Low-temperature elastic properties of YbSbPt probed by ultrasound measurements

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Abstract. The elastic properties of a single crystal of the half-Heusler compound YbSbPt have been investigated by means of the ultrasonic measurement. In particular, careful measurements of the temperature (T) dependent elastic constant \( C_{11}(T) \) was performed in the vicinity of its phase transition point near \( T_N \) of 0.5 K. A clear step-like anomaly accompanied by spin-density-wave type antiferromagnetic (AFM) phase transition was found in the \( C_{11}(T) \) curve. The low-temperature magnetic phase diagram is proposed on the basis of the results. The phase diagram consists of, at least two main distinct phases: a low-field and high-field regime with a transition field of approximately 0.6 T at zero field. We discuss the low-temperature elastic property based on analysis of Landau-type free energy.

1. Introduction
The discovery of a massive electronic state in YbBiPt, and thereafter YbCo₂Zn₂₀ has stimulated experimental and theoretical activity aimed at understanding fundamental electronic state and magnetic properties of these and related Yb-based intermetallic compounds. [1-5] In particular, an intriguing aspect of YbBiPt is the existence of spin-density-wave type magnetic phase transition at 0.4 K determined by a small but rather sharp peak in its specific heat. Furthermore, a sudden steep jump was observed in the temperature (T) dependence of the electrical resistivity at 0.4 K, suggesting the formation of an energy gap at the Fermi level. [1-4] Recent neutron scattering measurement determined the averaged ordered moment of 0.8 \( \mu_B \)/Yb with the AFM propagation vector \( q = (1/2, 1/2, 1/2) \) below 0.4 K. [6] Here, it should be noted that YbBiPt is a low-carrier-concentration semimetal, although most of systems with such a largely enhanced Sommerfeld coefficient \( \gamma \) in the vicinity of the quantum critical point (QCP) favor a metallic state characterized by a renormalized effective mass. [7-10] The origin of the massive electronic state in the low-carrier-concentration system YbBiPt is of particular interest. From the structural analogy, a significant enhancement of the Sommerfeld coefficient \( \gamma \) would be also expected in the isostructural system YbSbPt. The Sb substitution is regarded as a chemical pressure because of its smaller ionic radius than that of Bi, leading to the lattice contraction and its major effect on the system is to increase a hybridization between 4f states and valence electronic states. In fact, the massive electronic state and the similar magnetic phase transition have been clearly recognized in YbSbPt in the previous studies.[11] YbSbPt belongs to the series of cubic half-Heusler (space group F43m)\( R \)Pt\( X \) compounds (\( R \) = rare-earth, \( X \) = Sb, Bi) with...
the magnetic Yb ions forming a face-centered-cubic (fcc) magnetic sublattice, and is one of the few stoichiometric Yb-based HF compounds. In fact, it was recently found that YbSbPt also exhibits an enormous low-temperature Sommerfeld coefficient, $\gamma \sim 9 \, J/mol \, K^2$. Several hypotheses have been proposed to explain these observations. For example, the fcc structure produces frustrated Ruderman-Kittel-Kasuya-Yoshida interactions such that magnetic order cannot circumvent Kondo interactions. Very recently, several half-Heuslers are predicted to display band inversion at the $\Gamma$ point, leading to topologically nontrivial states.[12-14] These features could possibly lead to the formation of massive quasi-particles close to the Fermi level. Although there have been considerable experimental and theoretical efforts, the origin of the enormous $\gamma$ has not been yet clear at this stage.

An ultrasonic measurement is suited to study the $4f$ electronic state via quadrupolar response of the $4f$ electronic ground state split by the crystalline electric field effect if the $4f$ electrons are localized well. On the other hand, a narrow quasiparticle band formed by heavily renormalized quasiparticles causes elastic anomaly as well even if the $4f$ electrons are delocalized due to a deformation potential coupling to conduction bands.[15,16] In this paper, we report partial results of an investigation of the low temperature elastic properties of a single crystal of YbPtSb to deepen the understanding of the ground state properties in YbSbPt.

2. Experiment

The single crystal was grown from an excess Sb flux. The crystal structure was characterized by an X-ray diffraction measurement. The determined lattice parameters, $a = 6.4624 \, \AA$ and the half-Heusler MgAgAs structure with space group F43$\bar{m}$ are in agreement with previous studies.[17] Specimen used for the present ultrasonic measurement was cut into a rectangular shape with two axes along the $\langle 100 \rangle$- and $\langle 110 \rangle$-axis. The sound velocity, as the elastic constant was measured by an ultrasonic apparatus based on a phase comparison method. For low-temperature measurements, an Oxford helium dilution fridge adapted for ultrasonic measurements was employed with a 8 T superconducting magnet. 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 relative change of the $C_{11}$, $\Delta C_{11}$ of YbSbPt is used in this paper.

3. Experimental Results and Discussions

The relative variation of the elastic constant $C_{11}$ as a function of temperature is shown in Fig. 1 under selected fields along the $\langle 100 \rangle$ axis. The data were normalized to their value at 1 K and the curves have been shifted vertically for clarity. The $C_{11}$ is one of the three principal independent elastic constants for the cubic crystal, and was measured by the longitudinal sound wave with frequencies of 10 - 30 MHz propagating along the $\langle 100 \rangle$ axis. Although it is not shown here, the $C_{11}$ which denotes a pure compression along the $\langle 100 \rangle$ axis smoothly increases at high temperature. [18] This temperature dependence appears normal in view of the expected stiffening following the progressive disappearance of phonon anharmonic effects upon lowering the temperature. However, the $C_{11}$ shows a noticeable softening below around 20 K, as already reported by our group. [19] Here, we put a focus on the elastic property involving the low-temperature phase. A step-like elastic anomaly at the phase transition is observed clearly at zero magnetic field. The transition temperature shifts slightly to higher temperatures and the shape of the anomaly becomes sharper with increasing the magnetic fields up to around 0.6 T. In contrary, the transition temperature shifts to lower temperatures with the further increase of the magnetic field. Surprisingly, the shape of the anomaly changes dramatically, namely a sudden
Figure 1. Temperature dependence of one of the principal elastic constants $C_{11}$ of YbSbPt, measured in different applied magnetic fields. The data were normalized to their value at 1 K and the curves have been shifted vertically for clarity. The arrows indicate the phase transition temperature point, derived from the minimum or maximum in $dC_{11}(T)/dT$.

Figure 2. The relative change of the $C_{11}$, $\Delta C_{11}$ of YbSbPt in a zero field, (a) and in a field of 0.6 T, (b), being associated with the phase transition. $\Delta C_{11}$ is determined as shown the arrow.

increase (stiffening) appears at the transition temperature. The anomaly becomes suppressed with the further increase of the magnetic field, and invisible in the field above around 3 T. It should be noted that the precipitous increase of $C_{11}$ at the magnetic field of 0.6 T is characteristic of the low-temperature ordered phase. In order to discuss the magnetic field evolution of the temperature dependence of the elastic constant $C_{11}(T)$ in the vicinity of $T_N$, a relative of change of $C_{11}$: $\Delta C_{11}$ accompanied by the phase transition was estimated on the basis of the definition as shown in Figs 2(a) and (b). Figure 3 shows the obtained magnetic field dependence of the relative change of the elastic constant $\Delta C_{11}$ due to the phase transition. The dashed lines are
given as guides to the eye. One can recognize that the critical magnetic field of $H_c \sim 0.6$ T exists and the system changes its elastic property when crossing $H_c$. Furthermore, it should be additionally noted here that a sharp increase of the resistivity observed around $T_N$ is completely suppressed by a magnetic field above $H_c$, suggesting disappearance of the energy gap.

**Figure 3.** Magnetic field dependence of the relative change of the $C_{11}, \Delta C_{11}$ of YbSbPt. The dashed lines are a guide for the eye.

**Figure 4.** Magnetic phase diagram constructed and illustrated by data taken from the present measurements. The dashed lines are a guide for the eye. Orange regions indicate a low-field phase in which the $C_{11}(T)$ decreases below $T_N$: AFM I. Dark blue regions, being the left side of the dashed line indicate a high-field phase in which the $C_{11}(T)$ increases below $T_N$: AFM II.
Let us here discuss the obtained elastic anomalies from a coupling between elastic strain and order parameters including magnetic moment, or enhanced quasi-particles based on analysis of Landau-type free energy. Recall the relative change of the $C_{11}$, $\Delta C_{11}$ of YbSbPt below and above $H_c$, due to the phase transition are shown in Fig 3. In general, the $\Delta C_{11}$ gives us microscopic information for the coupling between the elastic strain $\varepsilon^{11}_\Gamma$ and the order parameter of the ordered phase $Q$ based on Landau phenomenological theory as follows,[20]

$$F = \frac{1}{2}aQ^2 + \frac{1}{4}bQ^4 - \zeta Q^2 \varepsilon^{11}_\Gamma + \xi Q^2 \varepsilon^{11}_\Gamma + \ldots$$

(1)

From the second derivative of the free energy $F$ with respect to the elastic strain, one can obtain the following formula

$$C_{11}(T) = \frac{\partial^2 F}{\partial \varepsilon^{11}_\Gamma} = C_{11}^{(0)}(T) - \frac{2\xi^2}{b} - 2Q^2 \xi$$

(2)

Here, $C_{11}^{(0)}(T)$ is the lattice part and originates mainly from anharmonic effect of the crystal. $a$ and $b$ denote the second- and fourth-order coefficient of free-energy. $\xi$ and $\zeta$ denote the fitting parameters related to the elastic softening and hardening, respectively. As mentioned above, the elastic softening of $C_{11}(T)$ below $H_c$ is primarily caused by $\xi$, while the elastic hardening above $H_c$ is primarily caused by $\zeta$ as shown in Figs. 2 (a) and (b), respectively. Furthermore, it is commonly known that the former corresponds to a possible change of transfer integrals of heavy quasi-particles formed near the Fermi energy, and the latter corresponds to a possible change of the coupling constant between the elastic strain and the order parameter $Q$, probably here being the magnetic moments ($M$) of the heavy quasi-particles. [21,22] If an energy gap appears i.e., the number of carriers decreases, it leads to an elastic hardening as seen in PrRu$_4$P$_{12}$, which is inconsistent with the behavior in the low-field regime below $H_c$.[23] This discrepancy remains unsettled at this stage. On the other hand, the significant decrease of the relative change of $C_{11}(T)$ above $H_c$ with increasing applied magnetic fields is probably due to the decrease of $\xi$, suggesting the suppression of spin-density-wave type magnetic phase with increasing the fields.

Viewed in this light, it is most likely that at least there are two different phases in the low-temperature ordered phase. The characteristics observed here are collected in the $H$ - $T$ phase diagram displayed in Fig. 4. The boundary was determined from the sharp peak position in $dC_{11}/dT$. The low-field phase is characterized by the elastic softening and semiconducting with an energy gap as labeled by AFM I. On the other hand, the high-field one is characterized by elastic stiffening and semi-metallic nature as labeled by AFM II. The higher-field phase is consistent with the previous results obtained from the magnetization, electric resistivity and specific heat measurements. The higher-field phase labeled by AF II, however does not fully agree with that determined by previous studies.[4] The AFM II boundary might be corresponding either to the crossover of $H^*$ on which the broad local maximum was observed in the $T$ dependence of the derivative $d\rho(T)/dT$, or to $T_{FL}$ which was determined by the upper limit of the $T^2$ dependence of the electrical resistivity in the reference [4]. This is an open question.

Finally, we would like to comment on the possible surface state in YbSbPt due to topological nature of surface conducting channel, reported recently in half-Heusler systems such as HoPdBi, ErPdBi, LuPdBi and others.[24-29] Since ultrasound measurements are sensitive and reliable volume probes of ordering phenomena in the bulk of solids, discrepancies might occur in physical interpretations between results of the electrical resistivity and present elastic constant near the phase transition temperature. Namely, formation of the energy gap and a very weak induced magnetic moment below $T_N$ might be due to topological surface nature. Very sensitive and
direct measurements at low temperatures, such as Scanning Tunneling Microscope and Angle-Resolved Photoemission Spectroscopy measurements are required in the future in order to make a sharp distinction between its surface- and bulk-nature.

4. Summary
In summary, we have investigated the low-temperature elastic properties of a single crystal of YbPtSb by means of the ultrasound measurement. A marked difference was found in the temperature dependence of the longitudinal elastic constant $C_{11}(T)$ between the low field- and the high field regime with $H_c = \sim 0.6$ T. The characteristic behavior would reflect the electronic state of strongly renormalized quasi particles including its energy gap and magnetic moment with the relatively lower carrier-concentration. The deeper investigation is necessary to understand its origin and to interpret properly the corresponding experimental data, including a possible scenario based on Dirac electrons formed in the vicinity of Fermi level in YbPtSb. For a future discussion, the same measurements for other kinds of elastic constants, $(C_{11} - C_{12})/2$ and $C_{44}$ are currently in progress. We hope that these observation will stimulate theoretical studies to understand the remarkable elastic properties of YbPtSb.

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