

1. Thermodynamic optimization of the Li-Pb system aided by first-principles calculations

By Zhou, Chenyang; Guo, Cuiping; Li, Changrong; Du, Zhenmin
From *Journal of Nuclear Materials* (2016), 477, 95-101. Language: English, Database: CAPLUS,
DOI:10.1016/j.jnucmat.2016.04.061

The Li-Pb system was optimized using CALPHAD (Calc. of PHase Diagram) method. The enthalpies of formation of eight intermetallic compds. Li_4Pb ($\text{Li}_{22}\text{Pb}_5$), Li_7Pb_2 , $\text{Li}_{10}\text{Pb}_3$, Li_3Pb , Li_8Pb_3 , Li_5Pb_2 , αLiPb and βLiPb at 0 K were calcd. from first-principles calcns. with DFT + GGA approxns. The liq. phase was treated as $(\text{Li}, \text{Li}_{0.8}\text{Pb}_{0.2}, \text{Pb})$ using an assoc. soln. model because a short-range-order phenomenon was proven to exist in liq. The soln. phases fcc and bcc were described as (Li, Pb) with a simple substitutional model. The intermetallic compds. Li_4Pb , Li_3Pb and Li_5Pb_2 were treated as stoichiometric compds. With certain soly. ranges, the intermetallic compds. Li_7Pb_2 , αLiPb and βLiPb were modeled as $\text{Li}_7(\text{Li}, \text{Pb})_2$, $(\text{Li}, \text{Pb})(\text{Li}, \text{Pb})$ and $(\text{Li}, \text{Pb})(\text{Li}, \text{Pb})$ using the two-sublattice model. A set of self-consistent thermodyn. parameters in the Li-Pb system was obtained in the present work.

~0 Citings

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2. Structure and electrophysical properties of liquid $\text{Pb}_{83}\text{Mg}_{17}$ and $\text{Pb}_{83}\text{Li}_{17}$ eutectics

By Mudry, S.; Shtablavyi, I.; Sklyarchuk, V.; Plevachuk, Yu.
From *Journal of Nuclear Materials* (2008), 376(3), 371-374. Language: English, Database: CAPLUS,
DOI:10.1016/j.jnucmat.2008.02.011

Short range order structure of $\text{Pb}_{83}\text{Mg}_{17}$ and $\text{Pb}_{83}\text{Li}_{17}$ liq. alloys was studied by x-ray diffraction method, in view of nuclear reactor coolant application. The structure factors and pair correlation functions are analyzed. Exptl. structure data were used to calc. the partial structure characteristics by Reverse Monte Carlo method. Also Li_4Pb significantly affects the structure of $\text{Pb}_{83}\text{Li}_{17}$ eutectic melt. For $\text{Pb}_{83}\text{Mg}_{17}$ eutectic melt the elec. resistivity and thermo-emf. were measured at 550-1300 K. Their anal. confirms the diffraction data concluding the heterocoordinated at. distribution Pb and Mg atoms.

~6 Citings

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3. Influence of strong heterocoordination on surface properties of Li-Pb melts

By Anusionwu, B. C.; Adebayo, G. A.; Orji, C. E.
From *Physics and Chemistry of Liquids* (2005), 43(6), 495-506. Language: English, Database: CAPLUS,
DOI:10.1080/00319100500186311

The influence of the strong heterocoordination tendency of the Li-Pb liq. alloy on its surface properties was studied using a statistical thermodyn. model based on compd. formation and that based on the layered structure near the interface. In addn. to the already proposed saltlike structure Li_4Pb compd. formed in the liq. alloy, the study shows that the compd. Li_3Pb also has a profound influence on the thermodyn. properties of the liq. alloy. The surface study suggests that the formed compds. in the liq. alloy segregate to the surface ~0.8 at fraction of Li. The calcd. surface tension of the liq. alloy exhibits a pronounced hump above equiat. compn.

~4 Citings

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4. 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

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5. 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 **Li₄Pb** 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 **Li₄Pb** are reported.

~0 Citings

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6. 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

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7. Thermodynamic study of liquid lithium-lead alloys using the EMF method

By Gasior, W.; Moser, Z.

From [Journal of Nuclear Materials \(2001\)](#), 294(1,2), 77-83. Language: English, Database: CAPLUS, DOI:10.1016/S0022-3115(01)00440-8

Liq. Li-Pb alloys were investigated by the emf. (emf) method at Li concns. of $0.025 \leq X_{Li} \leq 0.965$ mol fraction and at temps. from 775 to 975 K. The expts. were conducted at const. temp., and the Li concn. was changed by the coulometric-titrn. technique. The two-phase Li-Bi alloys and liq. lithium were used as the ref. electrodes. The dependence of emfs on temp. for each investigated alloy was linear, and from the linear equations ($E = a + bT$), partial Li excess Gibbs energies, partial enthalpies and entropies of lithium were calcd., and compared with previously published data. The excess stability function ES and the concn.-concn. partial structure factor $S_{cc}(0)$ were calcd. and discussed in relation to the neutron diffraction data and other properties. A change in the type of chem. bonding near the compn. **Li₄Pb** is indicated. This study was initiated since Pb-17Li eutectic alloy was proposed as a breeder blanket fluid for fusion reactors.

~8 Citings

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8. The ionic structure and the electronic states of liquid Li-Pb alloys obtained from ab initio molecular dynamics simulations

By Senda, Y.; Shimojo, F.; Hoshino, K.

From [Journal of Physics: Condensed Matter \(2000\)](#), 12(28), 6101-6112. Language: English, Database: CAPLUS, DOI:10.1088/0953-8984/12/28/307

Ab initio mol. dynamics simulations are carried out for liq. $Li_{0.8}Pb_{0.2}$ and $Li_{0.5}Pb_{0.5}$ alloys to investigate the ionic structure and the electronic states. In our simulation, the existence of the "chem. complex" **Li₄Pb** is not found; rather, a salt-like ordering of Pb ions is seen in the liq. $Li_{0.8}Pb_{0.2}$ alloy. It is found from the calcd. partial and total structure factors that this ordering leads to the characteristic behavior of the total structure factor, which agrees well with the results of a neutron diffraction expt. The compn. dependence of the electronic states is explained on the basis of the ionic configuration. The tendency towards ionicity or charge transfer is seen in both liq. alloys, though the valence-electronic charge distribution is not so localized around the ions.

~7 Citings

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9. 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

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10. Polyanionic complexes and short range order in liquid Li-based alloys

By Mudry, S.

From [Zhurnal Fizichnikh Doslidzhen \(1998\), 2\(3\), 331-334](#). Language: Ukrainian, Database: CAPLUS

A possible existence of polyanionic clusters in near-eutectic Li-Sn and Li-Pb alloy melts is detd. Using exptl. structural data, partial structural factors for polyanionic Zintl complexes are calcd. assuming the additive law for the intensity of scattered x-ray radiation from each structural unit. In the Li-Pb melts, the microinhomogeneity of the structure is expressed by tetrahedral polyanionic clusters and Li_4Pb -type microregions, whereas Li_3Sn -type assoc. only are present in the Li-Sn system.

~1 Citing

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11. Collective ionic dynamics in a molten binary alloy

By Fernandez-Perea, R.; Alvarez, M.; Bermejo, F. J.; Verkerk, P.; Roessli, B.; Enciso, E.

From [Physical Review E: Statistical Physics, Plasmas, Fluids, and Related Interdisciplinary Topics \(1998\), 58\(4\), 4568-4581](#). Language: English, Database: CAPLUS

A series of computer mol. dynamics studies are performed to investigate the details of the at. motions. From an anal. of the simulated structure factors for molten Li_4Pb , as well as by a comparison with those of liq. Li under different thermodyn. conditions, it is found that the high-frequency excitation found in the alloy shows characteristics remarkably different from those of pure Li. The relative phases of the atoms partaking in such motions, as well as the remarkably short excitation lifetimes, portray it as a fairly localized mode, with a frequency dependent polarization.

~41 Citings

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12. High-frequency dynamics in a molten binary alloy

By Alvarez, M.; Bermejo, F. J.; Verkerk, P.; Roessli, B.

From [Physical Review Letters \(1998\), 80\(10\), 2141-2144](#). Language: English, Database: CAPLUS, DOI:10.1103/PhysRevLett.80.2141

Heavily damped excitations are found in molten Li_4Pb by inelastic neutron scattering. The expt. covered a kinematic range which enabled an unambiguous characterization of such excitations by means of the study of the wave vector dependence of their frequencies, lifetimes, and signal amplitudes. The excitations exhibit features which substantially deviate from those expected for the propagation of an acoustic mode (which should involve in-phase at. displacements).

~41 Citings

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13. Bimetallic clusters of interest for liquid alloys.

By Alonso, J. A.; Molina, L. M.; Lopez, M. J.; Rubio, A.

From [Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17 \(1997\), COMP-120](#). Language: English, Database: CAPLUS

Different properties of liq. alloys formed by Pb and alkali metals (Li, Na, K, Rb, Cs) suggest the presence of two types of clusters: the first group comprises Li_4Pb and Na_4Pb clusters, and the second group, including Na_4Pb_4 , K_4Pb_4 , Rb_4Pb_4 and Cs_4Pb_4 , belongs to the Zintl class. The partial ionic character of the corresponding liq. alloys is expected to arise from charge transfer effects in the clusters. We have performed d. functional calcns. for free bimetallic clusters of the elements listed above, varying the no. of alkali and Pb atoms in the cluster, with the objective of providing some insight into the clustering in the liq. alloys. Indeed we have obtained that clusters of compn. A_4Pb and A_4Pb_4 (where A indicates an alkali element) are very stable. Gas phase expts. for mixed lead-sodium vapors indicate, in contrast, that Na_6Pb is an extremely abundant cluster in the gas phase, and this is also explained in our calcns.

~0 Citings

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14. Observation of fast sound in liquid Li_4Tl and liquid Li_4Pb by inelastic neutron scattering

By de Jong, P. H. K.; Verkerk, P.; de Vroege, C. F.; de Graaf, L. A.; Howells, W. S.; Bennington, S. M.
From *Journal of Physics: Condensed Matter* (1994), 6(44), L681-L686. Language: English, Database: CAPLUS

We performed inelastic neutron scattering expts. on liq. Li_4Pb and Li_4Tl . We obtained the first exptl. evidence for the existence of fast sound in a molten binary alloy of elements of strongly different wt. This phenomenon was obsd. for the first time ten years ago in a computer mol. dynamics (CMD) simulation. The results are compared with the results of the CMD simulation and with exptl. results for the sound dispersion of pure lithium.

~30 Citings

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15. Structure of covalent liquids

By Tosi, M. P.
From *Journal of Physics: Condensed Matter* (1994), 6(Suppl. 23A), A13-A28. Language: English, Database: CAPLUS, DOI:10.1088/0953-8984/6/23A/003

A review with 94 refs. Bond directionality and network formation from local structural units are the signature of covalent bonding. On melting, a three-dimensional (3D) network of covalent bonds tends to break into a metallic liq. (e.g., in Si, Ge, and GaAs), unless a sufficiently large electronegativity difference between the components stabilizes the electronic structure through chem. short-range order. The melt may then be a semimetal (e.g., Li_4Pb and KPb), an ionic semiconductor (e.g., CsAu) or an insulator (e.g., ZnCl_2). Bonding appears to be more stable in networks of lower dimensionality ($D = 2$ as in GeSe_2 and YCl_3 ; $D = 1$ as in Se and BeCl_2 ; and $D = 0$ as in P , SbCl_3 , and AlBr_3). Melting from $D = 2$ to $D = 0$ occurs in AlCl_3 . Intermediate-range order may be preserved in the melt through interat. correlations over distances of order 5-10 Å. Exptl. evidence and simulations on illustrative examples of these various trends are given, with emphasis on the interconnection between stable local coordination and intermediate-range order.

~28 Citings

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16. 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 thermodyn. 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

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17. Nuclear spin-lattice relaxation in liquid lithium-germanium alloys

By Van der Marel, C.; Heitjans, P.; Ackermann, H.; Bader, B.; Freilaender, P.; Schirmer, A.; Stoeckmann, H. J.
From [Zeitschrift fuer Physikalische Chemie \(Muenchen, Germany\) \(1988\), 156\(2\), 629-34](#). Language: English,
Database: CAPLUS, DOI:10.1524/zpch.1988.156.Part_2.629

In liq. Li-Ge alloys with ≤ 55 at.% Ge the spin-lattice relaxation rate $1/T_1$ of β -active ^8Li nuclei was measured as a function of temp. The relaxation rate decreases rapidly when Ge is added to Li, to ~ 20 at.% Ge: for higher Ge concns. $1/T_1$ is approx. const. Combining $1/T_1$ with ^7Li Knight shift data the enhancement factor η of the measured rate relative to the Korringa rate was obtained. η Exhibits max. at 20 and 50 at.% Ge. The man. at 20 at.% Ge is probably due to the formation of a liq. octet compd. similar to liq. Li_4Pb . The max. in η at the equiat. compn. was unexpected according to recent tight-binding calcns. in which the stability of tetrahedral clusters was considered as a function of the size of the alkali ion.

~0 Citings

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18. Ordering potential and the structural properties of binary Yukawa mixtures

By Gonzalez, D. J.; Silbert, M.

From [Journal of Physics F: Metal Physics \(1988\), 18\(11\), 2353-62](#). Language: English, Database: CAPLUS,
DOI:10.1088/0305-4608/18/11/008

Results are presented of numerical calcns., in the mean spherical approxn. (MSA), for model liq. binary alloys interacting via Yukawa potentials, namely $\phi_{ij}(r) = A_{ij} \exp(-\lambda r)/r$. Parameters were chosen which allow the description of the structural properties of liqs. Li-Na and Li-Pb at different concns. and Li_4Pb at 3 temps. It is shown that (1) that once the ordering potential, $v(r) = 1/2(\phi_{11}(r) + \phi_{22}(r) - 2\phi_{12}(r))$, is specified the total structure factor $S(k)$, the concn.-concn. partial structure factor $S_{cc}(k)$ and the no.-no. partial structure factor $S_{NN}(k)$ are insensitive to changes in the pair interactions $\phi_{ij}(r)$; and (2) that the thermodyn. properties-specifically $S_{cc}(0)$ and the correlation energy-are sensitive to changes in $\phi_{ij}(r)$.

~5 Citings

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19. Fast sound in liquid lithium-lead (Li_4Pb)

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

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20. 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 $\text{Li}_{.61}\text{Na}_{.39}$) 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

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21. Screened Coulomb model in a uniform background charge for temperature dependence of the structure of liquid lithium-lead (Li_4Pb)

By Aniya, Masaru; Ginoza, Mitsuaki

From [Journal of the Physical Society of Japan \(1987\), 56\(6\), 2046-55](#). Language: English, Database: CAPLUS, DOI:10.1143/JPSJ.56.2046

For understanding the temp. dependence of the static structure factor of liq. Li_4Pb , a 2-component system consisting of charged hard spheres with screened Coulomb interaction in a uniform neutralizing background charge was investigated in terms of the modified mean-spherical approxn. In respect to the structure reflecting the chem. short-range order, the calcd. temp. dependence agrees reasonably well with the measured one. This suggests that the effect of the background charge plays an essential role in the temp. variation of the static structure of liq. Li_4Pb .

~0 Citings

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22. On the concentration dependence of the ordering potential in liquid lithium-lead alloys

By Gallego, L. J.; Somoza, J. A.; Alonso, J. A.

From [Physics and Chemistry of Liquids \(1987\), 16\(4\), 249-58](#). Language: English, Database: CAPLUS, DOI:10.1080/00319108708078527

The expression for the free energy of mixing arising from the Bhatia and Young (1984) approach is used to study the concn. fluctuations $S_{cc}(0)$ of liq. Li-Pb alloy. The exptl. behavior of $S_{cc}(0)$ can be explained by this theory if the ordering potential is assumed to vary strongly with concn. near the stoichiometric compn. Li_4Pb .

~5 Citings

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23. Computer simulation studies of atomic structure and dynamics relevant to liquid and amorphous alloys

By Ronchetti, Marco; Jacucci, Gianni

From [NATO ASI Series, Series E: Applied Sciences \(1987\), 118\(Amorphous Liq. Mater.\), 82-98](#). Language: English, Database: CAPLUS

A review with 38 refs. on icosahedral quasicrystals, computer simulation of bond-orientational order in liqs. and glasses, dynamics of atoms in fluids, and collective modes in Li_4Pb liq. alloy.

~0 Citings

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24. Calculation of $C_p(T)$ for liquid lithium/lead alloys from experimental $\rho(T)$ and (ρ/T) s data

By Saar, J.; Ruppertsberg, H.

From [Journal of Physics F: Metal Physics \(1987\), 17\(2\), 305-14](#). Language: English, Database: CAPLUS, DOI:10.1088/0305-4608/17/2/003

The d. and the adiabatic variation of temp. T with pressure p , were measured for the whole concn. range of liq. Li/Pb alloys and for a temp. range of 200-700 K (depending on compn.) above the liquidus temp. T_L . The heat capacity (C_p), calcd. from these data exhibits a pronounced peak at the compn. Li_4Pb where at T_L it exceeds the ideal C_p^i by an excess value C_p^{xs} of about $0.8 C_p^i$. Linear variation of C_p with T was only obsd. for pure liq. Pb. Strongly bent curves with more or less pronounced min. were obsd. for the other compns., including pure liq. Li. C_p^{xs} of liq. Li_4Pb compares well with a value calcd. from neutron diffraction data by Ruppertsberg and Schirmacher (1984).

~15 Citings

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25. Model for the temperature dependence of the static structure of liquid lithium-lead (Li_4Pb)

By Aniya, Masaru; Ginoza, Mitsuaki

From [Journal of the Physical Society of Japan \(1986\), 55\(9\), 3281-2](#). Language: English, Database: CAPLUS, DOI:10.1143/JPSJ.55.3281

A possible explanation is discussed of the temp. dependence of the 1st peak height in the obsd. (H. Ruppertsberg et al., 1982) concn.-concn. structure factor $S_{cc}(k)$ within the screened Coulomb model.

~1 Citing

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26. Computer simulation of the liquid lithium-lead (Li₄Pb) alloy

By Jacucci, G.; Ronchetti, M.; Schirmacher, W.

From *Journal de Physique, Colloque* (1985), (C8), 385-9. Language: English, Database: CAPLUS, DOI:10.1051/jphyscol:1985858

For liq. Li₄Pb at 1085 K, partial radial distribution functions, static and dynamic structure factors, and Li and Pb self-diffusion coeffs. were obtained in mol.-dynamics simulations based on the model potential given by A. P. Copestake, et al., (1983). The results were compared with existing exptl. data.

~0 Citings

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27. Observation of the strongly anomalous temperature and composition dependence of ($\delta p/\delta T$)s in liquid lithium/lead alloys

By Saar, J.; Ruppertsberg, H.

From *Physics Letters A* (1985), 113A(3), 161-3. Language: English, Database: CAPLUS, DOI:10.1016/0375-9601(85)90164-1

The values ($\delta P/\delta T$), which are proportional to the sp. heat were measured between the liquidus temp. and 1250 K for the whole concn. range of liq. Li/Pb alloys. For all concns., there are pos. deviations from the values expected for an ideal soln. and there is a narrow peak close to the compn. Li₄Pb. At $0.2 < x_{Li} < 0.6$ a fall off after melting is followed by a broad max. at about 1000 K.

~0 Citings

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28. 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 Li₄Pb are discussed in detail.

~2 Citings

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

By Ruppertsberg, 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. Li₄Pb and Li₇Ag₃ 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. Li₄Pb 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 Li₇Ag₃ than in Li₄Pb and increases significantly with temp. for the latter.

~2 Citings

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

By Copestake, A. P.; Evans, R.; Ruppertsberg, 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. Li₄Pb 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 sepn. 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 Li₄Pb. 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 \AA^{-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

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31. Self-consistent study of chemical short-range order and charge transfer in liquid alloys as a function of temperature

By Holzhey, Christiane; Brouers, Francois; Franz, Judy R.; Schirmacher, Walter
From *Journal of Non-Crystalline Solids* (1984), 61-62(1), 65-70. Language: English, Database: CAPLUS,
DOI:10.1016/0022-3093(84)90531-3

A self-consistent theory of the electronic and at. structure of binary liq. alloys with strong ionic tendencies developed recently by the authors is applied to study the temp. variation of the electronic d. of states and the charge transfer of such systems. The dip in the d. of states at the Fermi level which indicates the tendency towards non-metallic behavior is reduced and the charge transfer decreases with increasing temp. This is consistent with recent measurements on liq. Li₄Pb indicating that the charge transfer which seems to occur in this substance is reduced at higher temps.

~0 Citings

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32. Lithium-8 spin relaxation in liquid lithium alloys with compound-forming tendency

By Heitjans, P.; Kiese, G.; Van der Marel, C.; Ackermann, H.; Bader, B.; Freilaender, P.; Stoeckmann, H. J.
From *Hyperfine Interactions* (1983), 16(1-4), 569-72. Language: English, Database: CAPLUS,
DOI:10.1007/BF02147317

In liq. Li-Bi, Li-Sn and Li-Si alloys, the spin-lattice relaxation rate T_1^{-1} of β -active ⁸Li probe nuclei was detd. over a wide concn. (c) and temp. (T) range. T_1^{-1} is governed by hyperfine contact interaction with the conduction electrons. Near the comps. Li₃Bi, Li₄Pb, Li₄Sn, and Li₄Si, both $(T_1 T)^{-1}$ and $d(T_1 T)^{-1}/dT$ vs. c show marked extremes. These data, when combined with Knight shift and/or cond. values, inform on the prolongation of the electron residence time and the redn. of the d. of states at the Fermi surface. There is progressive tendency to electron localization and compd. formation in the sequence Li₄Pb, Li₄Sn, and Li₃Bi with mainly ionic bonding in the case of liq. Li₃Bi.

~2 Citings

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33. A model for the structure of liquid lithium lead [Li₄Pb]

By Copestake, A. P.; Evans, R.; Ruppertsberg, H.; Schirmacher, W.
From *Journal of Physics F: Metal Physics* (1983), 13(10), 1993-2010. Language: English, Database: CAPLUS,
DOI:10.1088/0305-4608/13/10/011

Calcns. are presented of the partial structure factors and radial distribution functions of liq. Li_4Pb at different temps. Assuming that this alloy is partially ionic, the interionic forces are modeled by pairwise potentials that are strongly repulsive at small sepn. (r) and electronically screened Coulombic at large r . This model arises from the fact than an r -dependent ordering potential, which exhibits approx. screened Coulombic decay for large r , can be extd. from the neutron diffraction data for $S_{\text{CC}}(q)$ in Li_4Pb . The calcns., which are based on the mean-spherical and the hypernetted-chain approxns., show that the wavenumber dependence of the measured concn. structure factor $S_{\text{CC}}(q)$ can be reasonably well accounted for by the 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 \AA^{-1} . These parameters are consistent with values obtained from the ordering potential extd. from expt. In order to explain the obsd. temp. dependence of $S_{\text{CC}}(q)$ it is necessary to assume that the charge transfer between species decreases with increasing temp.

~18 Citings

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34. Structure of multicomponent hard-sphere mixtures: application to the liquid lithium-lead alloy

By Hoshino, Koza

From [Journal of Physics F: Metal Physics \(1983\), 13\(10\), 1981-92](#). Language: English, Database: CAPLUS, DOI:10.1088/0305-4608/13/10/010

A general formula for the partial structure factors of an m -component mixt. is derived. The compressibility of the mixt. obtained by J. G. Kirkwood and F. P. Buff (1951) can be written in terms of the partial structure factors in the long-wavelength limit. For the m -component hard-sphere system, the explicit expressions for the partial structure factors are obtained based on Hiroike's exact soln. of the Percus-Yevick equation. The formulas are applied to the liq. Li-Pb alloy, which is considered as a ternary mixt. of Li, Pb, and Li_4Pb . The theor. total structure factor agrees with that obsd. by H. Ruppersberg and H. Reiter (1982).

~25 Citings

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35. Kinetics of the cathodic formation of lithium-lead (Li_8Pb_3 and Li_4Pb) intermetallic compounds in propylene carbonate

By Kiseleva, I. G.; Tomashova, N. N.; Kabanov, B. N.

From [Elektrokhimiya \(1983\), 19\(4\), 532-6](#). Language: Russian, Database: CAPLUS

The kinetics were studied of the cathodic formation of the intermetallic compds. Li_8Pb_3 and Li_4Pb . In the presence of forming these compds., a substantial role is played by diffusion of the Li. During cathodic polarization together with the formation of Li_4Pb there also occurs its conversion to Li_8Pb_3 and recrystn.

~3 Citings

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36. Lithium-8 spin-lattice relaxation in liquid lithium-bismuth and lithium-lead alloys

By Kiese, G.; Heitjans, P.; Ackermann, H.; Bader, B.; Buttler, W.; Freilaender, P; Van der Marel, C.; Ruppersberg, H.; Stoeckmann, H. J.

From [Lecture Notes in Physics \(1982\), 172\(Ionic Liq., Molten Salts Polyelectrolytes\), 117-23](#). Language: English, Database: CAPLUS

The nuclear spin-lattice relaxation rate T_1^{-1} of β -active ^8Li ($T_{1/2} = 0.8 \text{ s}$) was measured in liq. Li-Bi and Li-Pb alloys. T_1^{-1} As function of concn. and temp. shows marked deviations from metallic behavior near the compns. Li_3Bi and Li_4Pb . Combining the relaxation data with Knight shift and/or cond. data the mean 'residence time' τ_e of the conduction electrons at a nuclear site and the d. of states at the Fermi surface $N(E_F)$ are obtained relative to the free-electron values. In liq. Li-Bi the tendency towards electron localization and compd. formation is significantly stronger than in Li-Pb. The melt $\text{Li}_{0.8}\text{Pb}_{0.2}$ seems to become metallic above 1400 K.

~0 Citings

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37. 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

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38. Thermodynamic investigations of liquid lithium-lead and lithium-silver alloys - a comparative study

By Becker, Werner; Schwitzgebel, Guenter; Ruppertsberg, Henner

From [Zeitschrift fuer Metallkunde \(1981\), 72\(3\), 186-90](#). Language: English, Database: CAPLUS

The Li activity was detd. by emf. measurements of 800-900 K. The integral mixing enthalpy and the integral excess free energy in Li-Pb show deep asym. min. Near the compn. Li_4Pb and LiAg, Darken's excess stability exhibits a max. The partial mixing entropy of Li develops an S-shaped curve near LiAg. In Li-Pb a sharp temp.-dependent neg. peak was obsd., which should be regarded as a part of an S-shape. These features are indications of cluster formation or assocn., and agree with the results of x-ray and neutron diffraction studies. This agreement between thermodyn. and structural considerations extends to the strength of interaction, which is very high in Li-Pb and low in Li-Ag.

~8 Citings

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39. Lithium-7 Knight shift of liquid lithium-lead and -tin alloys

By Van der Marcel, C.; Geertsma, W.; Van der Lugt, W.

From [Journal of Physics F: Metal Physics \(1980\), 10\(10\), 2305-12](#). Language: English, Database: CAPLUS

The ^7Li Knight shift was measured in liq. Li-Pb and Li-Sn alloys through the entire concn. range and at several temps. The Knight shifts in liq. Li-Pb are discussed together with previous measurements of the elec. cond. and the spin-lattice relaxation time, which also exhibit anomalous behavior near the compn. Li_4Pb . The results support the assumption of a partially saltlike mixt. around the compn. Li_4Pb .

~0 Citings

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40. Magnetic susceptibility of liquid alloys sodium-antimony, sodium-bismuth, lithium-antimony, lithium-bismuth and lithium-lead

By Hackstein, K.; Sotier, S.; Luescher, E.

From [Journal de Physique, Colloque \(1980\), \(C8\), 49-51](#). Language: English, Database: CAPLUS, DOI:10.1051/jphyscol:1980813

The d.c. magnetic susceptibility was measured of Na-Sb, Na-Bi, Li-Sb, Li-Bi and Li-Pb liq. alloys. Na-Sb, Na-Bi, Li-Sb and Li-Bi exhibit a strong variation in the susceptibility depending upon compn., with a metal-to-semiconductor transition near the stoichiometric compn. (Na_3Sb , Na_3Bi , Li_3Sb , Li_3Bi). At the stoichiometric compn., a relatively strong diamagnetic min. occurs. The susceptibility of Li-Pb shows a min. at the stoichiometric compn. Li_4Pb , but it is less pronounced than in the other alloys.

~0 Citings

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41. Dynamical concentration fluctuations in liquid lithium-lead (Li_4Pb)

By Soltwisch, M.; Quitmann, D.; Ruppertsberg, H.; Suck, J. B.

From [Journal de Physique, Colloque \(1980\), \(C8\), 167-70](#). Language: English, Database: CAPLUS, DOI:10.1051/jphyscol:1980843

A measurement of the quasielastic neutron scattering from liq. ${}^7\text{Li}_4\text{Pb}$ were performed. Corrections for background, absorption, self shielding, and multiple scattering were applied and the spectra were reduced to cross sections by normalization to V . Since the coherent scattering lengths av. to zero, the intensity obsd. is essentially due to the concn. fluctuation structure factor $S_{cc}(q, E)$. $S_{cc}(q, E)$ Shows a pronounced quasielastic peak around $q \approx 1.5 \text{ \AA}^{-1}$. In the region of the peak, the energy width narrows down by about a factor of 2. A fit in terms of a sum of Lorentzians is attempted which corresponds to an extrapolation of the description valid in the hydrodynamic limit. The self diffusion const. for Li is derived from the ${}^7\text{Li}$ incoherent scattering and an interdiffusion const. from $S_{cc}(q, E)$.

~0 Citings

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42. Volume of mixing of compound-forming molten alloys

By Bhatia, A. B.; Singh, R. N.

From [Physics Letters A \(1980\), 78A\(5-6\), 460-2](#). Language: English, Database: CAPLUS, DOI:10.1016/0375-9601(80)90424-7

The variations in mixing vols. (V) with concn. are examd. theor. for alloy systems with compd. formation. The results are compared with the exptl. data for LiPb and NaPb alloys at 950 and 700 K, resp. Max. in $|V|$ correspond to formation of Li_4Pb and Na_4Pb , resp.

~3 Citings

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43. Electrochemical power producing battery cell

By Panzer, Richard E.

From [No Corporate Source data available \(1965\), US 3189485 19650615](#), Language: Unavailable, Database: CAPLUS

The electrochem. system of $\text{U}|\text{LiCl-KCl-kaolin}|\text{LiCl-KCl-UO}_3|\text{Ni}$ is new in a long life high power cell. The anolyte consists of 65% LiCl-KCl eutectic or LiOH-LiCl eutectic and 35% 325-mesh kaolin pressed into a pill. The catholyte consists of 65% UO_3 as the active material and 35% electrolyte pressed into a pill. The anolyte and the catholyte are placed between the anode and the cathode collector of Ni. To increase the output of the cell, a U oxide glass coating is used on the cathode collector. This consists of U oxide and an oxide of B, P, or Si. Results of using U, Mg, or Li_4Pb alloy as the anode and UO_3 in a thermal cell are tabulated. By using Mg the cell reactions for UO_3 and V_2O_5 are compared. The reaction for V_2O_5 produced 295 w.-hrs./lb. with an efficiency of 10% due to side reactions, resulting in 29.5 w.-hrs./lb. The UO_3 produced 111 w.-hrs./lb. at an av. efficiency of 54.5% or 60 w.-hrs./lb. The UO_3 does not react with the electrolyte, has a reasonably high potential, and its coulombic capacity is high. The cell is operative above the m.p. of the electrolyte and below the m.p. of the cell electrodes.

~0 Citings

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44. The exchange of magnesium by lithium or sodium in magnesium plumbide

By Brauer, Georg; Tiesler, Joachim

From [Zeitschrift fuer Anorganische Chemie \(1950\), 262, 309-18](#). Language: Unavailable, Database: CAPLUS

To det. the effect of a type A_4B compd. on the antifluorite lattice of a type A_2B compd. the systems $\text{Na}_{15}\text{Pb}_4\text{-Mg}_2\text{Pb}$ and $\text{Li}_4\text{Pb-Mg}_2\text{Pb}$ were investigated. Powder patterns showed that the antifluorite structure of Mg_2Pb was distorted with small amts. of Na present but still gave strong lines with 43 mole % Li_4Pb . Up to 10 mole % Li_4Pb introduced no new lines to the Mg_2Pb pattern. Both the lattice const. and d. of the $\text{Li}_4\text{Pb-Mg}_2\text{Pb}$ system exhibit discontinuities at about 10 mole % Li_4Pb , and the d. data indicate that the mixed-crystal lattice is of the addn. type.

~0 Citings

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45. The γ phase of lead-lithium alloys, $\text{Li}_{10}\text{Pb}_3$

By Rollier, M. A.; Arreghini, Enrico

From [Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie \(1939\), 101, 470-82 \(Italian with German abstr.\)](#). Language: Unavailable, Database: CAPLUS

By melting Pb with 12% Li in an atm. of A, $\text{Li}_{10}\text{Pb}_3$ was formed. This was previously reported as Li_4Pb , Li_7Pb_2 and Li_3Pb . The compd. is cubic, with $a = 10.082$, $Z = 4$, space group T^1_d . The structure is similar to that of γ -brass, and corresponds to the arrangement given for Cu_9Al_4 by Bradley (C. A. 23, 1323).

~2 Citings

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46. Electrical conductivity and phase diagram of binary alloys. XV. The system lithium-lead

By Grube, G.; Klaiber, H.

From [Zeitschrift fuer Elektrochemie und Angewandte Physikalische Chemie \(1934\)](#), 40, 745-54. Language: Unavailable, Database: CAPLUS

The Li-Pb alloys were examd. according to the method of thermal analysis and also by detn. of the change of elec. cond. with change of temp. as previously used (C. A. 27, 934). From these measurements the complete phase diagram was set up. The intermetallic compds. LiPb , Li_5Pb_2 , Li_3Pb , Li_7Pb_2 and Li_4Pb were shown. Of these only LiPb , m. 482° , and Li_7Pb_2 , m. 726° , melt without decomn. Li_5Pb_2 exists at 642° Li_3Pb at 658° and Li_4Pb at 648° . LiPb exists in two forms, which are converted into each other at 214° . The form stable below 214° has a neg. and the form stable above 214° a pos. temp. coeff. of elec. resistance. With excess Pb, LiPb forms α -mixed crystals whose satn. concn. with temp. was detd. With excess Li, LiPb forms β -mixed crystals which change to β -mixed crystals at 214° . The satn. concn. of β -mixed crystals is at 53.3% Li. With excess Li, Li_7Pb_2 forms γ -mixed crystals in a narrow range of about 1%.

~8 Citings

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