

Lattice dynamics of ferromagnetic superconductor UGe₂

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Abstract. This paper reports the lattice dynamical study of the UGe₂ using a lattice dynamical model theory based on pairwise interactions under the framework of the shell model. The calculated phonon dispersion curves and phonon density of states are in good agreement with the measured data.

Keywords. Phonons; UGe₂; density of states.

PACS Nos 63.10.+a; 63.20.-e; 74.25.Ke

1. Introduction

Since the discovery of superconductivity and ferromagnetism together [1] in UGe₂, great interest is generated in this compound due to its unusual and interesting characteristics. The coexistence of ferromagnetism and superconductivity to this system is not new to this system and have been found earlier in many compounds [2,3], but the behaviour of UGe₂ under pressure brings it under focus. Shick and Pickett [4] reported that this compound shows two order higher Curie temperature ($T_{\text{Curie}} \sim 35$ K) than the superconducting transition ($T_c \sim 0.7$ K) at pressure 12 kbar. In other cases the Curie temperature is less than the transition temperature. The disappearance of superconductivity and ferromagnetism at the same pressure $P \approx 16$ kbar suggests that both these phenomena in this compound are cooperative [5]. Machida and Ohmi [6] have suggested that the triplet pairing is responsible for these phenomena based on a phenomenological theory of ferromagnetic superconductivity. However, the origin of the pairing mechanism is under debate and therefore other mechanisms of superconductivity have been proposed. One such proposal is the importance of screened phonons in ferromagnetic medium that was responsible for the mechanism. This fact has been further supported by the anomalous behaviour of the specific heat at ambient pressure. The behaviour of the ambient pressure specific heat indicates a substantial contribution from low energy phonons or any another soft mode [7]. The anomaly of excess specific heat occurring at $T = 30$ K and $P = 0$ is still puzzling and cannot be ignored as it is

found to be responsible for the phase transition. Watanabe and Miyake [8] tried to explain this specific heat anomaly using a methodology based on the coupling of spin and charge density waves which suggests that a Kohn anomaly occurs in the phonon spectrum similar to $\alpha - U$ [9]. The anomalous specific heat measurements [10] and large Sommerfeld coefficients obtained from the specific heat measurement indicates a heavy fermion behaviour in UGe_2 . To understand this unusual behaviour, several band structure calculations [11] and neutron scattering measurements of the ferromagnetic superconductor UGe_2 [1,12] have been performed. While the band structure calculations focused mainly on the spin and orbital magnetic state to understand the anomalous specific heat, the neutron scattering studies focus on its debatable structure [1,12]. It is observed from the literature on UGe_2 that while this compound gains focus due to its anomalous specific heat behaviour [10], the role of phonons has not been taken seriously so far except by Raymond and Huxley [13]. Raymond and Huxley [13] have performed the inelastic neutron scattering (INS) measurement of phonon spectrum of the ferromagnetic superconductor UGe_2 to understand the anomalous specific heat behaviour. They also simulated the phonon spectrum by using BvK lattice dynamical model with *ad hoc* force constants. However, they did not observe any significant change in the INS spectra (lattice dynamics) with the temperature and any phononic contribution to the anomalously predicted very high value of specific heat. A detailed investigation of lattice dynamics is desirable to understand the behaviour of phonons in this compound. It is indeed essential to perform the lattice dynamics of UGe_2 by using more accurate lattice dynamical model with physically significant model parameters or by using *ab initio* methods.

In the present paper we report a detailed and systematic investigation of phonon properties by using a lattice dynamical model theory in the framework of the shell model. We present the calculated frequency of zone centre Raman and infra-red (IR) active phonon modes and neutron weighted phonon density of states in addition to the phonon dispersion curves for UGe_2 compound. While the total phonon density of states has been used to calculate the specific heat, the partial phonon density of states is used to calculate the isothermal parameters and demonstrate the actual atomic contributions to the total phonon density of states. In §2, the interatomic potential and the computational methods for calculating the lattice vibrational properties are briefly discussed. Section 2 contains results and discussion on the phonon properties of UGe_2 followed by the main conclusions in §4.

2. Interatomic potential and computational methods

In the present study, the lattice dynamics of UGe_2 is carried out in the framework of the shell model. The model is not only appropriate for the complex systems but also has been quite successful in predicting the phonon properties of many systems including the MgCNi_3 which is quite similar to the present system [14]. In addition, it considers the ionic polarizability of the ions. In the present shell model every ion is represented by a shell coupled to a core through a harmonic force constant K , and the short-range interactions between ions are represented by pair potentials of the Born–Mayer form and the total potential along with the Coulomb interactions

Table 1. Short-range interactions and model parameters for UGe_2 .

Interactions	b (eV)	ρ (Å)
U–Ge	1500.0	0.3066
Ge–Ge	18764.0	0.5554
Shell model: Ge; $Y(e) -2.86902$, $K = 72.92 \text{ eV-Å}^2$		

are written as

$$U_{ij}(r_{ij}) = \frac{Z_i Z_j e^2}{r_{ij}} + b_{ij} \exp\left(-\frac{r_{ij}}{\rho_{ij}}\right), \quad (1)$$

where the first and the second term represent the long-range Coulomb potential and Born–Mayer repulsion energies, respectively. Here, r_{ij} is the interatomic distance between atoms i and j , Z_i and Z_j are the effective charges of the respective atoms, b_{ij} and ρ_{ij} are the short-range potential parameters for each pair of atoms usually found by fitting to experimental data. The cation–anion short-range (SR) potential parameters are obtained by ensuring that the total stress and forces for the given structure vanishes. However, it is ensured that the physically significant parameters are obtained which give nearly vanishing forces on all the atoms and right magnitude of the eigenfrequencies in the harmonic approximation. The electronic polarization of the lattice is included by the shell model in which an ion is represented by a massless shell of charge Y and a core of charge X which are coupled by a harmonic spring constant K . The free ionic polarizability is expressed by $\alpha = (Ye)^2/K$, where Y is the dimensionless shell charges and e is the absolute value of the electron charge. To calculate the phonon properties, the code LADY for lattice dynamical simulation is used which has been successfully applied by us [14]. The crystallographic data for UGe_2 for the calculations of phonon properties have been taken from ref. [8]. The model parameters are presented in table 1.

3. Results and discussion

UGe_2 crystallizes in orthorhombic $C_{mmm}(D_{3d}^6)$ space group, with two formulas per unit cell and its irreducible modes at zone centre can be given as

$$(D_{3d}^6) = 2A_g + 2B_{1g} + 2B_{3g} + 4B_{1u} + 4B_{2u} + 4B_{3u}, \quad (2)$$

where g and u modes are Raman and IR active respectively. In the orthorhombic C_{mmm} phase of UGe_2 , there are six atoms in the primitive cell and thus 18 phonon modes at each wave vector. The zone centre optical phonon frequencies calculated by using the present shell model are presented in table 2. The phonon dispersion curves for UGe_2 along the Λ -, Δ - and Σ -directions of the Brillouin zone (BZ) along with the experimental data obtained from the inelastic neutron scattering experiment [13] are presented in figure 1a. All the 18 phonon modes are distributed almost uniformly up to 215 cm^{-1} ($\approx 27 \text{ meV}$). In the present study, the low-lying

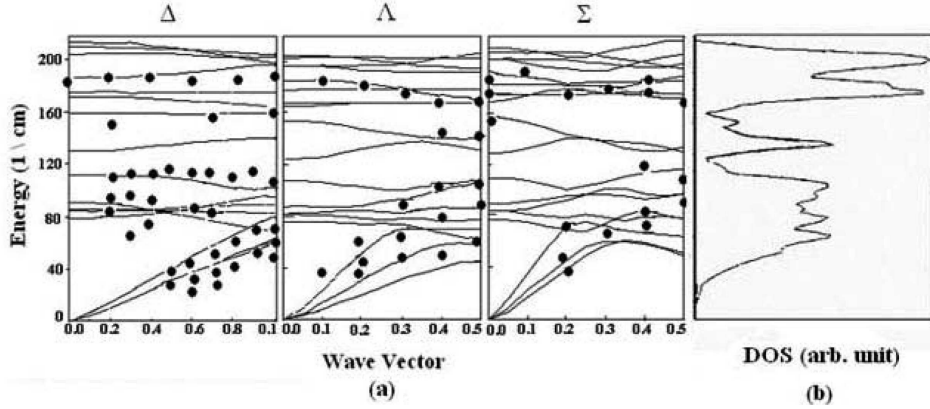


Figure 1. (a) Phonon dispersion curves of UGe_2 along the three principal symmetry directions. Filled circles represent experimental INS data obtained at 300 K [13]. (b) Neutron weighted phonon density of states (PDOS) of UGe_2 .

Table 2. Zone centre phonon modes of UGe_2 .

Modes	A_g	B_{1g}	B_{3g}	B_{1u}	B_{2u}	B_{3u}
Frequency (cm^{-1})	51.64, 118.67	44.11, 137.24	29.42, 85.87	55.96, 90.25, 132.12	66.48, 85.64, 96.20	57.64, 80.45, 130.00

phonon modes (acoustic phonon branches) are of special concern due to its unusual nature. In the case of Σ -direction the separation between two branches below $q=0.3$ has been correctly reproduced by the present calculation similar to the INS data than the force constant model. It is seen from the present figure that the low-lying phonon modes in Σ -direction of the BZ show significant bend near the zone edge similar to the experimental data but contrary to the BvK model. The present study predicts that the acoustic modes are linear in Δ -direction. The degeneracy of TA modes observed from the experimental data are better produced by the present model than by the BvK model. The agreement between the experimental and calculated data for the acoustic phonon branches is poor in the Λ -direction. The frequencies of the TA modes calculated from the present calculations are however lower than the experimental data which were predicted to be higher in the BvK model. The highest frequency region (optical frequencies) which is due to the vibrations of Ge atoms only contains more or less dispersionless optical phonon modes in the Λ - and Δ -directions while they show dispersion in the Σ -direction. We cannot comment on the success of the present model in predicting the optical phonons as more accurate measurements are needed. However, to overcome this we have started an *ab initio* lattice dynamics calculation for the UGe_2 compounds.

Figure 1b presents neutron weighted phonon density of states of UGe_2 . The two peaks observed in the higher frequency side of the spectrum are due to the Ge atoms only while in the middle region the contributions come from both Ge and

U atoms. The lower side of the spectra is due to the U atom vibrations. However, a significant feature in the phonon DOS is the absence of DOS below 25 cm⁻¹ in the phonon density of states. A similar structure in the experimental neutron scattering spectra is also observed [13]. The spectrum follows the mass relation.

Finally, in the present paper we report the phonon dispersion curves and neutron weighted phonon density of states of the UGe₂ compound. There is a reasonably good agreement with the experimental data. We observed the bending of transverse acoustic phonon modes near zone boundary in the Σ -direction and the absence of phonon DOS below 25 cm in the neutron weighted phonon density of states spectra.

Acknowledgements

Financial assistance from the DAE-BRNS, DST and UGC is highly appreciated.

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