mode analysis of any ferroic structure. As input only the ferroic distorted structure and the (real or virtual) non-distorted one of higher symmetry is required. With this information the program AMPLIMODES identifies the displacive distortion present in the structure and decomposes it in terms of modes of different symmetries associated with irreducible representations of the high-symmetry space group. The decomposition of the structure in collective symmetry-adapted distortion modes is given in terms of global amplitudes and normalized polarization vectors for each of the modes present. The importance and character of each of the allowed symmetry modes can be extracted from a comparison of their amplitudes and the internal structure of their polarization vectors. The polarization vector of each frozen mode is presented in a crystallographic way, as a list of relative atomic displacements within an asymmetric unit. This allows a straightforward construction of virtual structures corresponding to the sole presence with arbitrary amplitudes of any of the relevant modes. This type of analysis allows to distinguish and isolate the correlated atomic displacements that correspond to the structural instabilities at the origin of the ferroic distortion, i.e. the so-called primary modes. In this way, secondary weaker induced distortions of marginal relevance are separated. The Bilbao Crystallographic Server, where this tool can be used on-line, is a free web site with many other crystallographic databases and programs [1,2].

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Keywords: ferroic materials, structural phase transitions, symmetry modes

P11.01.67

New organic conductors based on cobaltacarborane anion and its derivatives

Oleg Dyachenko[1,2], Olga Kazheva[2]
[1]Russian Foundation for Basic Research, Leninskii prosp., 32a, Moscow, Moscow, 119991, Russia, [2]Institute of Problems of Chemical Physics of RAS, Semenov av., 1, Chernogolovka, 142432, Russia, E-mail：doa@icp.ac.ru

Just a few conducting radical cation salts containing metallacarborane anions have been described so far [1,2]. No radical cation salt derived from the cobalt bis(dicarbollide) anion $[3,3'-Co(1,2-C_2B_9H_{11})_2]^-$ or its halogen derivatives was reported. First molecular conductors with cobalt bis(dicarbollide) anion and its iodine and bromine derivatives were electrochemically synthesized and investigated by X-ray study [3-5]: $(TMTSF)_2[3,3'-Co(1,2-C_2B_9H_{11})_2]$ (1), $(TTF)[3,3'-Co(1,2-C_2B_9H_{11})_2]$ (2), $(ET)[3,3'-Co(1,2-C_2B_9H_{11})_2]$ (3), $(ET)_2[3,3'-Co(1,2-C_2B_9H_{11})_2]$ (4), $(ET)_2[8-I-3,3'-Co(1,2-C_2B_9H_{10})(1',2'-C_2B_9H_{11})]$ (5), $(BMDT)[3,3'-Co(1,2-C_2B_9H_{11})_2]$ (6), $(ET)_2[3,3'-Co(8-Br-1,2-C_2B_9H_{10})_2]$ (7), $(BMDT)_4[3,3'-Co(8-Br-1,2-C_2B_9H_{10})_2]$ (8), and $ET[3,3'-Co(8-BrC_2B_9H_{10})_2]$ (9). Salt (1) is a semiconductor with activation energy Ea=0.03 eV, conductivity S(293) = 15 $Ohm^{-1}cm^{-1}$, that is the maximum value of conductivity for all metallacarborane radical cation salts studied before [1,2].

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Keywords: organic conductors , carboranes, X-ray crystal structure analysis

P11.06.68

Phase and glass forming diagrams in the gallium borate and ternary barium gallium borate systems

Rafael M Hovhannisyan[1], Bella V Grigoryan[1], Hovakim A Alexanyan[1], Berta V Petrosyan[1], Vahan P Toroyan[2]
[1]Scientific-Production Enterprise of Material Science, Research & Development, 17 Charents Str., Yerevan, Yerevan, 25, Armenia, [2]Institute of General and Inorganic Chemistry of NAS RA, Argutyan st., district 2, 10, Yerevan, 0051 , Armenia, E-mail：hovhannisyan@netsys.am

The revealing of new stoichiometric compositions still actual problem for new acentric or non-centrosymmetric solids (single crystals, ceramics) development. The glass ceramic (GC) technology combines flexibility, simplicity and cheapness of glass technology with possibility to form crystal structures of the reference sizes and compositions through controlled and oriented crystallization. Alkaline earth binary borates and alkaline-earth ternary borates are the good candidate for this purpose, because they combine nonlinear characteristics with good glass forming ability. This was a motivation for study and construction both phase and glass forming diagrams in the binary gallium borate and ternary barium gallium borate systems. The glasses were melted from chemically pure" grade chemicals in platinum crucibles in air at 1300-1600 °C in electrical furnace.

Keywords: barium gallium borates, phase diagram , glass forming diagram

P11.05.69

SAXS investigation of SBA-15 vacuum calcination process

Francisco Mariano Neto[1], Marcia C. A. Fantini[1], Luis C. Cides Silva[2], Jivaldo R. Matos[2]
[1]Institute of Physics / University of Sao Paulo, Applied Physics Department, Trav. R da Rua do Matao, 187, Ed. Basilio Jafet, Sl. 124-B, Sao Paulo, Sao Paulo, 05508-900, Brazil, [2]Institute of Chemistry / University of Sao Paulo, E-mail：fmneto@if.usp.br

Ordered mesoporous silica (OMS) is a new alternative material for many technologies, ranging from microelectronics to medical applications. In this work, in situ analysis of the calcination process of SBA-15 was carried out in vacuum at the SAXS2 beamline of LNLS, Brazil. The as-synthesized powder was submitted to a heat treatment procedure at a pressure of about $1\cdot10^{-3}$ torr, from room temperature up to 540℃, at a constant temperature increase of around 2℃·min^{-1}. The sample was kept at this temperature for 6 hours. At around 300℃ the polymer starts to decompose and the lattice parameter decreases from a=12.8nm to a=12.4nm, until the temperature reaches 540℃, when the polymer decomposes. The lattice parameter reaches a final value of 12.3nm, remaining at this constant figure until the final cooling process. The peak areas do not change up to 300 ℃ . A strong and subtle increase of peak areas is observed at this temperature. During the isothermal calcination process, part of the ordered structure is destroyed, as indicated by the decrease of the diffracted intensities. A sample previously calcined in nitrogen and air showed a larger shrinkage effect, resulting in a=11.8nm. Also, the SAXS curve of this sample presented a larger background when compared to that registered in the measurements of the vacuum heat treated sample. This result is attributed to the presence of disordered pores, with maximum gyration radius of 7nm, to micropores and/or to inter-grain scattering. Ex-situ SAXS analysis of a similar sample submitted to vacuum heat treatments at 300℃, 400℃ and 540℃ was also carried