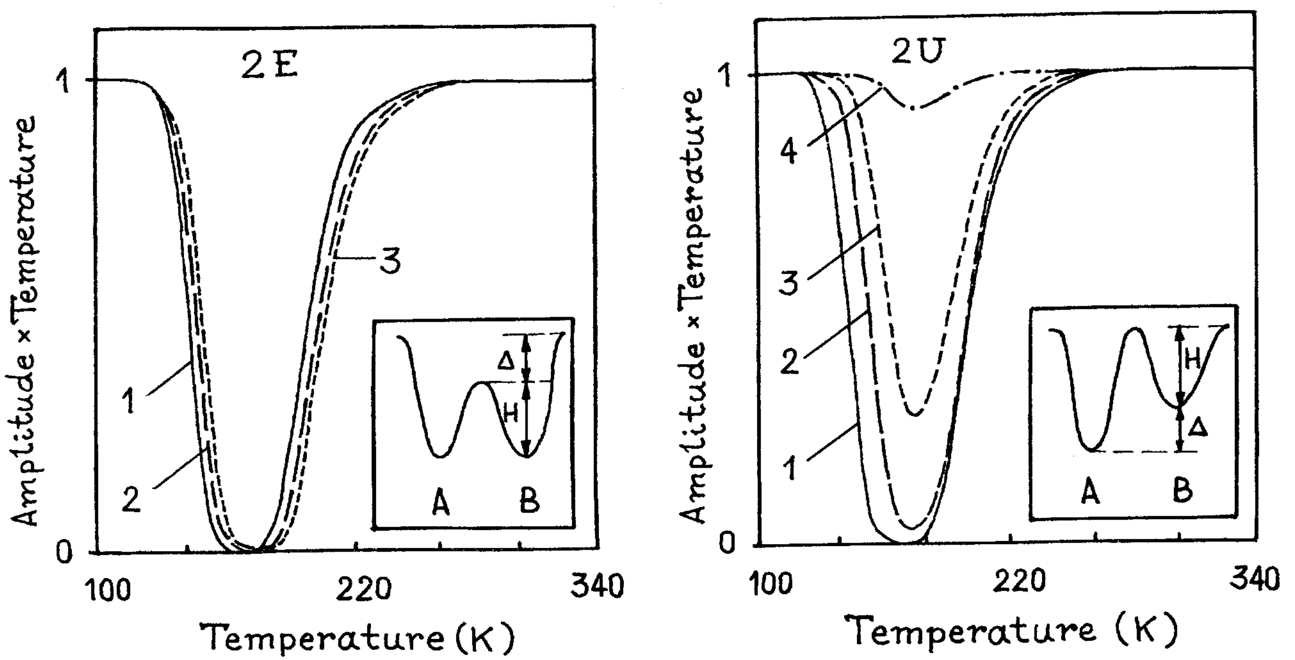

Fig.1. A normalised plot of Curie law corrected magic echo amplitude (N=2, τ = 5μs) versus temperature for the different double-minimum potentials and various values of Δ : 1 - Δ=0 kJ/mol; 2 - Δ=2.5 kJ/mol; 3 - Δ=4.2 kJ/mol; 4 - Δ=8.4 kJ/mol. H=29 kJ/mol, $\Delta M_2\tau^2 = 1$.

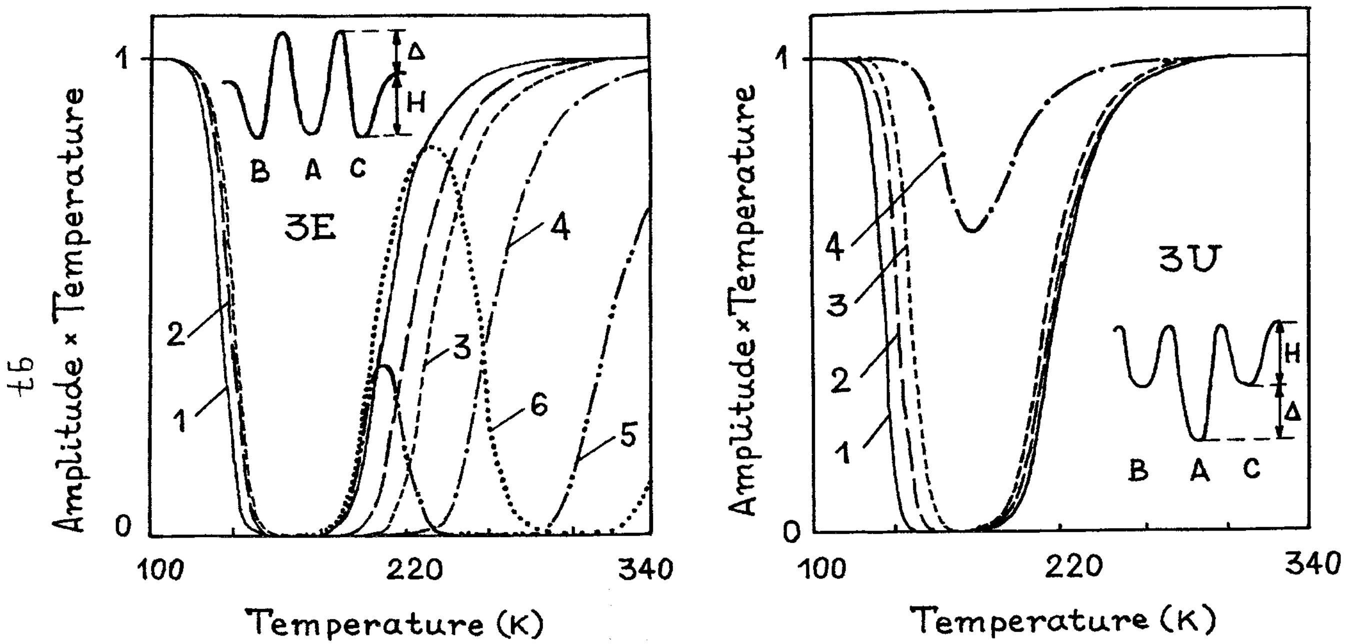

Fig.2. A normalised plot of Curie law corrected magic echo amplitude (N=2,τ=5μs) versus temperature for the different triple-minimum potentials and various values of Δ :1- Δ=0 kJ/mol;2- Δ=2.5 kJ/mol;3- Δ=4.2 kJ/mol;4- Δ=8.4 kJ/mol;5- Δ=16.7 kJ/mol;6- Δ= 25 kJ/mol.H=29 kJ/mol,$\Delta M_2\tau^2$= 1.

$$
\begin{aligned}
\left(T_{2e}^{-1}\right)_i &= \frac{1}{3}K_i\tau_{ci}\left(\frac{3}{2}+\sum_{k=1}^{\infty}\frac{a_k^2}{1+(k\omega\tau_{ci})^2}\right)+\frac{K_i}{6N}\frac{\tau_{ci}^2}{\tau}\left[\left(\exp(-\frac{4N\tau}{\tau_{ci}})-1\right)\times\right. \\
&\left(-\frac{1}{2}+\sum_{k=1}^{\infty}\frac{a_k}{1+(k\omega\tau_{ci})^2}\right)^2+\left(\exp(-\frac{4N\tau}{\tau_{ci}})-1\right)\left(\exp(-\frac{2N\tau}{\tau_{ci}})-1\right)\times \\
&\left.\left(-\frac{1}{2}+\sum_{k=1}^{\infty}\frac{a_k}{1+(k\omega\tau_{ci})^2}\right)+\left(\exp(-\frac{2N\tau}{\tau_{ci}})-1\right)\right],
\end{aligned}
\tag{3}
$$

In eq.(3)

$$
a_k=\frac{2}{k\pi}(-1)^{k+1}\sin(\frac{\pi}{2}k), \qquad \omega=\frac{\pi}{2\tau}.
$$

K_i $(i=1,2,\dots n)$ are the structural parameters which are determined by the shape of the potential barrier and τ_{Ci} are the correlation times, characterizing n modes of reorientation [4,5].

The temperature dependences of the magic echoes amplitude for the different potentials considered in [5] are shown in Fig.1 and Fig,2. So as in the case of the temperature dependence of the solid echo amplitude [4], the temperature dependence of the magic echo amplitude shows a strong dependence on Δ for the 2U, 3E and 3U potential wells. In the case of the 3E potential barrer the two well resolved minima in the temperature dependence of the magic echo amplitude may be observed.

The obtained results demonstrate that the study of the temperature dependence of the magic echo amplitude can yield valuable information about the shape of the potential barriers in solids.

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