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# Anisotropic intermediate valence in $Yb_2Rh_3Ga_9$

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**Abstract**

We report measurements of the inelastic neutron scattering spectrum for the anisotropic intermediate valence system $Yb_2Rh_3Ga_9$. Calculations for the Anderson impurity model with crystal field terms within an approach based on the non-crossing approximation have been performed for the inelastic neutron scattering spectrum as well as other thermodynamic quantities. These results corroborate the importance of crystal field effects in these materials. They also suggest that Anderson lattice effects are important to the physics of $Yb_2Rh_3Ga_9$.


*Keywords:* Intermediate valence; Anderson impurity model; Crystal fields

Recently, we have established that $Yb_2Rh_3Ga_9$ is an anisotropic intermediate valence (IV) system [1,2]. In these studies, we found that Anderson impurity model (AIM) calculations, including the effects of crystal field (CF) level splitting, were able to simultaneously reproduce the temperature dependence of the magnetic susceptibility and the 12 K inelastic neutron scattering spectrum (INS). However, the calculated 4f occupation number, $n_f(T)$, rises much more rapidly with temperature than the experimental data. Such effects have been observed previously in a number of cubic IV systems, and have been attributed to the fact that the crossover from the high temperature local moment regime to the low temperature Fermi liquid regime is slower for the Anderson lattice (AL) than for the AIM [3]. This is due to the requirement that the conduction band accommodates a finite number of additional electrons arising from the change of valence with temperature. To explore the importance of AL effects further, we have performed new INS experiments and AIM calculations at 100, 200 and 300 K.

The samples, experimental conditions and data reduction used in these studies are the same as those used in Ref. [2]. We emphasize that a standard method, which uses a non-magnetic analog, in this case $Y_2Rh_3Ga_9$, was used to determine the magnetic portion of the INS signal ($S_{mag}$) [4,5]. The AIM calculations were performed in the same manner as in Refs. [1,2].

Fig. 1 displays the INS data at 12, 100, 200 and 300 K. The solid lines in all panels indicate a fit to the data using a single Lorentzian (Table 1). The INS data evolve from an inelastic response at 12 K to a quasielastic response at 300 K. This is the behavior normally encountered in IV systems [4]. From the Lorentzian fits it is possible to extract the static susceptibility. Good agreement (Table 1) is found at all temperatures, except at 12 K where it appears that the INS response is not sensitive to the low temperature upturn (which is probably extrinsic) observed in the static susceptibility [1]. This agreement gives confidence in our determination of $S_{mag}$.

AIM calculations utilizing the Zwicknagl, Zevin and Fulde simplification of the non-crossing approximation

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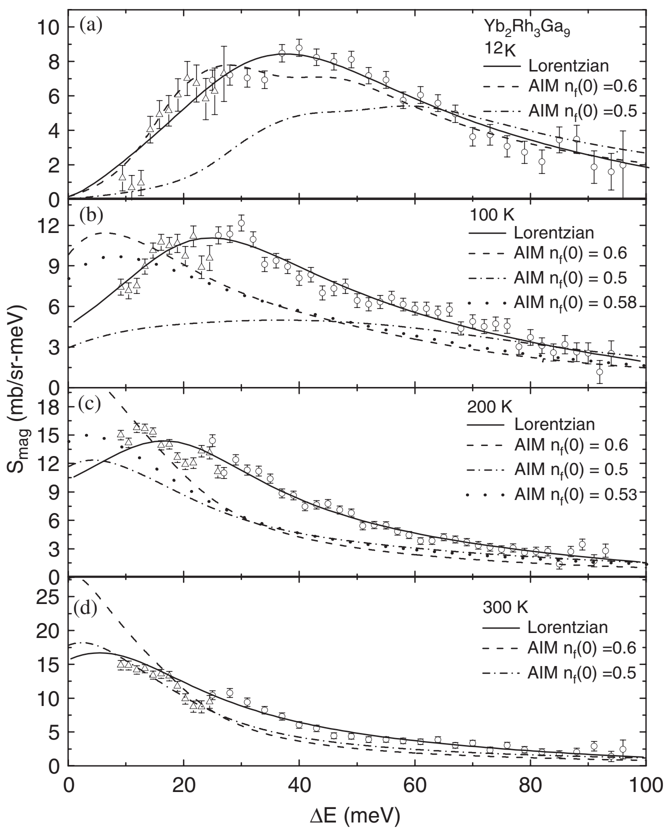


Fig. 1. $S_{mag}$ at 12, 100, 200 and 300 K. In all panels triangles (circles) denote incident energies of 35 (120) meV. Solid lines are Lorentzian fits as described in the text. Dashed (dash–dot) lines are AIM calculations with $n_f(0) = 0.6$ (0.5). The dotted lines in (b) and (c) are AIM calculations as described in the text.

Table 1
Lorentzian fit parameters

| | Susceptibility | $\Gamma$ | Position |
|---|---|---|---|
| 12 | 4.60 (5.73) | 27 | 27 |
| 100 | 6.39 (6.95) | 22 | 15 |
| 200 | 5.97 (6.23) | 19 | 12 |
| 300 | 4.70 (4.99) | 21 | 0 |

The numbers in parenthesis are the experimental values of the susceptibility from Ref [1]. Units are $10^{-3}$ emu/mol Yb, meV and meV.

(NCA) to the AIM [6] have been performed for various experimental quantities [1,2]. In the lowest order calculation the CF splits the eight-fold degenerate ground state of $Yb^{3+}$ into two quartets separated by the energy $\Delta$. The CF wave functions are taken as eigen states of the angular momentum operator $J_z$, where the ground state quartet consists of two doublets, $|\pm 7/2\rangle$ and $|\pm 5/2\rangle$, and the excited state quartet consists of the other two doublets, $|\pm 3/2\rangle$ and $|\pm 1/2\rangle$. By choosing the hybridization between the 4f and conduction electrons to have a value $\Gamma = 165$ K and the CF splitting to have a value $\Delta = 400$ K, we reproduce the temperature dependence of the anisotropic magnetic susceptibility as well as the 12 K INS data [2]. Improvements to the fits can be achieved by lifting the ground state degeneracy to two doublets separated by 100 K, lifting the degeneracy of the upper quartet to two doublets separated from the ground state by 280 and 340 K, and allowing the hybridization constant $\Gamma$ to be slightly different for the ground and excited multiplets [2]. Additional calculations have been performed with the same parameter set (in particular $n_f(0) = 0.6$) at 100, 200 and 300 K (Fig. 1). The fit at 12 K is reasonable; however, at elevated temperatures the fits progressively overestimate the scattering at low energy transfer.

To account for this, we performed the AIM calculation with the same parameter set, but with the value of $n_f(0) = 0.5$ chosen so that the calculation yields the experimental value of $n_f$ at 300 K. The agreement between the calculated and experimental $S_{mag}$ is remarkable (Fig. 1d). We have performed similar calculations with $n_f(0) = 0.5$ at 12, 100 and 200 K. At 12 K, the calculation utilizing $n_f(0) = 0.6$ provides a better fit. At 100 and 200 K, however, a better fit to the data at low energy transfer would be provided by curves utilizing values of $n_f(0)$ intermediate between 0.5 and 0.6. This is shown more clearly by the dotted lines in Fig. 1(b) and (c) where the AIM calculation has been perfomed by choosing $n_f(0)$ to give the experimental value of $n_f$ at 100 and 200 K. This reduction with increasing temperature of the value of $n_f$ required to fit the INS data implies that AL behaviour, in the form of the slow crossover mentioned above, is influencing the dynamic susceptibility of the anisotropic IV material $Yb_2Rh_3Ga_9$.

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