Ultrasonic investigation of a heavy fermion compound YbAgGe

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Abstract. We have performed ultrasonic measurements on a heavy fermion compound with geometrical frustration YbAgGe which undergoes a complex series of phase transitions of $T_{M1} = 0.8$ K, and $T_{M2} = 0.65$ K in zero field. A pronounced elastic softening toward the transition temperature $T_{M2}$ was observed in the temperature dependence of longitudinal elastic constants $C_{11}$ and $C_{33}$, and transverse one $C_{44}$, while no softening was observed in transverse one $C_{66}$. Furthermore, a sharp drop was observed at $T_{M2}$ in all the elastic constants. The data is difficult to explain only by crystalline electric field effect proposed previously. Alternately, the deformation potential approximation can reproduce the experimental data reasonably. It is found that the bandwidth $W$ of quasi-particles formed by hybridization between conduction electrons and 4$f$ localized ones derived from Yb ion increases gradually with increasing the applied magnetic field, indicating an increase of Kondo temperature $T_K$. A sudden change of the $W$ appears in a field of 5 T, suggesting that the application of field suppresses in part the magnetic frustration, and enhances the Kondo temperature $T_K$. We discuss our results with a model where the main contribution to the elastic softening arises from the deformation coupling between quasi-particles and elastic waves, and with an effect attributed to order-parameter fluctuations near $T_{M2}$.

1. Introduction
Over the past few years, a considerable number of studies have been conducted on the Ytterbium compounds since they display a rich variety of intriguing physical properties such as quantum critical behavior, non-Fermi liquid behavior, multipolar ordering and so on.[1] The unusual behavior is attributed to two energetically similar electronic configurations, trivalent 4$f^{13}$ and divalent 4$f^{14}$ of Yb ions, following the Hund’s rule tendency to fill the 4$f$ shell. As a result, a quantum mechanical admixture of these states leads to intermediate valence character. Furthermore, additionally geometrical frustration can cause sufficiently large quantum spin fluctuations leading to suppression of a long-ranged magnetic order as to drive a system into interesting types of intrinsically quantum-mechanical ground states. YbAgGe was recognized to be one of the few stoichiometric Yb-based heavy fermion compounds which ground state would be determined by the competition between the Kondo effect and the Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction derived from the exchange interaction between 4$f$ electrons and
conduction ones. In addition, a high degree of geometrical frustration plays also an important role in this compound.

YbAgGe, crystallizing in the hexagonal ZrNiAl-type structure, undergoes successive two magnetic phase transitions at \( T_{M1} = 0.8 \) K (second order) and \( T_{M2} = 0.65 \) K (first order), which disappear with the application of a magnetic field.[2-3] At the same time, non-Fermi liquid behavior is observed in specific-heat and resistivity measurements.[4] Furthermore, YbAgGe is recognized to be the moderate heavy-fermion (HF) compound with a Kondo temperature \( T_K \approx 20 \) K and high-temperature linear coefficient of the specific heat \( C_p/T = 150 \) mJ/mol·K\(^2\). It is worthwhile also to mention that the magnetic ordering temperatures are well separated from the Kondo temperature \( T_K \approx 20 \) K that is itself well below the estimated first excited crystal electric field (CEF) level \( T_{CEF} = 60 - 100 \) K.[5] As a result, most likely, the low temperature property would be governed by Kramers doublet including the competition between the Kondo effect and the RKKY interaction, and the geometrical frustration effect.

In this way YbAgGe really gives unique possibility to explore the possible interplay and the role of the Kondo effect, quantum criticality, intermediate valence, RKKY interaction and CEF effect using ultrasonic measurements. Ultrasound measurement has been used for the last three decades as a powerful method to investigate the elastic properties of Heavy Fermion HF compound. In particular, one can obtain detailed information concerning a ground state multiplet of rare-earth ions split mainly by the CEF effect and the character of a quadrupolar moment active in low-lying energy levels. We present in this communication the first ultrasonic investigation on the Yb-based moderate HF compound YbAgGe.

2. Experiment

Single crystal of YbAgGe was grown using a Ag-Ge rich self-flux method. The three Yb\(^{3+}\) ions per unit cell lie on a quasi-Kagome triangular lattice in the basal plane of the hexagonal non-centrosymmetric structure (space group \( P62\overline{m}, a = 7.05, c = 4.14 \) Å) Specimen used for the present ultrasonic measurement was cut into a rectangular shape with two axes along the \( a\)-and \( c\)-axis.

The sound velocity, as the elastic constant was measured by an ultrasonic apparatus based on a phase comparison method at temperatures down to 0.5 K in magnetic field up to 10 T. Plates of LiNbO\(_3\) was used for the piezoelectric transducer. The fundamental resonance frequency of LiNbO\(_3\) transducer is 10 - 30 MHz. The transducer was glued on the parallel planes of the sample by an elastic polymer Thiokol. The absolute value of the sound velocity was obtained by measuring the delay time between the ultrasonic echo signals with an accuracy of a few percent. The elastic constant was calculated as \( C = \rho v^2 \) by using the sound velocity \( v \) and the density \( \rho \) of the crystal. The lattice constant of YbAgGe at room temperature was used for the estimation of the density \( \rho = 9.801 \) g/cm\(^3\).

3. Deformation potential approximation

There are various couplings of lattice distortions and electronic states. In the case of intermetallic rare earth, especially for HF compounds a deformation potential coupling to conduction electrons plays an important role in their elastic property in addition to the quadrupolar response mentioned above. A large density of states of quasi-particles in the vicinity of Fermi level formed by a strong hybridization, a coupling constant \( d \) between the quasi-particles and a relevant elastic strain associated with sound waves becomes significantly strong. [6-7] This situation often brings about an elastic anomaly. For the simplicity, we employed here a rectangular density of states with a total band width \( W \). According to the deformation potential approximation with the rectangular density of states, the elastic constant \( C_T \) can be written by
\[ C_T(T) = C_T^{(0)}(T) - N \frac{4d^2}{W} \tanh\left(\frac{\beta W}{4}\right) \]  

(1)

where, \( C_T^{(0)} \), \( N \), \( d \) and \( W \) denote a background elastic constant, number of ions in a unit volume, coupling constant and total band width, respectively. \( \beta \) denotes \( 1/T \).

**Table 1.** Elastic constants at 4.2 K and fitting parameters in zero field in formula (1) of YbAgGe.

| \( C_{11} \) | \( C_{33} \) | \( C_{44} \) | \( C_{66} \) | \( d \) | \( W \) |
|---|---|---|---|---|---|
| 61.8 GPa | 39.7 GPa | 34.4 GPa | 25 GPa | 2.8 K | 6.0 K |

**Figure 1.** Temperature dependence of longitudinal elastic constants \( C_{11} \), \( C_{33} \) and transverse ones \( C_{44} \), \( C_{66} \) of YbAgGe.

4. Experimental Results and Discussions

Figure 1 depicts an overview of the longitudinal \( (C_{11}, C_{33}) \) and transverse \( (C_{44}, C_{66}) \) elastic constants as a function of temperature \( (T) \) for YbAgGe. The absolute values of each elastic constants are listed Table I. These data show normal behavior at higher temperature; a stiffening with decreasing \( T \). However, a softening was found below \( \sim 20 \) K in the \( T \) dependence of \( C_{11}, C_{33} \). Figure 2(a) depicts the \( T \) dependence of \( C_{11} \) at low temperatures under the selected magnetic fields \( (H) \) along \( a \)-axis, offset for clarity in ascending order bottom to top. The softening below around 10 K becomes suppressed gradually with increasing the \( H \), and finally disappear above 4 T. The solid blue lines in Fig. 2(a) show the calculated results based on the formula (1). These fits yield the important values: background \( C_T^{(0)}=a+bT \), deformation coupling constant \( d \), and band width \( W \) as summarized in Table I. Figure 2(b) depicts the \( H \) dependence of \( W \) and \( d \) under the selected \( H \) along \( a \)-axis. It is found that the both values increase dramatically around 4 T with increasing the \( H \).
Here, we discuss the low temperature property of YbAgGe. The softening observed is difficult to reproduce only by the CEF effect if the Kramers doublet is the ground state in YbAgGe as proposed by the experimental results of neutron inelastic scattering measurement.[5] Clearly, the quadrupolar degrees of freedom are not active on the same energy scale as the correlation or any exchange energy. Another factor need to be considered when understanding the strong softening observed. Now we examine the origin from a different angle. One can obtain better agreement if one applies the deformation potential approximation as stated above. This indicates that the coupling between quasiparticles and the relevant elastic strain associated with sound waves is of great importance and plays a crucial role at low temperatures. An increase in the band width $W$ with increasing $H$ suggests a tendency toward the broadening of $4f$ level to gain the Zeeman energy, leading to the suppressed HF behavior or/and suppression of a magnetic fluctuation due to the geometrical frustration. This point remains as a matter to be discussed further. We will discuss them more in detail in another article as space is limited.[8] Nevertheless, it might be reconfirmed, from this work, that the possible interplay and the role of the Kondo effect, quantum criticality, RKKY interaction and geometrical frustration effect would give rise to the novel ground state that the magnetic ordered state to the NFL one, being tuned by a $H$.

5. Summary
We have performed ultrasonic measurements on YbAgGe single-crystalline sample. Experimental results and the calculated fitting demonstrate that the coupling between quasiparticles and the relevant elastic strain associated with sound waves is of great importance, and also that the band width $W$ becomes broader with the application of a magnetic field when crossing the critical field $H_c \sim 4$ T. It seems that this notable feature would be associated with the field-induced non-Fermi-liquid behavior. The deeper investigation is necessary to understand its origin and to interpret properly the corresponding experimental data in the future. For a further discussion, the same measurements for the Au-substitution system YbAg$_{1-x}$Au$_x$Ge are currently in progress.
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