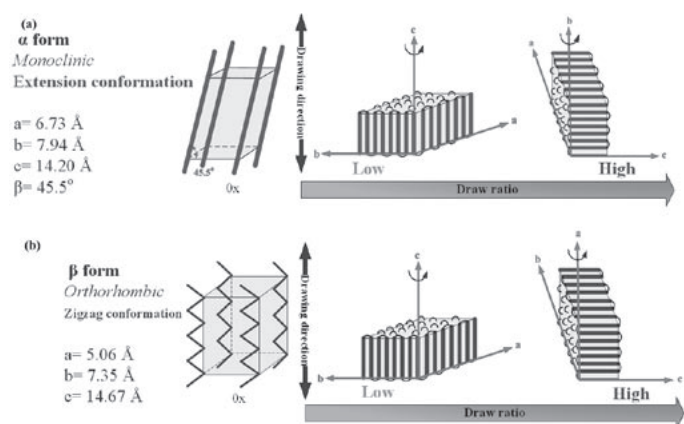


P11.08.74

Acta Cryst. (2008). A64, C530

Crystals orientation of polybutylene adipate/polyvinyl chloride blend under uniaxial drawingWei-Tsung Chuang¹, Yu-Rei Li², How-Shuenn Sheu¹, U-Ser Jeng¹, Po-Da Hong²¹National Synchrotron Radiation Research Center, 101 Hsin-Ann Road, Hsinchu Science Park, Hsinchu, Hsinchu, 30076, Taiwan, ²Department of Polymer Engineering, National Taiwan University of Science and Technology, Taipei, Taiwan, E-mail: weitsung@nsrrc.org.tw

The thin films of miscible Polybutylene adipate)/Polyvinyl chloride (PBA/PVC) 6/4 blend under uniaxial drawing behavior was studied by wide angle X-ray diffraction (WAXD), small angle X-ray scattering (SAXS) and grazing incidence wide angle X-ray scattering (GIWAXS). We study crystals orientation of polymorphic PBA crystals through different draw ratios. The polymorphic phase transition of PBA only depends on temperature and it does not change under strain. The c-axis parallels to the stretching direction at low drawing ratios on both PBA crystals of alpha- and beta- crystals. In contrast, the b-axis of the PBA alpha-crystal was oriented parallel to the stretching direction and the a-axis of the PBA beta-crystal was oriented parallel to the stretching direction at high drawing ratios. Figure 1 Models of PBA/PVC blend under drawing crystallization: (a) PBA alpha-crystal and (b) PBA beta-crystal .



Keywords: thin film of polymer, crystals orientation, crystallization under tension

P11.02.75

Acta Cryst. (2008). A64, C530

Crystallographic structure of LiCoO₂ based ruthenium catalyst for sodium borohydride hydrolysis

Eren Halit Figen, Aysel Kanturk, Nafi O. Guldal, Sema Z. Baykara, Sabriye Piskin

Yildiz Technical university, Chemical Engineering, Davutpasa Campus, Chemical Engineering Department, Esenler, Istanbul, 34210, Turkey, E-mail: hfigen@yildiz.edu.tr

As an energy carrier, hydrogen is a very clean fuel without greenhouse gases, ozone layer depleting chemicals, acid rain ingredients and pollution. Sodium borohydride (NaBH₄) can be used as a hydrogen storage medium due to high hydrogen storage capacity (10.8%wt). NaBH₄ in aqueous alkaline solution generates hydrogen and sodium borate (NaBO₂) as by product contact with catalyst according to the hydrolysis reaction which is known to run via zero

order kinetics. In the present study, Ru- LiCoO₂ catalyst has been manufactured to generate clean hydrogen from NaBH₄. Nano-sized ruthenium (Ru) dispersed on the LiCoO₂ surface by wash coating process to prepare the catalysis for NaBH₄ hydrolysis. The catalyst is characterized by scanning electron microscopy including EDX analysis (SEM-EDX), X-ray diffractometry (XRD). EDX analysis show the ~15wt. % Ru containing by the LiCoO₂, XRD patterns shows the Ru- LiCoO₂ catalyst display the characteristic peak of the LiCoO₂ structure. The analysis show Ruthenium particles coated the LiCoO₂ ceramics. A new study about the coating thickness has also been studied and the thickness of the Ruthenium coated on the surface of LiCoO₂ is measured.

Keywords: catalyst, ruthenium, lithium cobalt oxide

P11.02.76

Acta Cryst. (2008). A64, C530

Structural disorder in the Ce_{0.5}Zr_{0.5}O₂ catalyst: A possible factor of the high catalytic activityTakahiro Wakita^{1,2}, Masatomo Yashima²¹Daiichi Kigenso Kagaku Kogyo Co. LTD, Hirabayashiminami 1-6-38, Suminoe-ku, Osaka, Osaka, 559-0025, Japan, ²Tokyo Institute of Technology, Nagatsuta-cho 4259-J2-61, Midori, Yokohama, Kanagawa, 226-8502, Japan, E-mail: taka_wakita@yahoo.co.jp

Ceria-zirconia Ce_{0.5}Zr_{0.5}O₂ catalysts are widely used in the cleaning of exhaust gases from automobiles. The oxygen storage/release capacity is one of the most important factors to affect catalytic activity of Ce_{0.5}Zr_{0.5}O₂. Bulk oxygen diffusion is one of the steps of the oxygen storage/release process in Ce_{0.5}Zr_{0.5}O₂. The development of improved catalysts requires a better understanding of crystal structure and bulk oxygen ionic diffusion in ceria-zirconia materials. The Ce_{0.5}Zr_{0.5}O₂ solid solutions have been investigated by some researchers [1]. However, structural disorder and diffusion path of oxygen ions in Ce_{0.5}Zr_{0.5}O₂ remain poorly understood. Here we report the structural disorder and diffusion path of oxygen ions in Ce_{0.5}Zr_{0.5}O₂ [2, 3]. Nuclear-density distribution of cubic Ce_{0.5}Zr_{0.5}O₂ compound has been studied at 1831 K by the maximum-entropy method (MEM) and MEM-based pattern fitting combined with the Rietveld method using in situ neutron powder diffraction data. The oxygen ions show a large positional disorder and shift to the <111> directions. Possible bulk diffusion paths of the oxygen ions can be seen along the <100> and <110> directions. The spatial distribution of oxygen ions in Ce_{0.5}Zr_{0.5}O₂ is greater than that of CeO₂, which is consistent with the higher bulk diffusivity of oxygen ions in Ce_{0.5}Zr_{0.5}O₂. It is suggested that the greater disorder of Ce_{0.5}Zr_{0.5}O₂ is a factor of its higher catalytic activity.

References

- [1]. M. Yashima, K. Morimoto, N. Ishizawa, and M. Yoshimura, J. Am. Ceram. Soc., 76 (1993) 2865.
- [2]. T. Wakita and M. Yashima, Acta Crystallogr., Sect. B: Struct. Sci., 63 (2007) 384.
- [3]. T. Wakita and M. Yashima, Appl. Phys. Lett. 92 (2008) 101921.

Keywords: neutron powder diffractometry, *in-situ* powder diffraction, automotive catalyst