J. Phys. C: Solid State Phys., Vol. 8, 1975. Printed in Great Britain. © 1975.

LETTER TO THE EDITOR

High pressure metallic phase in cuprous chloride single crystals

C W Chu†, S Early‡, T H Geballe‡§, A Rusakov‡‖ and R E Schwall‡¶

† Department of Physics, Cleveland State University ,Cleveland, Ohio 44115
‡ Department of Applied Physics, Stanford University, Stanford, California 94305

Received 1 April 1975

Abstract. An insulator–metal–insulator sequence of transitions has been observed as a function of pressure in a freshly prepared single crystal of CuCl. The metallic phase is evidenced by a sudden drop in resistance by a factor of $\sim 10^7$ between ~ 40 Kbar and ~ 55 Kbar.

1. Introduction

Cuprous halides form tetrahedrally coordinated zinc blende structures and thus in some sense are related to the isoelectronic sequence of group IV elements, and III–V and II–VI semiconductors. However in many ways the cuprous halides are anomalous when compared to other members of the isolectronic sequence. Martin (1970) has shown that the reduced bulk modulus of CuCl is only $\leqslant 20\%$ of that expected by extrapolation, and that the reduced shear moduli are also unexpectedly soft. Inelastic neutron scattering results (Carabatos *et al* 1971, Hennion *et al* 1972) show that the transverse acoustic branches are low and flat over most of the zone, and that there is an intermediate maximum in the longitudinal acoustic $|110|$ branch of CuCl. Extensive optical, ultraviolet and x ray photoemission data (Tono *et al* 1973, Goldman *et al* 1974) give evidence that the 3d levels in Cu are strongly hybridized into the valence band as might be anticipated solely from the structural dissimilarity of the cuprous halides and the alkali metal halides. In CuCl the upper branch of the valence band arises mainly from the 3d states (Tono *et al* 1973, Goldman *et al* 1974) of Γ_{15} symmetry and the spin–orbit splitting at the top of the valence band is inverted (Cardona 1963, Shindo *et al* 1965).

Increase of pressure causes covalent and moderately ionic 4-coordinated zinc blende structures to collapse to the (4 + 2)-coordinated white tin structure. Highly ionic zinc blende structures on the other hand collapse directly to the insulating 6-coordinated NaCl structure (Klement and Jayaraman 1966). Again the cuprous halides are anomalous in that many phases, (Edwards and Drickamer 1961, Van Valkenburg 1964, Rapoport and Pistorius 1968, Bradley *et al* 1969) as yet not well characterized, have been observed by a number of workers as a function of pressure below the melting curve. Van Valkenburg has

§ Also at Bell Laboratories, Murray Hill, New Jersey 07974.
‖ Permanent address: Department of Theoretical Physics, Moscow Institute of Steel and Alloys, Moscow 117049, USSR.
¶ Permanent address: Oak Ridge National Laboratory, Bldg. 9201–2, PO Box Y, Oak Ridge, Tennessee 37830.