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X-Ray Study of Metal-Insulator Transition in  $\text{NiS}_2$

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Abstract

An X-ray diffraction study under pressure has shown that a metal-insulator transition in pyrite-type  $\text{NiS}_2$  is accompanied by a decrease in volume of about 0.4 % with no change in crystal structure.

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.<sup>1)</sup> Recently, by high pressure electrical measurement Wilson and Pitt<sup>2)</sup> have found that a metal-insulator transition in NiS<sub>2</sub> occurs in the vicinity of 32 kbar at room temperature. They also have pointed out that for the semiconducting NiS<sub>2</sub> there is a lattice parameter greater by 0.03Å than would have occurred in a metallic phase.

In the present study, we carried out X-ray diffraction measurement on NiS<sub>2</sub> 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.<sup>3)</sup>

A pressure clamp vessel including the anvils was mounted on a goniometer of a Guinier focusing camera. Diffraction pattern by Mo-K $\alpha$  radiation was recorded on a curved film with a radius of 114.6 mm that allows a dispersion equal to maximum  $2\theta$  angle of  $45^\circ$ . The pressure on the sample was calibrated by intimately mixing NiS<sub>2</sub> with CsCl as an internal standard for pressure because almost every line of NaCl overlaps the lines of NiS<sub>2</sub>. The pressure-volume relation for CsCl calculated by Decker<sup>4)</sup> was used

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  $\pm 1$  kbar.

The pressure-volume data for  $\text{NiS}_2$  are shown in Fig. 1. The volume for  $\text{NiS}_2$  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.<sup>2)</sup>

Moreover, any new diffraction lines indicating a change in the structure of  $\text{NiS}_2$  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  $\text{NiS}_2$  is a Mott transition associated with delocalization of d-state of  $\text{Ni}^{2+}$ ,

as discussed by Wilson and Pitt.<sup>2)</sup>

The compressibilities of  $\text{NiS}_2$  at room temperature were obtained from the results of the present study;  $(9.2 \pm 0.5) \times 10^{-4} \text{ kbar}^{-1}$  for insulating phase and  $(7.1 \pm 0.5) \times 10^{-4} \text{ kbar}^{-1}$  for metallic phase.

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#### References

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Figure Caption

Fig. 1 Pressure-volume relationship for NiS<sub>2</sub>.

