

ELECTRICAL TRANSPORT AND PHASE TRANSITIONS IN POLYMERIZED AC₆₀ (A=K, Rb)

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We have measured the resistivity of polymerized KC₆₀ and RbC₆₀ as a function of temperature, pressure, and magnetic field. We find that the zero-pressure resistivity of KC₆₀ decreases from 400 K to 50 K, below which temperature the material shows a semiconducting-like behavior. Applied pressure causes the resistivity to decrease, and suppresses the transition to the semiconducting phase. In contrast, the zero-pressure resistivity of RbC₆₀ shows semiconductor-like behavior between 300 K and 1.5 K. Under applied hydrostatic pressure, RbC₆₀ undergoes a phase transition, possibly structural, to a better-conducting state when cooled.. No magnetoresistance is observed in either material.

1 Introduction

In spite of their structural similarity, the orthorhombic polymerized phases of KC₆₀ and RbC₆₀ exhibit remarkably different electrical and magnetic properties. ESR¹ and NMR² give evidence that RbC₆₀ is a quasi-1D conductor with a transition to an insulating magnetic ground state near 50 K, and that KC₆₀, in contrast, is a 3-dimensional conductor with no magnetic transition. The dc resistivity of RbC₆₀ is semiconducting, while that of KC₆₀ is metallic. Since many properties of the doped C₆₀ materials are primarily lattice-constant dependent, study of the AC₆₀ materials under applied hydrostatic pressure can be useful in probing the transition between the metallic behavior of KC₆₀ and the semiconducting behavior of RbC₆₀.

2 Experimental Techniques

2.1 Sample Synthesis

Samples of both materials were made by stoichiometric doping of pristine C₆₀ crystals. The doped crystals were annealed at high temperature (400 °C) for 7 days and cooled to room temperature over 12 hours. The crystals were then exposed to air and immersed in toluene for another 7 days to eliminate all other phases. The structure of the insoluble material was confirmed to be orthorhombic AC₆₀ by X-ray diffraction.

2.2 High-Pressure Measurements

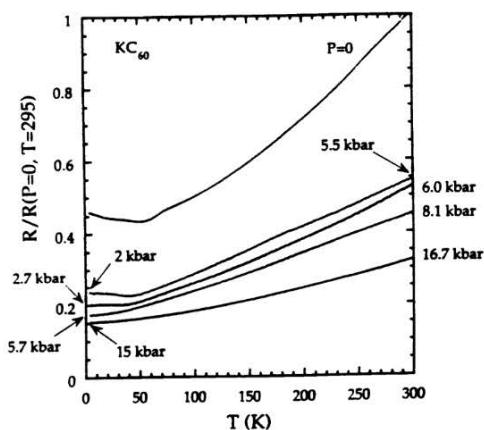
High-pressure resistivity was measured by the standard 4-probe technique in a self-clamping hydrostatic pressure cell with Fluorinert FC-75 as the pressure medium. The high-pressure measurements are not isobaric: the pressure in the cell drops as the cell cools, and so the pressure is monitored using a calibrated manganin coil.

3 KC_{60}

Figure 3.1 shows the dc resistivity of polymerized KC_{60} from 300 K to 4.2 K, at zero pressure and at pressures up to 16.7 kbar. At zero pressure, the resistivity decreases with decreasing temperature down to 50 K. Between 300 K and 100 K, the resistivity can be fit to the empirical form $\rho(T) = a + bT + cT^2$, similar to the $a + bT^2$ form in A_3C_{60} ³. Upon cooling below 50 K, the resistivity increases, giving evidence for a phase transition to a weakly insulating state. This material does not show evidence of a magnetic transition at low temperature, and shows no magnetoresistance (<0.1%), so the nature of this low-temperature phase is still unclear.

Figure 3.1. Resistivity of polymerized KC_{60} at $P=0$ and under pressures up to 16.7 kbar.

The resistivity of KC_{60} decreases dramatically under applied pressure: at room temperature, it saturates at a minimum of about one third of its zero-pressure resistivity. Under pressure, the low-temperature transition is suppressed: it flattens out, and the resistivity minimum decreases in temperature. Figure



3.2 is a proposed phase diagram for KC_{60} at low temperatures; it is quite similar to the phase diagram of quasi 1-D organic compounds which undergo a charge-density wave transition.

4 RbC_{60}

Figure 4.1 shows the resistivity of polymerized RbC_{60} at zero pressure and at pressures up to 10.6 kbar, from 300 K to 4.2 K. At zero pressure, the resistivity shows semiconducting-like behavior, although it is not truly activated. There is only a small bump in the resistivity at ≈ 40 K to give evidence of the magnetic phase transition which occurs at this temperature. Once again, the resistivity is highly pressure-dependent, decreasing to one-fifth of its room-temperature value at 10.6 kbar. Under applied pressure, RbC_{60} becomes metallic, with resistivity that decreases with decreasing temperature. More surprisingly, at intermediate pressures there is a sharp transition between semiconducting and metallic behavior.

Figure 4.1. Resistivity of polymerized RbC_{60} at 0 pressure and at pressures up to 10.6 kbar.

Figure 4.2 is an enlargement of the data shown above, and shows clearly that the material undergoes a transition to a "better conducting" phase, which causes a sharp change in the slope of the resistivity: the behavior is similar at all

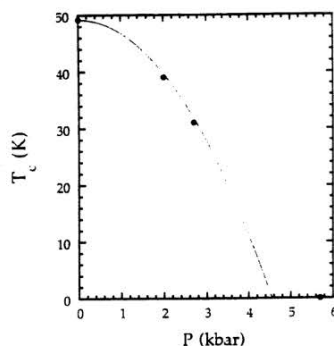
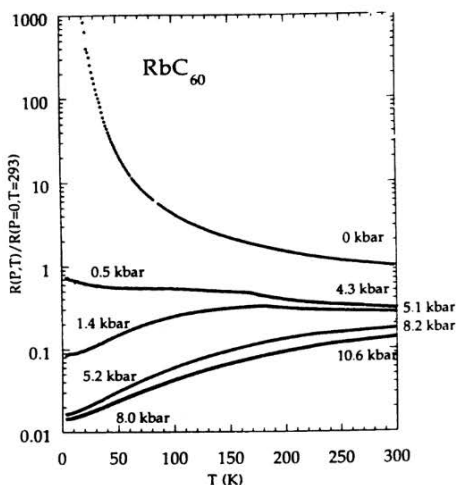


Fig. 3.2. Phase diagram of KC_{60} at low T



pressures, regardless of whether the material is metallic or semiconducting. The transition is hysteretic, as is shown in the inset. The phase transition is even clearer when the derivative of the resistivity is examined, as in figure 4.3. At all pressures, the derivative exhibits a rapid increase below a critical temperature T_C . The transition temperature increases fairly linearly with pressure, as is shown in the inset.

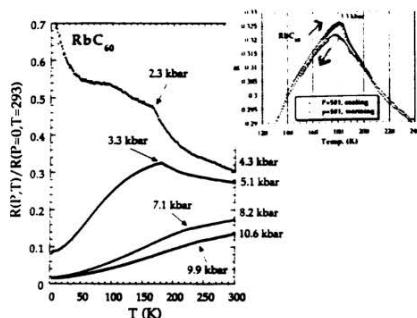


Figure 4.2. Resistivity of RbC₆₀ under pressure. The inset shows the hysteresis in the insulator-metal transition at 3.3 kbar and 180 K.

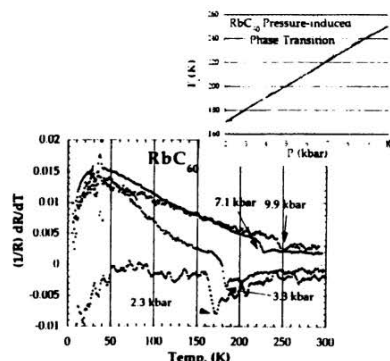


Figure 4.3. Logarithmic derivative $1/R dR/dT$ of RbC₆₀. Inset: the pressure dependence of the transition temperature.

Because the RbC₆₀ phase transition is hysteretic and occurs for both metallic and insulating states, it is likely to be structural. Determining the nature of this structural phase transition should elucidate the reason for the different behavior of KC₆₀ and RbC₆₀.

Acknowledgements

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