

## Second Order Phase Transition of FeS under High Pressure and Temperature

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There have been many investigations about high pressure behavior of stoichiometric FeS (troilite). The aim of the present study is to observe details of temperature behavior of FeS under high pressure condition near by the minimum thermal expansion, which was reported in our previous study.

The same material (Fe<sub>0.998</sub>S) used in previous studies was used for the present work. High pressure and temperature experiments were carried out using a 180ton press apparatus with a DIA-6 type vessel installed at BL14B1 in Spring-8. The *in-situ* X-ray observation was carried out by an energy dispersive type X-ray powder diffraction method

Figure 1 shows energy dispersive type X-ray powder diffraction patterns of FeS. The X-ray diffraction pattern at 4.84GPa and 500°C could be explained by the simple NiAs type phase, of which unitcell parameters were  $a_f=3.417(1)\text{\AA}$  and  $c_f=5.638(2)\text{\AA}$ . All diffraction lines of the pattern at 4.48GPa and 27°C could be indexed by the super-structured hexagonal phase with  $a=2a_f=6.699(5)\text{\AA}$  and  $c=c_f=5.692(5)\text{\AA}$ .

Unitcell parameters of the fundamental hexagonal cell ( $a_f$  and  $c_f$ ) normalized by those values at 27°C versus temperature are plotted in Fig. 2. Continuous changes in  $a_f$ ,  $c_f$  versus temperature between 500°C and 27°C suggest that the NiAs type - the super-structured phase transition is a second order transition. Figure 2 also shows an anisotropic thermal expansion of the hexagonal phase; the  $c$  axis contracted with elevating temperature up to 400°C, just the phase transition point to the

NiAs type phase, although the  $a$  axis showed a normal thermal expansion.

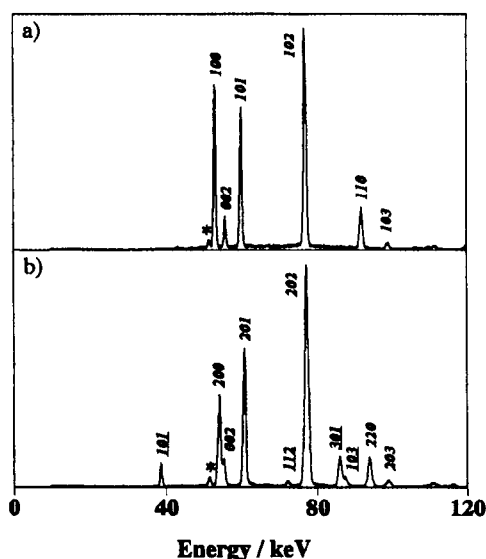


Fig. 1 X-ray diffraction patterns of FeS.  
a) at 4.84GPa and 500°C.  
b) at 4.48GPa and 27°C.

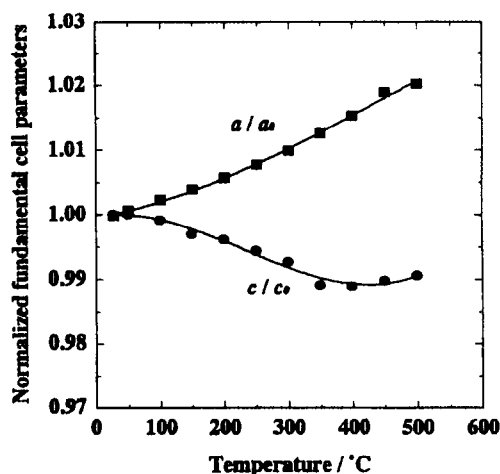


Fig. 2 Temperature dependence of unitcell parameters of FeS.