Coupling of rare earth moment and charge density wave ordering in a single crystal Er₂Ir₃Si₅

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Abstract. Charge Density Wave (CDW) transitions are well known phenomena in a large variety of quasi-low dimensional conductors. Their appearance is basically due to the low dimensionality which facilitates Fermi surface nesting. We have shown that both Lu₂Ir₃Si₅ and Er₂Ir₃Si₅ are two new CDW compounds whose structure is 3-D in nature [1,2]. The nesting of Fermi surfaces leads to the appearance of a periodic lattice distortion with an accompanying energy gap opening at the Fermi level [3]. In this work, we report the bulk characterization of a high quality single crystal of Czochralski pulled Er₂Ir₃Si₅ using transport and magnetization measurements. These studies establish multiple charge density wave transitions in this crystal with coupling of the Er moments to the CDW ordering as evidenced by the magnetization measurement. Such a coupling is rather unusual in rare earth compounds that display CDW transition. Possibility of modulated magnetism of Er moments due to CDW will be discussed.

1. Introduction

The charge density wave (CDW) ground state occurs in low-dimensional materials as a consequence of electron-phonon interactions in that the electronic instabilities lead to structural modulations. The periodic charge density modulation accompanied by a periodic lattice distortion has a tendency to achieve nesting of the Fermi surface and to open an energy gap at the Fermi level. The Rare earth ternary silicides, forming in various crystal structures with their unusual ground states, are known to exhibit various interesting phenomena like superconductivity, coexistence of magnetism and superconductivity, reentrant superconductivity and magnetic ordering. Of the R₂T₃X₅ [4,5] series (R=Rare-earth metal, T=Transition metal and X=Si and Ge), Lu₂Ir₃Si₅ single crystal is reported to show coexistence of charge density wave and superconductivity while polycrystalline Er₂Ir₃Si₅ is also reported to exhibit CDW ordering [1]. In the backdrop of intense efforts to understand the coexistence of magnetism and superconductivity, the interplay between magnetism and CDW could provide important clues to achieve a global understanding of the different degrees of freedom in a solid. Although ferromagnetism appears due to Coulomb repulsion between electrons whereas CDW is due to attractive electron-electron interaction mediated by phonons, theoretical works by Balseiro et al [6] showed that ferromagnetism can induce a periodic lattice distortion and coexist with CDW. Subsequent calculations by Gulacsi et al [7] showed that a CDW, spin density wave, and ferromagnetism could coexist in the presence of an external magnetic field. On the other hand, in rare-earth intermetallic SmNiC₂, CDW was reported to be destroyed by ferromagnetism [8]. CDW has been observed in nonmagnetic metal adlayers like Sn or Pb on Ge [9], In/Cu [10], and in bulk metal like uranium, [11] while in Er₂Ir₃Si₁₀ it is strongly coupled to the local moment antiferromagnetism [12]. In uranium metal, the CDW is associated with significant phonon softening that is related to the martensite transition [13]. Here we report an unusual coupling of local rare-earth moments to the CDW ordering itself as confirmed by magnetic measurements. The electrical transport
measurement data and magnetic susceptibility of Er$_2$Ir$_3$Si$_5$ single crystal along the (001) direction are reported in this paper.

2. Experimental details

The Er$_2$Ir$_3$Si$_5$ single crystal was grown in a tetra-arc furnace using a modified Czochralski technique. The constituent elements (Er = 99.99 %, Ir = 99.99 %, Si = 99.9999%) were taken in stoichiometric proportion to make 10 g melt in the tetra arc furnace. A thin tungsten rod was immersed into the melt and pulled at a speed of 11 mm/h in a pure and dry argon atmosphere. The phase homogeneity of the crystal ingot is confirmed by Laue diffraction and powder X-ray diffraction (XRD) using Cu-K$_\alpha$ radiation in PANalytical commercial diffractometer. The room temperature powder X-ray diffraction pattern of the sample could be indexed to the orthorhombic structure (U$_2$Co$_3$Si$_5$, space group = Ibam) with no impurity lines. For brevity, the XRD and Rietveld simulated patterns are not shown here. Earlier studies showed that the sample undergoes a structural transition (along with CDW) below 160 K. The electrical resistivity measurement, in the temperature range of 1.6 K to 300 K, was performed using four probe dc technique in a homemade setup. And a commercial Superconducting Quantum Interference Device (SQUID, MPMS, Quantum Design, USA) magnetometer was used to measure the temperature dependence of the magnetic susceptibility $\chi$ in a field of 1 kOe for temperatures between 1.8 K to 300 K.

3. Discussions

A sharp transition in the electrical transport measurement is observed along all the crystal axes. As Fig. 1. displays the electrical resistivity of the crystal along the (001) direction while warming and cooling between the temperature range of 4 K and 300 K. A large hysteresis anomaly is observed during the thermal cycle. A similar electrical transport behavior exhibited by charge density wave or spin density wave (CDW/SDW) materials due to the partial opening up of a gap in the electronic density of states are observed in the case of Lu$_2$Ir$_3$Si$_5$ between 150 K to 225 K range [3]. It has been suggested that the observed difference during the thermal cycling in the electrical resistivity measurement is due to the CDW transition itself and the residual stress after the transition in the sample. The striking feature in this system is that even in the CDW state, the compound still retains metal-like behavior indicating that the energy gap is not fully opened i.e., there is a definite electronic density of states within the gap itself. The electronic structure study of the compound is done and will be published elsewhere.

The magnetic susceptibility data between 140 K to 175 K is displayed in Fig. 2 which is performed in a field of 1 kOe and it obeys Curie- Weiss law except in the temperature region where the cooling

![Figure 1](https://via.placeholder.com/150)

**Figure 1.** Temperature dependence of electrical resistivity of Er$_2$Ir$_3$Si$_5$ showing CDW transitions at high temperatures, along (001) direction, for both warming and cooling of the sample.
and warming magnetic data exhibits sharp transitions with hysteresis. This type of anomaly is not observed in CDW materials like Er$_2$Ir$_3$Si$_5$ [12] which shows normal Curie-Weiss behavior between 20 K to 300 K which can be explained by a large local moment contribution of Er$^{3+}$ that overwhelms any changes in Pauli paramagnetism which might have occurred due to the loss of the density of states due to the CDW transition. Though the susceptibility fitting dictates full local moment contribution of Er$^{3+}$, it is interesting to observe a prominent anomaly in the magnetic data which suggests that the local moments are strongly coupled to the underlying transition. This could be either due to the change in the underlying crystal field states before and after CDW transition or due to the change in the magnetic moment across the temperature region of the hysteresis. Inelastic neutron scattering measurements are required to settle this issue.

From the inset we also observe a paramagnetic nature of the susceptibility of this crystal in the higher temperature regime. A sudden decrease in the moment is seen at a temperature of 165 K while the sample is being warmed up, which is consistent with the transition temperature of 162 K as observed in the resistivity measurement while warming as in figure 1. As for the cooling down measurement of the susceptibility, a sudden slight increase in moment occurs at ~143 K with a small delay as compared to ~146 K in resistivity measurement result in figure 1. It can be inferred from the magnetic data that though rare-earth moments are localized, they are not totally isolated from the onset of spatial modulation of charge density.

As we have mentioned before both magnetism and CDW either coexists [12,14] or destroys [8]. Such occurrence is rare and even in those cases, there is no direct evidence of the CDW coupling to the magnetic moments in the paramagnetic state. In this sense the observation of the coupling of the Er$^{3+}$ moments with the CDW in Er$_2$Ir$_3$Si$_5$ is rather novel requires microscopic investigations to fully understand this phenomena.

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