Thermoelectric power of barium up to 8 GPa

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The present measurements indicate that the thermoelectric power (TEP) of barium at room temperature and pressure is 15 $\mu V K^{-1}$, and decreases with increasing pressure, reaching about 4 $\mu V K^{-1}$ just before the bcc→hcp transition. The TEP shows a discontinuous increase at the bcc→hcp transition beyond which it continues to decrease with increasing pressure.

Barium at room temperature and pressure has a body-centered-cubic (bcc) structure and transforms to hexagonal close-packed (hcp) structure at 5.7 GPa.[1-3] In the bcc phase, the resistivity of barium increases with pressure. The bcc→hcp transition is accompanied by a nearly 25% increase in resistivity. In the hcp phase, the resistivity continues to rise with pressure. In this Brief Report the thermoelectric power (TEP) of barium up to 8 GPa has been reported.

The barium specimens (99% pure from BDH Chemicals, England) were pressurized using a tungsten carbide opposed anvil setup (the diameter of the flat faces 12.5 mm) with pyrophyllite gasket and talc or epoxy as the pressure-transmitting medium. The specimen pressure was calibrated in terms of the ram pressure using Bi I—II (2.55 GPa), Tl II—III (3.67 GPa), Bi III—V (7.6 GPa) transitions. The procedure for measuring the thermoelectric power is described in detail elsewhere.[4] Briefly, a flat specimen measuring $0.5\times0.5\times5$ mm^3 was placed between the anvils. A temperature gradient across the length of the specimen was set up by heating one end of the specimen. The temperature difference and the Seebeck emf were measured using Chromel-Alumel thermocouples and a nanovolt potentiometer (Leeds and Northrup, K-5 model). The precision with which the TEP could be measured was 5%.

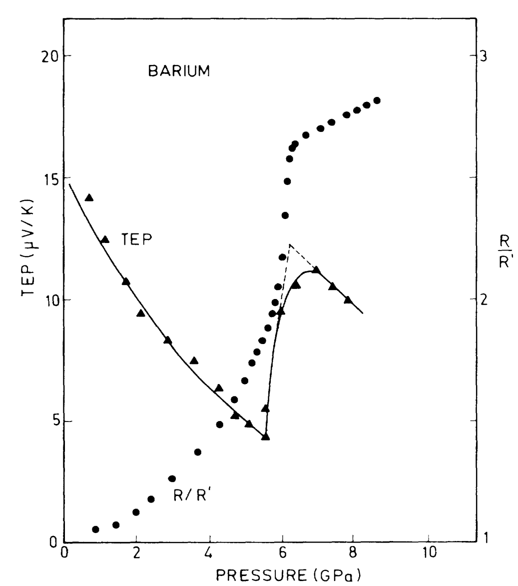

FIG. 1. Thermoelectric power and resistivity of barium as a function of pressure. R' denotes the resistivity at 0.5 GPa.

The TEP of barium as a function of pressure is shown in Fig. 1. The resistance-pressure data (also shown in Fig. 1) for these samples agree well with those obtained earlier.[3] The TEP of barium is large and positive (15 $\mu V K^{-1}$) at 1 atm and decreases with increasing pressure reaching 4 $\mu V K^{-1}$ just before the bcc→hcp transition. The bcc→hcp transition is accompanied by an increase in the TEP. In the hcp phase the TEP decreases with increasing pressure.

Theoretical estimates of the TEP of barium are extremely difficult because of the complexity of the band structure. Earlier attempts to explain the resistivity of barium under pressure[5,6] met with only partial success. These calculations, however, clearly indicated that the band structure, which is nearly free-electron-like, does not have the simple form of *sp* bands at the Fermi level, but that a strong admixture of *d* character is present. The free-atom ground state of barium which has a $6s^2$ configuration, acquires substantial $5d$ character in the solid state. The occupation numbers of the $6s$ and $5d$ bands have been calculated as a function of lattice constant by Herbst.[7] These calculations indicate that occupation numbers of the $6s$ and $5d$ bands are equal at 1 atm. As the pressure is increased the occupation number of the $6s$ band decreases and that of the $5d$ band increases. The pressure dependence of the TEP before the bcc→hcp transition appears to be related to the continuous change with pressure in the occupation number of the $6s$ and $5d$ bands.

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