

to obtain the pressure values based upon the lattice parameter. The diffraction lines, 110, 111, 200, 210, and 211 were used for the calculation of the lattice parameter of CsCl. The error in pressure calibration is ± 1 kbar.

The pressure-volume data for NiS_2 are shown in Fig. 1. The volume for NiS_2 was determined from the six diffraction lines, 111, 200, 210, 211, 220, and 311. The error in V/V_0 is $\pm 0.1\%$. It is seen from the figure that the low pressure phase (insulating) and the high pressure phase (metallic) have the different compression curves. The transition point with volume discontinuity appears to lie between 37 and 48 kbar and the volume change at the transition is $-0.4 \pm 0.1\%$. The volume change between the two phases at atmospheric pressure and room temperature is tentatively estimated to be $-1.6 \pm 0.3\%$ by a linear extension of the compression curve of the metallic phase. This value is in good agreement with one estimated by Wilson and Pitt.²⁾

Moreover, any new diffraction lines indicating a change in the structure of NiS_2 were not observed in the pressure range up to 100 kbar. The pyrite structure remains in this pressure range because any change in the intensities of the lines of pyrite structure was not found. It seems that the pressure-induced first order transition in NiS_2 is a Mott transition associated with delocalization of d-state of Ni^{2+} ,