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Semiconducting ytterbium at high temperatures

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Abstract. We report in this communication some new results on the resistivity behaviour of ytterbium in its semiconducting phase. In the high temperature region ($T > 150°\text{C}$) the temperature coefficient of resistance is strongly positive like that in a degenerate semiconductor. This correlates well with our earlier work on the thermoelectric behaviour of ytterbium at high pressures and high temperatures.

Our measurements of the resistivity against pressure at room temperature and above show a distinct change in the slope accompanying the metal to semiconductor transition previously reported to be unobservable by other workers.

1. Introduction

Ytterbium undergoes a semimetal to semiconductor transition under pressure (Souers and Jura 1963). There have been several resistivity studies at high pressure but the data are all confined to temperatures less than 25°C (Souers and Jura 1963, McWhan *et al* 1969; Jerome and Rieux 1969). The available data near room temperature do not show a characteristic change in the slope of the resistance against pressure graph accompanying the semimetal–semiconductor transition.

Our recent study on the thermoelectric behaviour of Yb at high pressures and high temperatures gives clear evidence of the semimetal–semiconductor transition in the thermopower against pressure graph (Ramesh *et al* 1977). Further the variation of thermopower in the high temperature region strongly suggests that Yb behaves like a degenerate semiconductor. This prompted us to undertake a detailed study of the resistivity behaviour of Yb at high pressures and temperatures and to correlate these results with our earlier thermopower work.

In this paper we report resistivity measurements at pressures up to 30 kbar and temperatures up to 600°C. The semimetal to semiconductor transition is observed as a distinct change in the slope of the resistance against pressure graph. In the semiconducting phase of ytterbium the temperature coefficient of resistivity is strongly positive for temperatures greater than 150°C. These results are consistent with the thermoelectric behaviour.

2. Experimental

The ytterbium samples used in the present investigation were cut from an ingot supplied by Research Chemicals, USA. High pressures were generated in a conventional piston and cylinder apparatus. Experimental data at temperatures less than 150°C were collected using the teflon cell technique with silicon fluid as the pressure transmitting medium (Jayaraman *et al* 1967). In the higher temperature region up to 600°C talc was used as a pressure transmitter. The high-pressure and high-temperature cell arrangement and the automatic recording facility for plotting resistivity against temperature have been described elsewhere (Shubha and Ramesh 1977).

3. Results

Figure 1 gives the continuous record of relative resistance against pressure at 25°C. This data was collected under truly hydrostatic pressure conditions using the teflon cell technique. It can be clearly seen that a change in slope occurs near 12–13 kbar pressure. We attribute this to the semimetal–semiconductor transition. For $P < 13$ kbar $(\mathrm{d}R/\mathrm{d}P) \simeq 0{\cdot}11\,\mathrm{m}\Omega/\mathrm{kbar}$ and for $P > 13$ kbar $(\mathrm{d}R/\mathrm{d}P) \simeq 0{\cdot}23\,\mathrm{m}\Omega/\mathrm{kbar}$. Also shown in the diagram is the thermopower against pressure behaviour of ytterbium at 42°C. The change in slope near 13 kbar is more marked in the thermopower than in the resistivity curve.

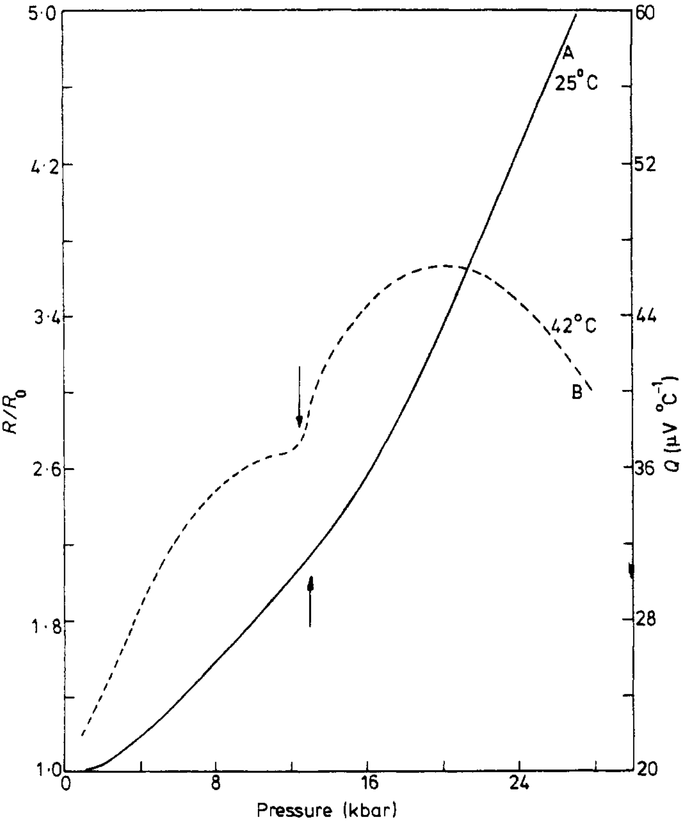

Figure 1. Relative resistance (curve A) and thermopower (curve B) against pressure. R_0 is the resistance at 25°C and atmospheric pressure. Position of arrows indicate the metal to semiconductor transition.

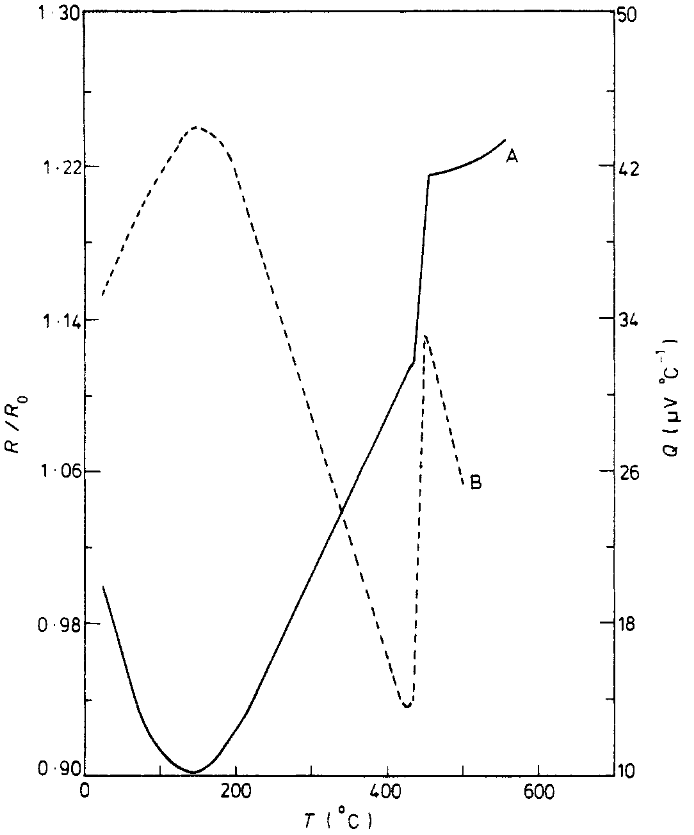

Figure 2. Relative resistance (curve A) and thermopower (curve B) as a function of temperature at 22 kbar pressure.

Figure 2 gives the relative resistance against temperature at 22 kbar pressure. Also shown in the diagram is the thermopower variation under identical pressure and temperature conditions. The main feature of the resistivity curve is the increase in resistivity with temperature in the semiconducting phase above 150°C. It may be noted that in this region the thermopower decreases linearly with temperature. For temperatures less than 150°C the resistivity decreases exponentially with temperature in conformity with earlier studies. The discontinuous increase in resistivity near 435°C is due to the first-order phase transition from the FCC to BCC phase. Thermopower also exhibits a discontinuous change near this transition.

Figure 3 gives the isobaric curves of resistivity against temperature in the semiconducting phase of ytterbium. The rate of increase of resistivity with temperature decreases with increase of pressure. We remark that the temperature coefficient of resistance is of the same order of magnitude as that of a metal. The minimum in the R/R_0 against T plot shifts towards higher temperatures with increasing pressures.

4. Discussion

The metal–semiconductor transition in ytterbium is due to the continuous removal of the overlap between the 6s and 5d bands with the application of pressure. The

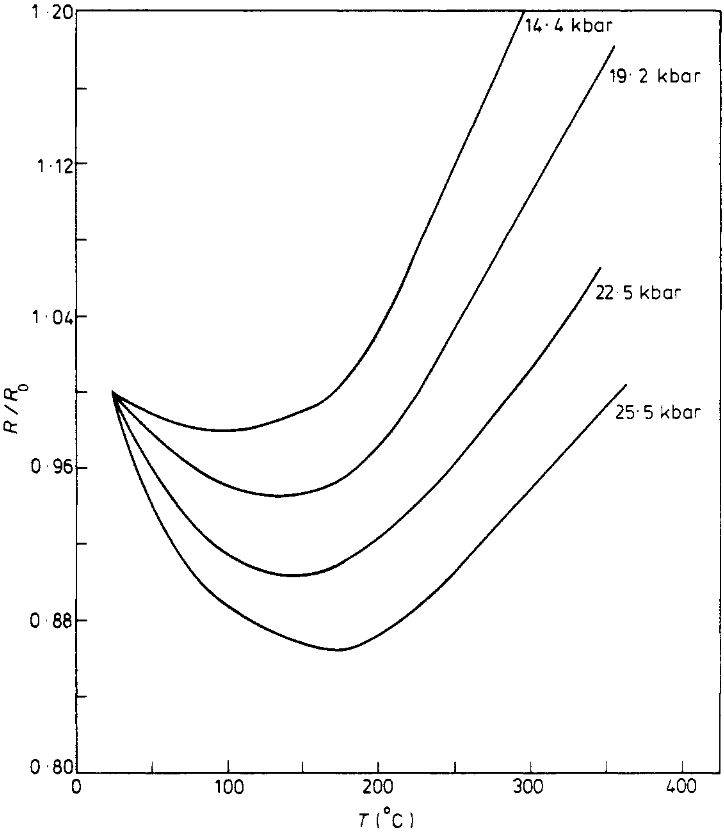

Figure 3. Isobars of the relative resistance against temperature in the semiconducting phase of ytterbium. R_0 for each isobar is the value of resistance at 25°C and corresponding pressure.

two-band model appropriate to divalent metals like Ca, Sr and Yb (Mott and Jones 1936, Vasvari *et al* 1967, Johansen and Mackintosh 1970) provides a general framework for understanding electronic properties like resistivity (Souers and Jura 1963, Jerome and Rieux 1969, McWhan *et al* 1969), Hall effect (Holzapfel and Severin 1971) and thermopower (Ramesh *et al* 1977) under pressure.

It is clear from figure 1 that the rate of increase in the resistivity with pressure is much greater in the semiconducting phase ($P > 13$ kbar) than that in the semimetallic region ($P < 13$ kbar). Qualitatively, the resistivity increases with pressure, because the number density of carriers is reduced by the removal of the overlap. However in the semiconducting phase, due to the opening up of a positive energy gap, the effective number of carriers decreases more rapidly with pressure than in the semimetallic region. This is also reflected in the thermopower graph (curve B) where Q, the thermoelectric power, increases rapidly with pressure up to 20 kbar. The decrease in Q after 20 kbar has been qualitatively explained elsewhere (Ramesh *et al* 1977).

The high-temperature resistivity behaviour in the semiconducting phase is very striking (figures 2 and 3) and correlates well with the thermoelectric behaviour. The linear increase in the resistivity with temperature after 200°C and the linear decrease in thermopower (figure 2) suggests strongly that ytterbium behaves like a degenerate semiconductor. The onset of degeneracy is aided by the small energy gap and a smaller effective mass for the carrier concerned.

The Hall coefficient at 300 K becomes negative in the semiconducting phase and its magnitude increases with pressure after the semimetal to semiconductor transition (Holzapfel and Severin 1970). This suggests that the effective mass of the electrons is much smaller than that of the holes. Thus the smaller density of states near the bottom of the 5d conduction band leads to the electron gas becoming degenerate near 150°C. This has the important consequence that the carrier density varies only slightly with temperature and the contribution from the mobility term (relaxation time τ) becomes significant. This accounts for the increase in the resistivity with temperature.

The linear variation of thermopower in the same temperature region can be understood only on the basis that the electron gas is behaving like a degenerate system. The linear increase of resistivity with temperature provides supporting evidence to this hypothesis.

The shift of the minimum in the R/R_0 against T graph (figure 3) towards higher temperatures with increasing pressure is due to the increase in the energy gap. Thus at higher pressures the electron system becomes degenerate at higher temperatures. Another important feature illustrated in figure 3 is that the temperature coefficient of resistance α decreases considerably at higher pressures. Typically α at 14·4 kbar is $0{\cdot}0017^\circ C^{-1}$ and at 25·5 kbar is $0{\cdot}000\,85^\circ C^{-1}$. It appears plausible that τ is very sensitive to temperature in systems where the energy gaps are small.

In conclusion we have made a detailed investigation of the resistivity behaviour of ytterbium at high temperatures in the semiconducting phase. The linear increase in resistivity with temperature (above 200°C) together with the linear decrease in the thermopower in the same temperature region strongly suggest that ytterbium behaves like a degenerate semiconductor.

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