1. Modeling of electric conductivity processes during metal-nonmetal phase transition in melts of lead and gallium systems with alkali metals

By Kiselev, A. I.; Gorbunov, V. A.
From Materialovedenie (2011), (11), 2-7. Language: Russian, Database: CAPLUS

The results of calcn. of elec. resistivity in the melts of the systems of lead and gallium with alkali metals are presented. The theory of elec. cond. of metal melts of G. Simon describes the exptl. effects of the increase of elec. resistivity in the phase transition 'metal-nonmetal' in the systems of lead with alkali metals. The results of the above theory predict similar qual. effects of the change of elec. resistivity in the systems of melts of gallium with alkali metals.

~0 Citings

2. Collective dynamics in binary liquids: spectra dependence on mass ratio

By Bryk, Taras; Mryglod, Ihor
From Journal of Physics: Condensed Matter (2005), 17(3), 413-427. Language: English, Database: CAPLUS, DOI:10.1088/0953-8984/17/3/002

We discuss the spectrum of longitudinal propagating collective excitations in a liq. metallic alloy Li_4Pb and a Lennard-Jones binary mixt. obtained by an eight-variable approach of generalized collective modes. Reported wavenumber-dependent amplitudes of contributions from high- and low-frequency propagating excitations to dynamical structure factors in Li_4Pb permit a new viewpoint on the 'fast sound' phenomenon. A three-variable anal. model for slow and fast mass-concn. fluctuations is used for explanation of the high-frequency branch in the long-wavelength region. An addnl. anal. of longitudinal dynamics in liq. binary mixts. with different mass ratio of components permits us to establish a tendency in frequency and damping coeffs. of the high-frequency propagating excitations.

~21 Citings

3. Collective excitations and generalized transport coefficients in a molten metallic alloy Li4Pb

By Bryk, T.; Mryglod, I.
From Condensed Matter Physics (2004), 38, 285-300. Language: English, Database: CAPLUS

Collective dynamics of a molten metallic alloy Li_4Pb is studied using a combination of anal. multivariable approach of generalized collective modes and mol. dynamics simulations. Dispersion and damping of 2 branches of propagating collective excitations are analyzed in a wide range of wavenumbers. The features in collective dynamics connected with the large difference in species mass are discussed. Generalized k-dependent transport coeffs. for Li_4Pb are reported.

~0 Citings

4. Octet composition in alkali-Pb solid alloys

By Molina, L. M.; Alonso, J. A.; Stott, M. J.
From Physical Review B: Condensed Matter and Materials Physics (2002), 66(16), 165427/1-165427/8. Language: English, Database: CAPLUS, DOI:10.1103/PhysRevB.66.165427

D. functional calcns. have been performed to investigate some features of the phase diagrams of Pb-alkali metal alloys. Alkali metal-rich intermetallic compds. occur for Pb with Li and Na, but not with the heavier alkalis. But although for the Li-Pb and Na-Pb systems compds. form near the octet stoichiometry, there are no exact 4:1 stoichiometric compds. Calcns. for free clusters already provide some qual. insight into these questions. In addn. simulations of the assembling of solid compds. using free clusters as building blocks were done. There is substantial rearrangement during the assembling process as the clusters coalesce to form the solid, but the trends in the alloys varying down the alkali group seem to be closely related to such characteristic properties of the clusters as the HOMO and LUMO gap, and alkali at. size effects. The striking absence of octet stoichiometric compds. in the Li-Pb and Na-Pb systems is accounted for as a result of competition between compds. with slightly different compns. The enhanced stability of the nonstoichiometric compds. can be understood in terms of preferential filling of bonding orbitals leading to enhanced ionic binding.

~0 Citings

5. Conditions for cluster assembled solids

By Molina, L. M.; Alonso, J. A.; Lopez, M. J.; Rubio, A.; Stott, M. J.
From Recent Advances in Computational Chemistry (2002), 1(Recent Advances in Density Functional Methods, Part 3), 234-246. Language: English, Database: CAPLUS

D. Functional Theory is used to investigate the conditions required for the successful assembling of metallic clusters to yield stable or metastable clustered-solids. Some solid alloys of Pb and alkali metals contain clusters and to understand this feature we have studied in detail the chem. binding and electronic structure of those alloys. Assembling of Zintl (A_4Pb_4, with A = alkali atom) and octet (A_4Pb) clusters into solid alloys has been simulated. A high stability of the free clusters and a weak cluster-cluster interaction are the two main requirements for assembling cluster-solids. The second condition is achieved in the Zintl solids by the coating effect of the alkali cations, which prevents the interaction between the charged Pb_4 clusters.

~1 Citing

6. Computer simulation of cluster assembling

By Duque, F.; Mananes, A.; Molina, L. M.; Lopez, M. J.; Alonso, J. A.
From International Journal of Quantum Chemistry (2002), 86(2), 226-238. Language: English, Database: CAPLUS, DOI:10.1002/qua.1603

D. functional theory is used to investigate the assembling of metallic clusters to yield stable or metastable cluster solids. Motivated by the obsd. high stability of the $Al_{13}H$ cluster, which has a substantial highest occupied and LUMO (HOMO-LUMO) gap, we have modeled the assembling of those clusters. For a favorable relative orientation of each cluster with respect to all its neighbors, a cluster solid is predicted and its structure appears to be stable at least up to 150 K, which is the highest temp. in our simulations. We have also studied the chem. bonding in the stoichiometric solid alloys PbA, where A is one of the alkali elements Na, K, Rb, or Cs. Those crystals exist in an ordered phase formed by tetrahedral Pb_4 clusters surrounded by the alkali atoms. The study of this family of natural cluster compds. reveals the coating role played by the cations, providing further insight into the favorable conditions required for the formation of cluster solids.

~19 Citings

7. A generalized model for the structural investigation of liquid Li4Pb

By Satpathy, Alok
From Indian Journal of Physics, A (2001), 75A(1), 87-90. Language: English, Database: CAPLUS

A generalized model for partial structure factors of charged-hard-sphere mixt. of arbitrary charge and size is employed for the structural investigation of liq. Li-Pb in stoichiometric compn., treating the sample as partially charge transfer system. The computed concn.-concn. structure factor $S_{cc}(k)$ is in satisfactory agreement with the expt.

~0 Citings

8. Optic-like excitations in binary liquids: transverse dynamics

By Bryk, Taras; Mryglod, Ihor
From Journal of Physics: Condensed Matter (2000), 12(28), 6063-6076. Language: English, Database: CAPLUS, DOI:10.1088/0953-8984/12/28/305

The generalized collective mode approach was applied to study the transverse dynamics of binary mixts. The scheme is based on simultaneous treatment of the conserved total mass current and the mutual mass-concn. currents, as well as their time derivs. The condition for existence of optic-like transverse modes in a binary system was derived. The strong mutual diffusion and the tendency towards demixing prevent the emergence of transverse optic-like modes. Optic-like excitations were found in a Lennard-Jones Kr-Ar fluid and the liq.-metallic alloys $Mg_{70}Zn_{30}$ and Li_4Pb, while in the "fast-sound" dense gas mixt. $He_{75}Ar_{25}$ they do not appear for small wavenumbers.

~47 Citings

9. Anode materials for secondary nonaqueous-electrolyte batteries and batteries using these materials

By Shimamura, Harunari; Okamura, Kazuhiro; Nitta, Yoshiaki
From Eur. Pat. Appl. (1998), EP 883199 A1 19981209, Language: English, Database: CAPLUS

The composite title materials comprise a core formed by a solid phase A, and a solid phase Q partly or entirely wrapping the core. The amt. of Li intercalation and deintercalation by the phase A resulting from the charge and discharge is higher than that by the phase Q, however, the discharge capacity decrease of the phase Q resulting from battery cycling is low. The solid phase A comprises 1 of the materials selected from Li, ≥1 of the elements which is able to alloy with Li, solid soln. including ≥1 of the above elements being able to alloy with Li, or an intermetallic compd. including ≥1 of the above elements being able to alloy with Li. The solid phase Q has a different compn., but comprises the same kind of materials except Li by itself as those of the solid phase A. It is essential that the solid phase Q is a mixed conductor having electronic as well as Li ionic cond. When these materials are used in the anode, a secondary nonaq.-electrolyte battery can be realized featuring high reliability, high cycle characteristic, a high capacity, and excellent high-rate charge and discharge characteristics.

~15 Citings

10. Mixed lead-alkali clusters in the gas phase and in liquid alloys

By Molina, L. M.; Lopez, M. J.; Rubio, A.; Alonso, J. A.; Stott, M. J.
From International Journal of Quantum Chemistry (1998), 69(3), 341-348. Language: English, Database: CAPLUS, DOI:10.1002/(SICI)1097-461X(1998)69:3<341::AID-QUA12>3.0.CO;2-5

Ab initio d. functional calcns. for Na_nPb, Li_nPb, Na_nPb$_4$, and Li_nPb$_4$ are reported. The abundance of Na_6Pb obsd. in gas-phase expts. is explained as a consequence of evaporative cooling, which stops at Na_6Pb because of the high evapn. energy of this cluster. Insight is also provided into the clustering in the liq. Li-Pb and Na-Pb alloys. Anomalies in several electronic, structural, and thermodn. properties were detected at certain compns. (20% Pb in Li-Pb; 20% Pb and 50% Pb in Na-Pb) and our calcns. support the interpretation of those anomalies in terms of the formation of octet and clusters given by E. Zintl and G. Woltersdorf (1935).

~8 Citings

11. Effective interactions between concentration fluctuations and charge transfer in chemically ordering liquid alloys

By Akdeniz, Z.; Tosi, M. P.
From Nuovo Cimento della Societa Italiana di Fisica, D: Condensed Matter, Atomic, Molecular and Chemical Physics, Fluids, Plasmas, Biophysics (1993), 15D(2-3), 393-8. Language: English, Database: CAPLUS, DOI:10.1007/BF02456921

The correlations between long-wavelength fluctuations of concn. in a liq. binary alloy are detd. by a balance between an elastic-strain free energy and an Ornstein-Zernike effective interaction. The latter is extd. from thermodn. data in the case of the Li-Pb system, which is known to chem. order with stoichiometric compn. corresponding to Li_4Pb. Strong attractive interactions between concn. fluctuations near the compn. of chem. ordering originate from electronic charge transfer, which is estd. from the electron-ion partial structure factors as functions of compn in the liq. alloy.

~0 Citings

12. Thermodynamic properties of compound-forming liquid alloys

By Sommer, Ferdinand
From Journal of Non-Crystalline Solids (1990), 117-118(Pt. 2), 505-12. Language: English, Database: CAPLUS, DOI:10.1016/0022-3093(90)90580-F

The exptl. detd. properties of compd.-forming liq. alloys show specific concn. and temp. dependences, which are caused by the existence of chem. short range order in these alloys. The concn. and temp. dependences of thermodn. mixing functions are explained on the basis of homogeneous equil. reactions within an assocn. model for a simple description of chem. short range order. The ability of this model to predict thermodn. properties of a binary liq. alloy from exptl. results and to extrapolate it to ternary liq. alloys is demonstrated.

~19 Citings

13. Fast sound in liquid lithium-lead (Li4Pb)

By Bosse, J.; Jacucci, G.; Ronchetti, M.; Schirmacher, W.
From Zeitschrift fuer Physikalische Chemie (Muenchen, Germany) (1988), 156(1), 379-84. Language: English, Database: CAPLUS, DOI:10.1524/zpch.1988.156.Part_1.379

Authors report the results of a computer simulation performed on the liq. alloy Li_4Pb at 1085 K. A new high frequency and short wavelength collective mode was found which was termed "fast sound". Its propagation velocity is three times higher than that of the ordinary sound, and it is much less damped. The data are analyzed in terms of the Zwanzig Mori formalism. Fast sound should not exist only in this particular system but quite generally in alloys with a large mass difference.

~0 Citings

14. Hard spheres - Yukawa reference system of liquid binary alloys

By Gonzalez, D. J.; Silbert, M.
From Zeitschrift fuer Physikalische Chemie (Muenchen, Germany) (1988), 156(2), 657-62. Language: English, Database: CAPLUS, DOI:10.1524/zpch.1988.156.Part_2.657

Numerical calcns. were made by using the mean spherical approxn. (MSA) for model liq. binary alloys (Li_4Pb and $Li_{.61}Na_{.39}$) interacting via Yukawa potentials. For a const. ordering potential, the concn.-concn. partial structure factor $S_{cc}(k)$ is insensitive to changes in the pair interactions of the model liq. binary alloys.

~1 Citing

15. Dynamical properties of classical liquids and liquid mixtures

By Jacucci, G.; Ronchetti, M.; Schirmacher, W.
From NATO ASI Series, Series B: Physics (1984), 112(Condens. Matter Res. Using Neutrons), 139-61. Language: English, Database: CAPLUS

A review with 18 refs. is given with discussion of d. fluctuations, individual and collective motions, and mol. dynamics of liqs. and liq. mixts. Computer simulations of liq. alkali metals and Li_4Pb are discussed in detail.

~2 Citings

16. Ordering potential in liquid lithium-lead (Li4Pb) and lithium-silver (Li7Ag3) calculated from neutron diffraction data

By Ruppersberg, H.; Schirmacher, W.
From Journal of Physics F: Metal Physics (1984), 14(12), 2787-95. Language: English, Database: CAPLUS, DOI:10.1088/0305-4608/14/12/004

The structure factor $S_{CC}(q)$ data obtained by neutron diffraction at different temps. for liq. Li_4Pb and Li_7Ag_3 are used to calc. curves for a function $W(r)$ which, according to Copestake et al., (1982), correspond approx. to the ordering potential $V(r)$ at distances r larger than the hard-core diam. σ. Further support for this assumption is found from the fact that for liq. Li_4Pb the ordering enthalpy ΔH_{ord} introduced by Hafner et al., calcd. from $W(r)$ and the Fourier transform of $S_{CC}(q)$, is almost identical to the value given by Hafner et al., (1984), as it should be if $W(r > \sigma)$ are really identical to $V(r > \sigma)$. The diffraction data also yield meaningful values for the temp. deriv. of ΔH_{ord}. In all cases, the decreasing part of $|W(r > \sigma)|$ behaves similarly to a Yukawa potential $W_y(r)$. If the effective interat. interaction is assumed to arise from a pos. charge at the Li site and a corresponding neg. charge at the site of the other component, and if the electron screening is treated with the help of local pseudopotentials and the Thomas-Fermi approxn., the amt. of charge transfer in the two alloys is approx. the same and varies only a little with temp. The electronic screening, however, is much stronger in Li_7Ag_3 than in Li_4Pb and increases significantly with temp. for the latter.

~2 Citings

17. A model for the structure of liquid lithium-lead (Li4Pb)

By Copestake, A. P.; Evans, R.; Ruppersberg, H.; Schirmacher, W.
From Journal of Non-Crystalline Solids (1984), 61-62(1), 231-6. Language: English, Database: CAPLUS,
DOI:10.1016/0022-3093(84)90556-8

The results of calcns. of the partial structure factors and radial distribution functions of liq. Li_4Pb at different temps. are given. By assuming that this alloy is partially ionic, the interionic forces are represented by pairwise potentials that are strongly repulsive at small sepns. r and electronically screened Coulombic at larger r. This model was motivated by the fact that a r-dependent ordering potential which exhibits approx. screened Coulombic decay for a large r, can be extd. from the neutron diffraction data for $S_{cc}(q)$ in Li_4Pb. These calcns., which are based on the mean-spherical and the hyper-netted-chain approxns., show that the wave no. dependence of the measured concn. structure factor, $S_{cc}(q)$, can be accounted for reasonably well by a model with effective electron charges of ~0.5 and -2.0 at the Li and Pb sites, resp., and an inverse screening length of 1.1 Å^{-1}. These parameters are consistent with values obtained from the ordering potential extd. from expt. In order to explain the obsd. temp. dependence of $S_{cc}(q)$ it is necessary to assume that the charge transfer between species decreases with increasing temp.

~0 Citings

18. Charge ordering in molten salts and in some liquid semiconducting alloys

By Copestake, A. P.; Evans, R.
From Lecture Notes in Physics (1982), 172(Ionic Liq., Molten Salts Polyelectrolytes), 86-91. Language: English,
Database: CAPLUS

The screened Coulomb model was applied to calc. the partial structure factors and radial distribution functions for Li_4Pb alloy. For small charge transfers, the calcd. results for the charge-charge structure factor and the Fourier transform of this quantity agrees with the exptl. results. The model gives an adequate description of the near salt-like charge ordering in the alloy.

~0 Citings

19. Structure factors of compound forming liquid mixtures

By Bhatia, A. B.; Ratti, V. K.
From Physics Letters A (1975), 51A(7), 386-8. Language: English, Database: CAPLUS, DOI:10.1016/0375-9601(75)90740-9

Expressions for the structure factors of a compd. forming A-B mixts. are derived by using the idea of formation of appropriate chem. complexes $A_\mu B_\nu$. Numerical results are given for Li-Pb.

~0 Citings