

## S K-edge EXAFS study of the hydrogen trapping by amorphous cobalt oxosulfide

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### Introduction

Release of radiolytic hydrogen is a source of serious safety problems in the management of nuclear waste. To diminish its negative impact, hydrogen traps can be used, to decrease explosion or swelling risks. Among the hydrogen traps that are efficient at ambient conditions, some inorganic sulfide compounds such as basic cobalt and nickel sulfides (CoS(OH), NiS(OH)) have been reported. However, if the efficiency of these sulfides has been evidenced, no clear depiction of the mechanism of their action exists in the literature. Recently, we demonstrated that the absorption of hydrogen by such systems does not depend on the radiolytic events, but is limited to a solid-gas interaction [1]. In the present work, we give insight on the mechanism of hydrogen trapping by amorphous cobalt oxysulfide. To reach this goal, evolution of S K edge was studied upon interaction of amorphous sulfide with hydrogen.

### Experimental details and results

The measurements were carried out on the BL-9A. In situ cell was specially constructed for these measurements, which included sample holder, heater and gas flow assembly. The in situ cell was installed in the measurement box flushed by helium in order to decrease soft X-rays absorption (Fig. 1). Spectra were collected in the fluorescence mode.

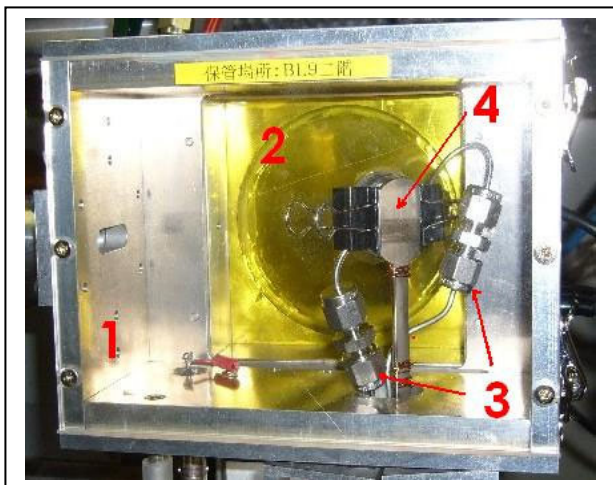


Fig.1. Experimental setup: helium flushed box (1); detector window (2); gas flow inlet and outlet (3); sample holder (4).

The measurements were carried out for the CoS(OH) solid before and after hydrogen as well as reference compounds including relevant sulfides of Cobalt, other transition metals sulfides and sulfur. Both XANES and EXAFS part of the spectra were examined.

In situ measurements demonstrated that S K spectra of CoS(OH) were modified after interaction with hydrogen during several hours. As shown in fig.2, at the end of experiment we observed the shape change of XANES part which is consistent with the formation of small crystallites of CoS. Comparison with the spectra of other cobalt sulfides allows ruling out their presence. However for the EXAFS part of spectra no significant modification of the spectra which means that the coordination state of sulfur was modified only marginally (hydrogen neighbor cannot be detected because of its small mass).

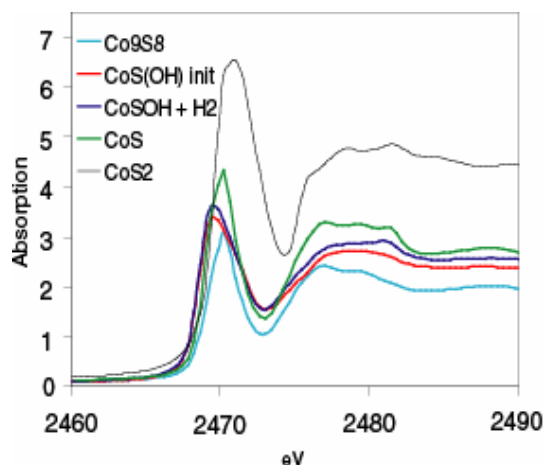


Fig. 2 XANES spectra of the initial CoSOH, its product of interaction with H<sub>2</sub> and several reference sulfides.

The results of this study help us to advance in better understanding of the hydrogen trapping mechanism by amorphous sulfides under ambient conditions which is new intriguing phenomenon.

### References

[1] C. Lussot, et al, Chem. Mater. 18, 5659 (2006).

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