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Calculation of Spin Relaxation Rate of Iron Ion

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Abstract

The present paper discusses the spin relaxation process and calculates the spin relaxation rate of Iron ion (Fe^{+3}). We also have discussed the variation of the spin relaxation rate with different low temperature and from this result, it has been shown that at low temperature this mechanism is in-effective in the temperature range up to 300K. We have extended this work to apply the temperature range up to 500K and showed that the relaxation rate at low temperature, relaxation rate at low temperature due to Hamiltonian doublet and relaxation rate at low temperature using strain operator increase with increasing the temperature. This also concludes that indirect two phonon process cannot be dominant mechanism for spin relaxation of S-state Iron ions and not able to produce any observable effect on the Mossbauer hyperfine spectrum.

Keywords: Spin relaxation rate, Temperature and Phonon

1. Introduction

In 1936, Heitler and Teller proposed to discuss the modulation of the crystalline electric fields by the lattice vibrations and to agree that these effects could account for the discrepancies between Waller's theory and the experiment. They did not attempt actually quantitative calculations, but did show that modulation of the crystalline field led to spin-lattice interactions [1]. In 1938, Fertz also discussed the modulation of the crystalline electric fields by the lattice vibrations [2]. In 1950, Benzie and Cooke have showed that paramagnetic relaxation is a complex phenomenon and obtained that relaxation times are of the order of 10^{-2} sec., with a temperature dependence[3,4] Heitler and Teller also developed a theory for the nuclear relaxation in the metals redefined by Korringa [5]. In 1961, Orbach explained the spin-lattice relaxation times observed in rare earth salts to estimate their magnitude and to predict quantitatively their field and temperature dependence [6]. In 2001, Malaecu et al. studied the magnetic relaxation processes in two ferro fluids with two samples MnO.4ZnO.6Fe2O4 and MnO.6FeO.4Fe2O4 of the mixed ferrite particles and observed for both samples at frequencies of tens MHz, assigned with relaxation processes with evaluation of the effective anisotropy constant K of the particles [7]. Reich also studied the different type of relaxation process and relaxation time specially with NMR spectroscopy [8].

In the present paper, we have discussed spin relaxation process and have calculated the spin relaxation rate of Iron ion (Fe^{+3}) on the basis of dynamic spin Hamiltonian. We also have discussed the variation of the spin relaxation rate with different low temperature and from this result, it has been shown that at low temperature this mechanism is in-effective in the temperature range up to 300K. We also have extended this work theoretically to apply the temperature range up to 500K for the calculation of relaxation rate at low temperature, relaxation rate at low temperature due to Hamiltonian doublet and relaxation rate at low temperature using strain operator.

2. Theoretical Discussion

The relaxation time between the two Eigen-states of doublet is given by the following equation.

$$\frac{1}{T_{SP}}=\frac{1.296\times10^{3}}{\pi^{3}\rho^{2}v^{10}\hbar^{2}}\int_{0}^{\omega_D}{\frac{\omega^{4}\exp(\hbar\omega/KT)}{1-[\exp(\hbar\omega/KT)]^{2}}}^{2}.d\omega \tag{1}$$

Hence ω_D is the Debye frequency of the lattice.

At low temperature, the relaxation time reduces by the following equation.

$$\frac{1}{T_{SP}}=\frac{3.1\times10^{4}}{\pi^{3}\rho^{2}\hbar^{2}v^{10}}(E'G')^{2}\left(\frac{KT}{\hbar}\right)^{5} \tag{2}$$

Data used:

$\rho=4gm^{-3}cm^{-3}$, $\hbar=10^{-27}$,
$v=4\times10^{5}cms^{-1}$, $E=0.2cm^{-1}=0.2\times1.95\times10^{-16}erg$
$G'=E'$, $K=1.38\times10^{-16}$,

Using the data in the above box and solving, we have

$$\frac{1}{T_{SP}}=9.1\times10^{-9}T^{5}s^{-1} \tag{3}$$

When the Spin-phonon Hamiltonian are added, the relaxation time will be doubled and is given by the following equation.

$$\frac{1}{T_{SP}}=1.8\times10^{-8}T^{5}s^{-1} \tag{4}$$

When the strain operator is used the relaxation time at the low temperature is given by the following equation

$$\frac{1}{T_{SP}}=7.1\times10^{-8}\times T^{7}s^{-1} \tag{5}$$

Table 1: Relaxation rate of various spin doublets calculation

S. N.	Temperature (in Kelvin)	Relaxation rate at low temperature (in per second). $(1/T_{SP}=9.1\times10^{-9}T^5)$	Relaxation rate at low temperature due to Hamiltonian doublet (in per second). $(1/T_{SP}=1.8\times10^{-8}T^5)$	Relaxation rate at low temperature using strain operator (in per second). $(1/T_{SP}=7.1\times10^{-8}\times T^7)$
1	1K	9.1×10^{-9}	1.8×10^{-8}	7.1×10^{-8}
2	10K	9.1×10^{-4}	1.8×10^{-3}	7.1×10^{-1}
3	20K	291.2x10^{-4}	57.6x10^{-3}	908.8x10^{-1}
4	30K	2211.3x10^{-4}	437.76 x10^{-3}	15527.7x10^{-1}
5	40K	9318.4 x10^{-4}	1843.2 x10^{-3}	116326.6 x10^{-1}
6	50K	28437.5 x10^{-4}	5625.0 x10^{-3}	554687.5 x10^{-1}
7	60K	70761.2 x10^{-4}	13996.8 x10^{-3}	1987545.6 x10^{-1}
8	70K	152943.7 x10^{-4}	30252.6 x10^{-3}	5847155.3x10^{-1}
9	80K	298188.8x10^{-4}	58982.5x10^{-3}	18844876.4x10^{-1}
10	90K	537345.9x10^{-4}	106288.6 x10^{-3}	33959079.9x10^{-1}
11	100K	910000 x10^{-4}	180000 x10^{-3}	71000000 x10^{-1}
12	200K	29120000x10^{-4}	5760000x10^{-3}	9088000000x10^{-1}
13	300K	221100000.3x10^{-4}	43700000.76 x10^{-3}	155270000000.7x10^{-1}
14	400K	931800000.4 x10^{-4}	184300000.2 x10^{-3}	11632600000.6 x10^{-1}
15	500K	2843700000.5 x10^{-4}	562500000.0 x10^{-3}	554687000000.5 x10^{-1}

3. Results and Discussion

In the present work, we have used three models due to Relaxation rate at low temperature (in per second) $(1/T_{SP}=9.1\times10^{-9}T^5)$, Relaxation rate at low temperature due to Hamiltonian doublet (in per second). $(1/T_{SP}=1.8\times10^{-8}T^5)$ and Relaxation rate at low temperature using strain operator (in per second) $(1/T_{SP}=7.1\times10^{-8}\times T^7)$ respectively for the comparative study of the relaxation rate from the temperature range 1K to 500K. The calculations regarding the spin relaxation rate calculation of Fe^{+3} ion on the basis of dynamic spin Hamiltonian shows that the spin relaxation rate increases with increase in temperature rapidly. The results gives relaxation rate as of the order of $10^5\times Ts^{-1}$ .and can be expected even at 300K. In the temperature range of 1K to 30K, the relaxation rate remains between 10^5 to 10^6 s^{-1} and therefore the nature of the magnetic hyperfine spectra will almost remains unchanged. The work is extended to apply the temperature range up to 500K and showed that the relaxation rate at low temperature, relaxation rate at low temperature due to Hamiltonian doublet and relaxation rate at low temperature using strain operator increase with increasing the temperature. This also concludes that indirect two phonon process cannot be dominant mechanism for spin relaxation of S-state Iron ions and not able to produce any observable effect on the Mossbauer hyperfine spectrum.

4. Conclusion

The relaxation rate at low temperature, relaxation rate at low temperature due to Hamiltonian doublet and relaxation rate at low temperature using strain operator increase with increasing the temperature. This process is dominant at low temperature and gives the light effect at high temperature region.

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