Vol. **113** (2008) *ACTA PHYSICA POLONICA A* No. 1

Proceedings of the CSMAG'07 Conference, Košice, July 9–12, 2007

Infrared Reflection of $MnTe_2$ under High Pressure

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The IR reflection measurements of $MnTe_2$ were performed at room temperature under various pressures. It is observed that the reflectivity increases at the pressure range of 8–25 GPa and becomes almost constant at the higher pressure. The carrier concentrations obtained from the reflectivity spectra at the highest pressure region are the order of 10^{22} cm^{-3}. Therefore it is concluded that pressure-induced semiconductor–metal transition occurs at the pressure range of 8–25 GPa.

PACS numbers: 71.30.+h, 78.30.–j

1. Introduction

$MnTe_2$ is a charge-transfer type ($\Delta = 1.5$ eV, $U = 5.5$ eV; Δ — charge transfer energy, U — intra-atomic Coulomb energy) semiconductor [1] with the pyrite structure and undergoes a second-order antiferromagnet-paramagnet phase transition at $T_{\mathrm{N}} = 86.5$ K [2]. The nature of its magnetic structure was shown to be non-collinear with the magnetic moments of the four manganese ions of the unit cell pointing along the body diagonals of the cube ($\mu_{\mathrm{Mn}} \parallel \langle 111 \rangle$) [3]. In recent high pressure study, a drastic decrease in electric resistance accompanied with a structural change was observed around 8 GPa [4, 5]. There is a possibility that a metallic phase transition occurs at the pressure and it is worth to study this material also by optical procedures. For clarifying that whether a phase transition is true metallic or semimetallic, it is the best and simplest way to show the high infrared (IR) reflectivity and its pressure insensitivity [6].

2. Experimental

We performed the IR reflection measurements under high pressure up to 38 GPa, which have been obtained by using a diamond anvil cell (DAC) at room temperature. The diameters of culet of diamond and sample room are 300 and 100 μm, respectively. The compression rate was less than 1 GPa/day. Applied pressure was estimated by conventional ruby fluorescence method. The reflection spectrum for the interface between the sample and diamond in mid-IR range was measured utilizing a Fourier transform infrared spectrometer FT/IR-610 (JASCO) combined with an infrared microscope installed with two mirror objectives and a HgCdTe detector. The incident condition in microscope system is not just normal. However deviation angle of the incident light on sample from the normal is smaller than 8 degree because of high reflective index of anvil diamond. Therefore we regarded as the condition is nearly normal. In order to obtain the reflectivity accurately, the powdered sample was compressed directly by diamond anvil without using any pressure mediums.

3. Results and discussion

The reflection spectra obtained under various pressure conditions are shown in Fig. 1. Many dips at the wave number region lower than 4000 cm^{-1} are mainly due to the absorptions by the diamond anvil and air.

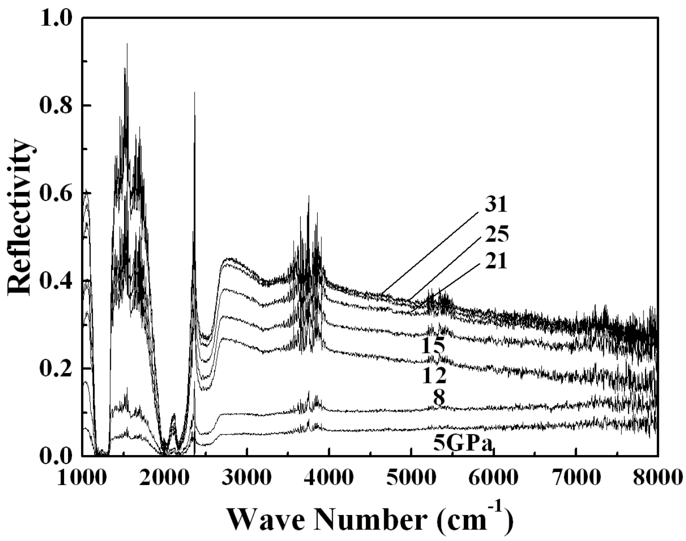

Fig. 1. Reflection spectra of $MnTe_2$ obtained under various pressures.

The pressure dependence of reflectivity monitored at 4000 cm^{-1} is illustrated in Fig. 2. The reflectivity starts to increase from 8 GPa. Let us note that this critical pressure coincides with that of the decreasing in resistance [5]. However, the increasing nature is not abrupt but relatively gradual. Since the compression was performed very slowly (less than 1 GPa/day), the pressure equilibrium condition was almost satisfied. Moreover since the reflection occurs at

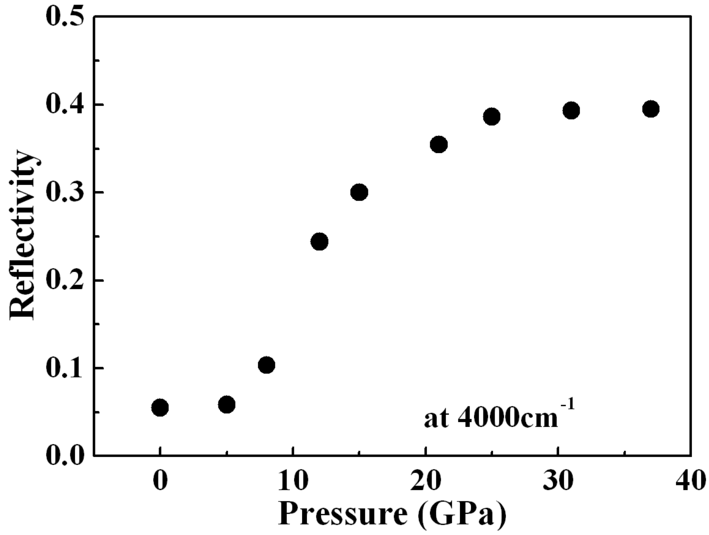

Fig. 2. Pressure dependence of the reflectivity at the point of 4000 cm^{-1}. The reflectivity increases from 8 GPa and saturates around 25 GPa.

the sample–diamond interface, in-plane uniformity of pressure was checked by the Raman spectra of anvil diamond [7] and the obtained inhomogeneity was less than 3 per cent. Therefore it is unlikely that the origin of the graduality is due to the pressure inhomogeneity of the sample room. Perhaps this result suggests that the transition does not occur at once but advances gradually through the step by step growing of high reflection domain with pressure. It becomes insensitive to pressure around 25 GPa. If the reflectivity increasing with pressure comes from the semimetallic band overlapping, the reflectivity should increase without saturation in contrast with present experimental results. The insensitivity to pressure from 25 GPa indicates that the band reconstruction to a metallic phase occurs at 8–25 GPa instead of the increased band overlap. Furthermore the parameter fitting of the spectrum obtauned at 38 GPa was performed using Drude model and obtained carrier concentration is the order of 10^{22} cm^{-3} which is 10–100 times higher than that of typical semimetal. Therefore it is concluded that the phase transition at 8 GPa reported in previous works is metallic one.

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