NMR LINE SHAPES FOR QUADRUPOLAR GLASS STATE OF SOLID HYDROGEN

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Introduction

One of the few rigorously established examples of short range glass-type ordering is the low temperature state of ortho- para-hydrogen mixtures with percentages of ortho-hydrogen below 55%. At low temperatures the molecular orientations become frozen at random with the local quadrupole moments, not just the alignments, exhibiting only short range order. These systems characterized by high frustration of the interactions that determine the molecular alignments is believe to be in the same family as fragile glasses where broken replica symmetry occurs. This orientational glass ordering was determined form careful analysis of the line shapes for bulk samples, but there have been inconsistencies and ambiguities about the analysis of line shapes for hydrogen films because of the influence of the restricted geometries on the interactions [1].

Results and Discussion

In order to obtain a better understanding of the low temperature behavior as deduced from the NMR studies, computer simulations of the NMR line shapes have been carried out to fit the observed line shapes in terms of local order parameters. This method allows one to determine the distribution of order parameters over allowed phase space for the parameters that provide the best fit to the experimental data. One of the important considerations for understanding the behavior of films is consideration of the crystal field interactions that are very strong in these geometries, typically of the order of 1K, while in bulk the fields are of the order of 0.02K. As a result of this contribution, one does not observe the characteristic *bell* shape for the NMR lines seen for bulk systems, and strong extended wing components can occur in the line shape. This tendency was previously reported for bulk systems without glass ordering by Dubault and Legrand [2] who interpreted the lines as resulting for an ensemble of hindered rotors.

Conclusions

The two-dimensional glass line shapes for films of hydrogen adsorbed onto substrates are very different form those observed for bulk samples. The simulations show that the two-dimensional line shapes can be understood in terms of a broad distribution of local order parameters. The unusual line shapes observed experimentally result from the dimensionality and the presence of strong crystal fields at the substrate that compete with the quadrupole-quadrupole interactions between ortho-hydrogen molecules.

References

1. Kim, K., *et al*., J. Low Temp. Phys., **114**, 173 (1999)
2. Dubault, A., Legrand, A.P., J. Chem. Phys. **B17**, 5016 (1978).