Electrochemical properties for $Cu_{5-x}Li_xFeS_4$

Atsuhsi Hirano
Department of Chemical for Materials, Faculty of Engineering, Mie University
1577 Kurimamachiya-cho,Tsu, Mie 5148507, JAPAN
hirano@chem.mie-u.ac.jp
http://material.chem.mie-u.ac.jp/~hirano/

Introduction

Iron sulfides and lithium iron sulfide have been investigated as an electrode material in a solid state lithium battery [1, 2]. When Li_2FeS_2 or FeS_2 are reduced, the final products were reported to Li_4FeS_2 [1] or Fe metal [2]. The reduction mechanism of Fe-S series materials are not yet clear. Another Fe-S series materials may available as an electrode material in lithium batteries.

Copper iron sulfides, $CuFeS_2$ (chalcopyrite) and Cu_5FeS_4 (bornite) have been reported as a Cu ion and electron mixed conductor [3]. $Cu_{5-x}Li_xFeS_4$ have been synthesized and electorchemcal properties have been studied.

Experimental

Cu_5FeS_4 and $Cu_{5-x}Li_xFeS_4$ were synthesized from Cu_2S, FeS, Li_2S and S. For Cu_5FeS_4, the mixture with variable mixing ratio, Cu_2S/FeS=1.5~2.5, were heated at 750 C for 24h under nitrogen gas flow. For $Cu_{5-x}Li_xFeS_4$, several mixing ratio of Cu_2S, FeS and Li_2S were heated. The powder x-ray diffraction patterns and electrochemical properties using conventional coin-type cell were measured.

Results and Discussion

Figure 1 shows the x-ray diffraction patterns for Cu_5FeS_4 with various mixing ratio of Cu_2S / FeS = 1.5 ~ 2.5. All samples show the Cu_5FeS_4 pattern. However, the samples with the mixing ratio of 2.0 and 2.5 showed the impurity phase which determined as Cu_2S. The single phase was obtained at the samples with the mixing ratio of 1.75. The oxidation state in this sample, $Cu_{3.5}FeS_4$, is not yet determined. Further study on the structure and oxidation state is necessary.

Figure 2 shows the charge-discharge corves for Cu_5FeS_4 with mixing ratio of Cu_2S / FeS = 1.75. At first discharge curve differ to second discharge curve. This results suggests the structural change among the first discharge state. In the charge state, three plateau observed at 1.7V, 2.3V and 2.6V. The capacity of first and second plateau decreased with the cycle. The intercalation mechanism and the structural change on first deintercalation will be discussed.

The x-ray diffraction pattern of the sample with high Li_2S ratio is similar to Li_2FeS_2 pattern. The

electrochemical properties of $Cu_{5-x}Li_xFeS_4$ will be discussed.

References

[1] Kazunori Takada, Kazuya Iwamoto, and Shigeo Kondo, *Solid State Ionics*, **117**, 273-276 (1999).

[2] R. A. Guidotti, F. W. Reinhardt, in: Proceedings of the 9th International Symposium on Molten Salts, 1994, 820 (1994).

[3] R. Berger and R. V. Bucur, Diffusion in copper sulfides; An experimental study of chalcocite, chalcopyrite and bornite, Report to Swedish Nuclear Power Inspectorate (Dec. 1995).

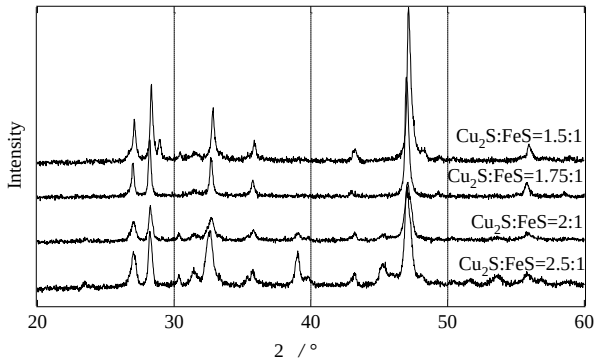

Fig. 1 X-ray diffraction patterns for Cu_5FeS_4 with various mixing ratio of Cu_2S / FeS = 1.5 ~ 2.5.

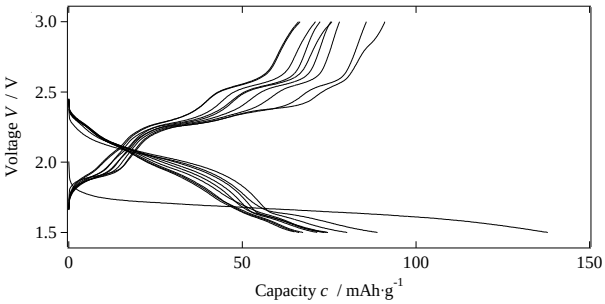

Fig.2 Charge-discharge curves for Cu_5FeS_4 with mixing ratio of Cu_2S / FeS = 1.75.

About Myself

Name: Atsushi Hirano
Nationality: Japanese
Hometown ikeda, Osaka, Japan
Degree Ph. D (Kobe Univ., Japan)
Study Solid state chemistry
Hobby Internet, Movie, Mah-jongg