

There has been considerable interest in the 3d transition metal disulfides having pyrite structure to study metal-insulator transition in connection with the Mott-Hubbard model.¹⁾ Recently, by high pressure electrical measurement Wilson and Pitt²⁾ have found that a metal-insulator transition in NiS_2 occurs in the vicinity of 32 kbar at room temperature. They also have pointed out that for the semiconducting NiS_2 there is a lattice parameter greater by 0.03\AA than would have occurred in a metallic phase.

In the present study, we carried out X-ray diffraction measurement on NiS_2 at room temperature up to 100 kbar in order to clarify if the transition is associated with a change in crystal structure and/or volume.

Single crystals having pyrite structure with a parameter $a=5.687\text{\AA}$ were prepared by chemical vapour transport with chlorine. A powdered sample of the single crystals was filled in a 0.3 mm hole in the center of a boron-epoxy disk, which was pressed between Bridgman anvils.³⁾

A pressure clamp vessel including the anvils was mounted on a goniometer of a Guinier focusing camera. Diffraction pattern by Mo-K α radiation was recorded on a curved film with a radius of 114.6 mm that allows a dispersion equal to maximum 2θ angle of 45° . The pressure on the sample was calibrated by intimately mixing NiS_2 with CsCl as an internal standard for pressure because almost every line of NaCl overlaps the lines of NiS_2 . The pressure-volume relation for CsCl calculated by Decker⁴⁾ was used