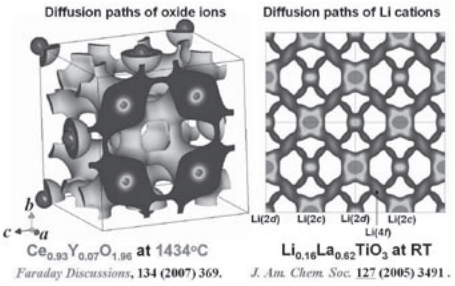
$(La_{0.8}Sr_{0.2})(Ga_{0.8}Mg_{0.15}Co_{0.05})O_{2.8}$ [CPL380(2003)391], CeO_2 [APL84(2004)526], $Bi_{1.4}Yb_{0.6}O_3$ [APL87(2005)221909], $Ce_{0.93}Y_{0.07}O_{1.96}$ [Farad.Discuss.134(2007)369], and $La_{0.64}(Ti_{0.92}Nb_{0.08})O_3$ [Chem.Mater.19(2007)32604], $Y_{0.79}Ta_{0.21}O_{1.72}$ [ChemMater19(2007)3539], $La_{0.6}Sr_{0.4}CoO_3$ [JApplCryst40 (2007)1166], $(La_{0.6}Sr_{0.4})(Co_{0.8}Fe_{0.2})O_{3-x}$ [SolStIon179(2008)1939], $(Pr_{0.9}La_{0.1})_2(Ni_{0.74}Cu_{0.21}Ga_{0.05})O_{4+x}$ [JACS139(2008)2662], $La_{0.62}Li_{0.16}TiO_3$ [JACS127 (2005)3491] and CuI [JMaterChem16 (2006)4393] (Figure). It was found that the disorder and path depend on the crystal structure.



Keywords: neutron and X-ray diffractometry, *in-situ* powder diffraction, ionic conductors

P11.13.81

Acta Cryst. (2008). A**64**, C532

Short-range to long-range order structure change of Mg-Fe alloys

Yasuhiro Yoneda[1], Hiroshi Abe[2], Takeshi Ohshima[2], Ryo Morimoto[3], Hirohisa Uchida[3]

[1]Japan Atomic Energy Agency, Synchrotron Radiation Research Unit, 1-1-1, Kouto, Sayo-cho, Sayo-gun, Hyogo, 679-5148, Japan, [2]Japan Atomic Energy Agency, 1233 Watanumi, Takasaki, Gunma, 370-1292, Japan, [3]Dept. of Applied Physics, Graduate and Undergraduate School of Engineering, Tokai University, 1117 Kitakaname, Hiratsuka, Kanagawa, 259-1292, Japan, E-mail：yoneda@spring8.or.jp

We performed structure analysis of Mg-Fe alloy system prepared by mechanical alloying. For Mg concentrations up to about 15 mol%, mechanical alloying can produce single-phase bcc alloys. By using the conventional average structure analysis and X-ray pair-distribution function method, we can bridge the long-range and short-range order structure of Mg-Fe alloys. The substituted Mg atoms arranged randomly in the low-Mg composition, but Mg atoms came to have the order structure as the Mg composition increases. It can explain this new finding as a kind of short-range order to long-range order phase transition.

Keywords: Mg-Fe, mechanical alloying, pair-distribution function

P11.13.82

Acta Cryst. (2008). A**64**, C532

Development of a new type of Li-battery materials based on the milarite-family

SoHyun Park

Ludwig-Maximilians-Universitaet-Muenchen, Earth and Environmental Sciences, Section Crystallography, Theresienstr. 41, Munich, Bavaria, 80333, Germany, E-mail：sohyun.park@lmu.de

Over the last three decades, enormous efforts have been devoted to advance Li-ion based batteries by exploiting a variety of electrode and electrolyte materials [1]. However, demands for lighter and smaller batteries exceed the dimension offered by the modern technology. In this respect, it is try-worthy continuing to develop new battery materials. The milarite-family $(A_2B_2C[T(II)_3T(I)_{12}O_{30}]$: A = Sn^{4+}, Ti^{4+}, Zr, Al, Fe^{3+},⋯; B = Na, H_2O; C = Na, K; T(I) = Si, Al; T(II) = Li, Be, Mg,.. [2, 3] is a highly interesting candidate due to: 1) the presence of short pathways available for conducting Li; 2) the presence of a crystal-chemical basis for the formation of solid-solutions and defect-engineering; 3) a high thermal stability up to 1200 K. In fact, our recent studies showed ionic conductivity in Li-bearing milarite-type minerals, sogdianite and sugilite, for the first time [4, 5]. The ionic conductivity in sogdianite could be assigned to site exchange processes of Li between T(II) and A sites parallel to the (001)-plane at elevated temperatures. Interestingly, the ionic conductivity in this topology is proportional to the amount of Na cations at B sites [5]. These Na cations may play a relevant multiple role, as carrying and transferring charges for the negative-charged framework $[Li_3Si_{12}O_{30}]^{9-}$. Here, the state of the art development of Li-Na-bearing milarite-type Li-battery materials will be presented.

1. J.-M. Tarascon, M. Armand (2001), Nature, 414, 359-367.
2. F.C. Hawthorne, et al. (1991), Am. Mineral., 76, 1836-1856.
3. F.C. Hawthorne (2002), Can. Mineral., 40, 699-710.
4. S.-H. Park, et al. (2007), J. Solid St. Chem., 180, 1306-1317.
5. S.-H. Park, Abstract, 16. Jahrestagung der DGK, 03-06.03.2008, Erlangen.

Keywords: ionic conductors, milarite, sogdianite

P11.13.83

Acta Cryst. (2008). A**64**, C532−533

Optimization of energy parameters indemnification of impurity levels in lead and bismuth

Mehmet Burcin Piskin[1], Emek Moroydor Derun[2], Nurcan Tugrul[3]

[1]Yildiz Technical University, Bioengineering, YTU Chemical and Metallurgical Faculty Department of Bioengineering Davutpasa Campus Davutpasa Esenler, Istanbul, Istanbul, 34590, Turkey, [2]Yildiz Technical University, YTU Chemical and Metallurgical Faculty Department of Chemical Engineering Davutpasa Campus Davutpasa Esenler, Istanbul, Istanbul, 34590, Turkey, [3]Yildiz Technical University, YTU Chemical and Metallurgical Faculty Department of Chemical Engineering Davutpasa Campus Davutpasa Esenler, Istanbul, Istanbul, 34590, Turkey, E-mail：meburp@hotmail.com

In impurity semiconductors except for the impurity giving the basic carriers of a charge, there are compensating impurities. Usually for their characteristic the measure of indemnification is entered and properties of semiconductors in a wide interval of a degree of indemnification are investigated. Influence of indemnification on properties of alloys is expressed that in the forbidden zone there are additional resolved power levels. Indemnification influences dispersion of carriers of a charge. These two factors strongly change such characteristics, as concentration and mobility of carriers of a charge (including electro-conductivity and thermoelectromotive of semiconductors). Influence of indemnification on properties of chalcogenides of bismuth and lead is investigated. Crystals PbTe-$PbCl_2$-B and Bi_2Te_3 <CdCl -B with low concentration of the hole carriers of current. The measured and calculated parameters (electro-conductivity, thermoelectromotive, concentration of carriers of current testify the strong compensating influence of boron. Adjusting with complex impurity ($PbCl_2$ -B) and ($CdCl_2$ -B) it was possible to receive a set of samples with concentration of the hole carriers down to P=6,2-1017 cm^{-2}, . The reason of strong indemnification is, on seen, linkage of vacancies of lead in complexes with ions of chlorine (in case PbS and PbTe). In Bi_2Te_3, strong p-type influence of boron results in indemnification of donor levels of chlorine.