**Density Functional Theory Study of Diffusion of Lithium in Li-Sn Alloys**

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**Abstract**

Diffusion of Li in LixSn alloys was investigated using a density functional theory in order to fully understand the lithiation process in these types of Li ion batteries. Variation of the calculated open circuit voltages of the LixSn alloys was found to agree well with experimental results. Diffusion coefficients of the Li in the LixSn alloys were calculated to be in the range between 6.6×10-8 cm2s-1 to 5.6×10-7 cm2s-1 at room temperature, which is within the range between 8.0×10-8 cm2s-1 to 5.9×10-7 cm2s-1 obtained from the experimental measurement.

**Key words**: Density functional theory, LixSn alloys, Voltage, Diffusion, Molecular dynamics

1. **Introduction**

Lithium ion batteries (LIBs) with a high energy density operated at a high power are being widely investigated as rechargeable energy storage devices for electric vehicles, smart grids, and medical apparatus [[1](#_ENREF_1),[2](#_ENREF_2)]. Further increasing the energy density of the LIBs can be realized through increasing the capacity or the open circuit voltage (OCV) of electrode materials [[3](#_ENREF_3)]. LixSn alloys have been received great attention recently owing to their large Li storage capacities (e.g., with a theoretical capacity value of 994 mAhg-1 for Li22Sn5) [[4](#_ENREF_4)]. Sn anode materials synthesized using an electrodeposition method showed an initial discharge capacity of 757 mAhg-1 [[5](#_ENREF_5)], and those synthesized using an electron-beam evaporation method showed a discharge capacity of about 800 mAhg-1 [[6](#_ENREF_6)]. Whereas those synthesized using a magnetron sputtering technique showed an initial discharge capacity over 800 mAhg-1 [[7](#_ENREF_7)]. Although these experimentally obtained discharge capacities of the Sn anode materials prepared using different methods are less than their theoretical maximum reading, they are much higher than those reported for the LIBs using graphite (372 mAhg-1) as anode materials [[8](#_ENREF_8),[1](#_ENREF_1)]. However, currently the Sn anodes have not been commercialized due to their poor cyclic performances because of their huge volume expansion/contraction during lithiation/delithiation processes, which causes mechanical disintegration of the Sn anode electrode materials [[9](#_ENREF_9),[6](#_ENREF_6),[10](#_ENREF_10)]. Various methods have been applied to improve the cyclic performances of the Sn anodes, such as using nanostructured Sn or Sn-based anode materials (i.e., nano-crystallized Sn-based intermetallic alloys, Sn nanoparticles/C nanotubes, Sn nanoparticles, SnO2 nanoparticles) [[11-17](#_ENREF_11)], and Sn-M (M=Fe, Co, Ni, Li) alloys [[18](#_ENREF_18),[19](#_ENREF_19)].

There are six types of LixSn alloy phases according to the literature: i.e., LiSn, Li7Sn3, Li5Sn2, Li13Sn5, Li7Sn2 and Li22Sn5 [[20](#_ENREF_20)]. These intermetallic phases of the LixSn alloys formed upon lithiation process have been investigated using electrochemical techniques in literature for potential LIB applications [[21-23](#_ENREF_21),[20](#_ENREF_20),[24](#_ENREF_24)]. The OCV?? ~~Open circuit voltage~~ and diffusion coefficient of Li ions in these Li-Sn alloys are important parameters if the Sn is to be used as an anode for the LIBs, since larger OCVs represent a larger energy density, and a larger diffusion coefficient indicates that the anode materials can be charged/discharged with a higher rate. Experimental results and theoretical calculation showed that the plateau potentials (*vs* Li/Li+) of the LixSn alloys were in the range of 0.3~0.8 V [[22](#_ENREF_22),[25](#_ENREF_25)]. Diffusion barriers of an isolated lithium atom in the α-Sn and β-Sn were reported to be 0.21 eV and 0.39 eV, respectively [[26](#_ENREF_26)]. The diffusion barrier of Li in Sn also showed a dependence on the Li content, and those for the Li diffusion paths with or without the influence of an adjacent Li ion were calculated to be 0.33 or 0.39 eV, respectively [[27](#_ENREF_27)]. The diffusivity value of the Li+ ion in a nano-crystallized Sn anode prepared using a laser-assisted vapor deposition was measured to be 4.15×10-8 cm2s-1 [[28](#_ENREF_28)]. Whereas the reading for a thin film Sn/Cu6Sn5 anode prepared using an electron-beam evaporation deposition was 1.91×10-7 cm2s-1, which is much higher than those of pure Sn and nano-crystallized Sn because of the significantly reduced crystal sizes of Cu6Sn5 [[6](#_ENREF_6)]. Simulation results from Genser et al. [[27](#_ENREF_27)] showed that the diffusivity values of Li in the LiSn and Li4Sn alloys were 3.7×10-5 cm2s-1 at 765K and 1.21×10-4 cm2s-1 at 1040 K, respectively. Xie et al. [[29](#_ENREF_29)] reported that the Li diffusivity values in the Sn films prepared by radio frequency magnetron sputtering were in a range between 10-16 and 10-14 cm2s-1, which shows a large difference compared with experimental results of other groups discussed above.

Clearly, the previously mentioned simulation work has been focused on diffusion behavior of an isolated Li ion in the Sn anode, but the results cannot predict the lithiation process at higher Li concentrations. Also systematic studies of the Li+ ion diffusion in the LixSn alloys with varied Li concentrations are urgently required in order to fully understand the lithiation process. In this work, a first principle simulation based on density functional theory (DFT) was used to systemically study the OCVs of lithiation/delithiation processes in the LixSn alloys and the diffusivity of Li in the LixSn alloys with varied concentrations of Li from 0.4 to 3.5.

1. **Computational details**

The average voltages of two neighboring elements of LixSn (x=0, 0.4, 1, 2.33, 2.5, 2.6, 3.5) alloys and their diffusion kinetics were calculated using the SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) code [[30](#_ENREF_30)] based on the DFT [[31](#_ENREF_31),[32](#_ENREF_32)]. The exchange-correlation energies were described using a generalized gradient approximation (GGA) with the Perdew-Burke-Emzerhof (PBE) function. Numerical atomic orbits were described using a double zeta basis set. An energy cut-off of 150 Ry was used for the Fourier expansion of the density and the Monkhorst Pack of special *k* points was used for sampling Brillouin zone for the LixSn alloys with different unit cell dimensions as listed in Table 1. Conjugate gradient algorithm was used in geometric relaxations to obtain converged results until the force on every atom was smaller than 0.02 eV/Å. It should be noted that during calculating the average voltage, a dense Brillouin zone sampling was applied to obtain the convergent values.

The average voltage was calculated from the energy difference of two neighboring phases of LixSn alloys by neglecting the volume and entropy effects.

 (1)

where *F* is Faraday constant.

 (2)

where are the cohesive energies of the and the metallic, respectively.

The diffusion kinetics were calculated using *ab* *initio* molecular dynamics (MD) simulations with the canonical (NVT) ensemble [[33](#_ENREF_33)], in which numbers and values of atoms, volume and temperature were kept as constant values. Temperature was controlled using a Nose-Hoover thermostat. A special k-point sampling with 2×2×2 k-grid with the Monkhorst-Pack scheme for the LixSn (x=0.4, 1, 2.33, 2.5, 2.6, 3.5) alloys was used for the Brillouin zone sampling. A denser Brillouin zone sampling of 4×4×4 k-grid was also tested for the LixSn alloy at 1100 K, and results from the mean square displacements (MSDs) with such a denser Brillouin zone sampling were overlapped with those with a k-grid of 2×2×2, indicating that a 2×2×2 k-grid is enough for the *ab initio* MD simulations. In simulation, the LixSn alloys were firstly annealed at 3000 K for 3000 steps with a time step of 1.0 fs, and then rapidly quenched to 300 K with a cooling rate of 1.0 K/fs. The structural evolution of the crystalline structure for the LixSn (x=0.4, 1, 2.33, 2.6, 3.5) alloys after quenching was characterized using a pair-distribution function (PDF)  (, where and are the average number densities of atoms at the distance *r* and the number density of atoms in the LixSn system, respectively. The PDF is a pair correlation representing the probability of finding atoms as a function of distance *r* from an average center atom. The quenched structure was used as a start model and the atom positions were relaxed at temperatures between 700 and 1200 K for 15 *ps* with a time step of 1.0 *fs*. The atom positions were recorded upon the relaxation, and the readings of MSDs for the Li and Sn atoms as a function of time were calculated in order to obtain the diffusion coefficients at different temperatures. The obtained data were then extrapolated to acquire the diffusion coefficients at room temperature according to the Arrhenius equation: [[34](#_ENREF_34)], where is the temperature,  is the diffusion energy barrier and  is the Boltzmann constant.

The diffusion coefficients () from the MD simulation is dependent on the Einstein relation:

 (3)

where  is diffusion time of atom .  is initial position of the  atom and  is the position of the  atom at , respectively. The item of  represents the MSDs.

1. **Results and discussions**

The OCV is an important parameter which can be used to characterize how large the driving forces to attain an equilibrium between the cathode and anode once they are connected. A larger value of the OCV is preferred for high power-consuming devices [[35](#_ENREF_35)]. The OCV of a lithium cell is determined by the difference of Li chemical potentials between the cathode and anode materials [[36](#_ENREF_36)]. The average voltages of two neighboring Li*x*Sn alloy phases calculated using equation (1) are shown in Fig. 1 along with two experimentally obtained charge/discharge curves from references of [[25](#_ENREF_25),[37](#_ENREF_37)]. The calculated curves agree well with the experimental ones. As *x* value of the Li*x*Sn alloy is smaller than 1.0, a higher average voltage was obtained. Whereas as *x* is in the range between 1.0 and 2.6, a voltage plateau appears. When *x* is increased to a value large than 2.6, the average voltages are reduced suddenly and much less than those of Li-deficient Li-Sn alloys.

The diffusivity of Li in the LixSn is an important parameter which can reveal if Sn can be efficiently used in high-power applications. The experimental results showed that the diffusivity values of Li in the LixSn at room temperature are in a wide range between 8×10-16 and 5.9×10-7 cm2 s-1 [[6](#_ENREF_6),[23](#_ENREF_23),[38](#_ENREF_38),[24](#_ENREF_24),[19](#_ENREF_19)]. The diffusivity of the Li in the LixSn (x=0.4, 1, 2.6, 3.5) was studied using *ab initio* MD. The PDF values characterizing the structural evolution of the LixSn (x=0.4, 1, 2.6, 3.5) alloys in both crystalline structure and after melting/quenching at 300 K are shown in Fig. 2. In Fig. 2, the data from left to right in a sequence represent the PDFs of Li2Sn5, LiSn, Li13Sn5 and Li7Sn2; and those from top to bottom represent the PDFs of Li-Li, Sn-Sn, Li-Sn and LixSn alloys; whereas the sharp curves and smooth curves represent the PDF values of the crystalline LixSn and the LixSn after quenching, respectively. Sharp peaks can be clearly observed for the crystalline LixSn alloys, and that at 3.16 Å in the crystalline Li2Sn5 for Li-Li bonds represents the nearest neighbors of Li-Li. After the samples were annealed at 3000 K and quenched to 300 K, the sharp peaks disappear except for the first one. This indicates that the long-range order disappears, and the crystalline LixSn (x=0.4, 1, 2.6, 3.5) alloys were transformed into amorphous phases.

The positions r*i*(*t*) of all atoms as a function of time *t* were recorded for all the amorphous phases as they became relaxed at a given temperature. The MSDs of Li in amorphous LixSn (x=0.4, 1.0, 2.6, 3.5) alloys as function of time are shown in Fig. 3. For all the alloys, the slope of the MSDs increases with increasing the simulation temperature, which demonstrates that the Li diffuses much faster at a higher temperature. The diffusion coefficients calculated using equation (4) are plotted in Fig. 4 (a). Those of the Li in the LixSn at room temperature were then extrapolated using the Arrhenius equation based on the data obtained at high temperatures, and obtained results are 5.6×10-7, 3.3×10-7, 6.6×10-8 and 5.1×10-7 for the LixSn alloys with x=0.4, 1.0, 2.6 and 3.5, respectively. The obtained diffusion coefficients as a function of Li content are shown in Fig. 4 (b), along with the reported experimental results. Our calculated results are within the range between 8.0×10-8 cm2s-1 to 5.9×10-7 cm2s-1 obtained from the previous experimental work [[6](#_ENREF_6),[23](#_ENREF_23),[38](#_ENREF_38),[24](#_ENREF_24),[19](#_ENREF_19)].

1. **Conclusions**

A systematic study of the Li+ ion diffusion behavior in the LixSn alloys with varied Li concentrations was performed in order to fully understand the lithiation process of Sn for the Li ion batteries. The average voltages and diffusion coefficients of the Li in the LixSn alloys were calculated using the density functional theory. The variation trends of the calculated average voltages agreed well with those from the experimental observations. The diffusion coefficients of Li in LixSn were calculated to be in the range between 6.6×10-8 cm2s-1 to 5.6×10-7 cm2s-1 at room temperature, and these agreed with the experimental measurement results.

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**Compliance with Ethical Standards:**

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**Conflict of Interest**: The authors declare that they have no conflict of interest.

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Table 1 The average voltage of the LixSn alloys between two neighboring phases.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| # | Δx | Space group | K points | U/V |
| Li | - | Im3m | 11×11×11 | - |
| Sn | 0.00 | I4/amd | 11×11×11 | - |
| Li2Sn5 | 0.40 | P4/mbm | 5×5×11 | 0.9925 |
| LiSn | 0.60 | P2/m | 11×11×5 | 0.7585 |
| Li7Sn3 | 1.33 | P21/m | 9×11×9 | 0.4839 |
| Li5Sn2 | 0.17 | R-3m | 11×11×2 | 0.4905 |
| Li13Sn5 | 0.10 | P-3m1 | 11×11×2 | 0.5383 |
| Li7Sn2 | 0.90 | Cmmm | 5×3×11 | 0.1792 |

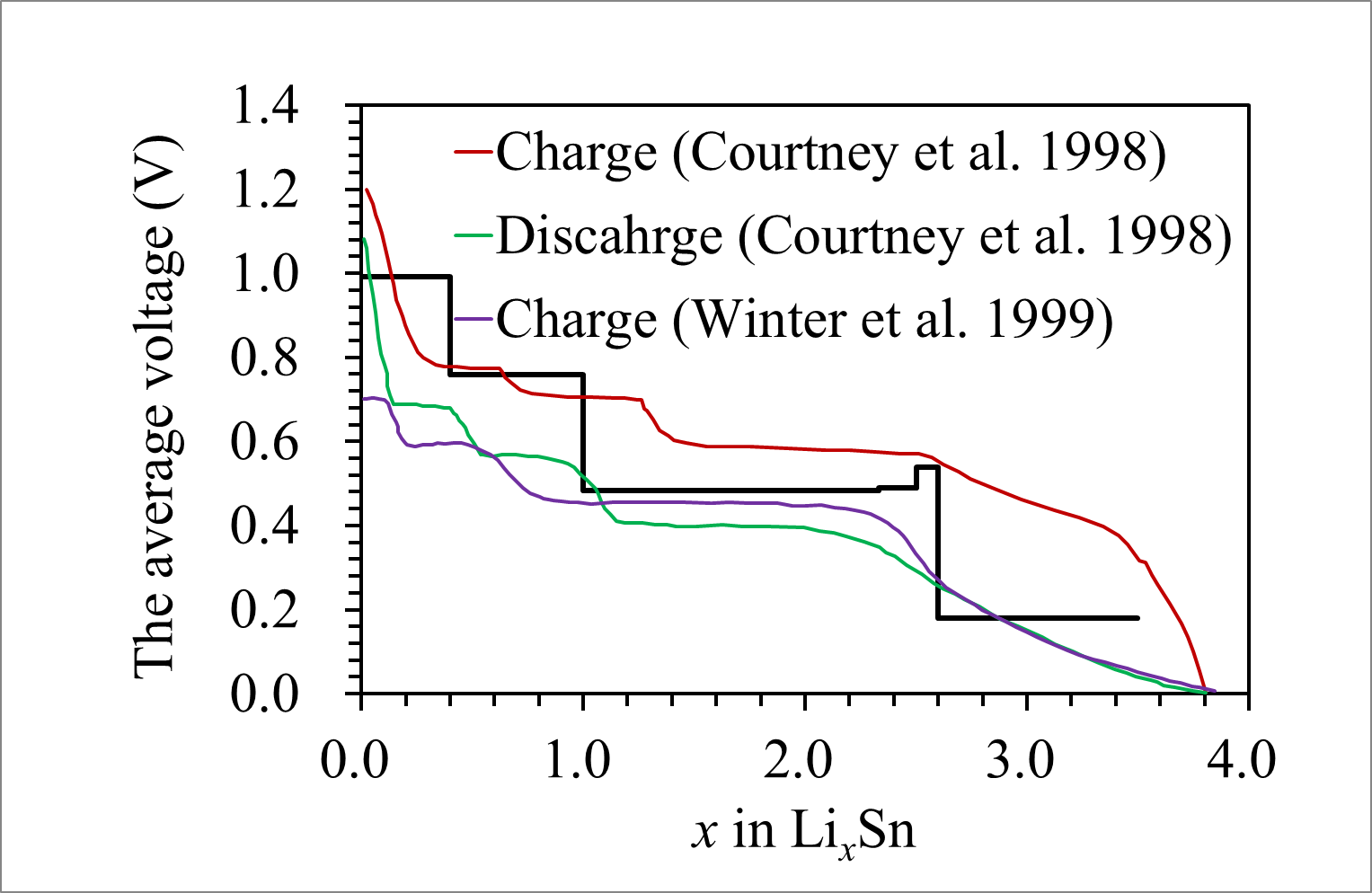
Lists of figure captions:

Figure 1 The average voltage of LixSn alloys between two neighboring phases.

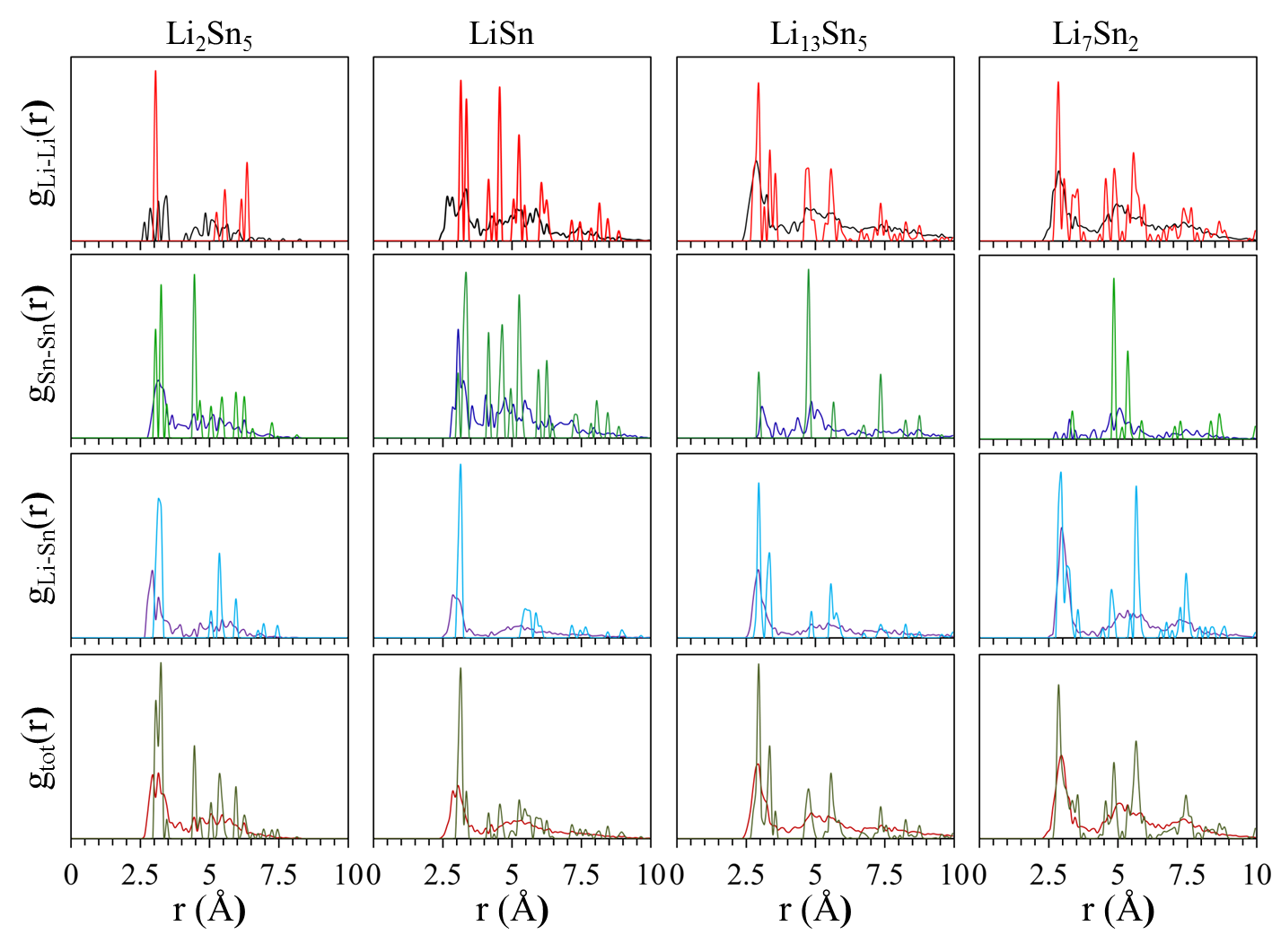
Figure 2 Total and partial pair distribution functions for LixSn (x=0.4, 1.0, 2.6, 3.5) alloys, where the sharp and smooth lines represent the PDF of the crystal LixSn and the quenched LixSn, respectively.

Figure 3 MSD of Li as a function of simulation time in LixSn alloys with (a) x=0.4, (b) x=1.0, (c) x=2.6, and (d) x=3.5.

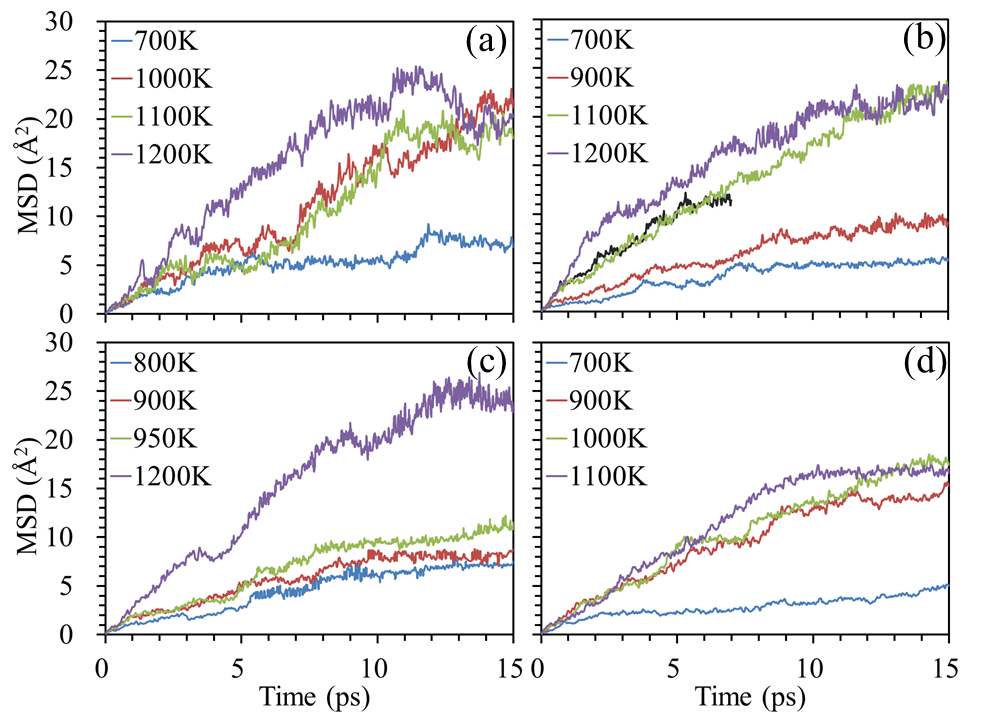
Figure 4 (a) Diffusion coefficients of Li in LixSn alloys as a function of the inverse of temperature. The value of diffusivity at 300K is extrapolated using an exponential fit. (b) The diffusion coefficients of Liin LixSn alloys as function of lithium content.



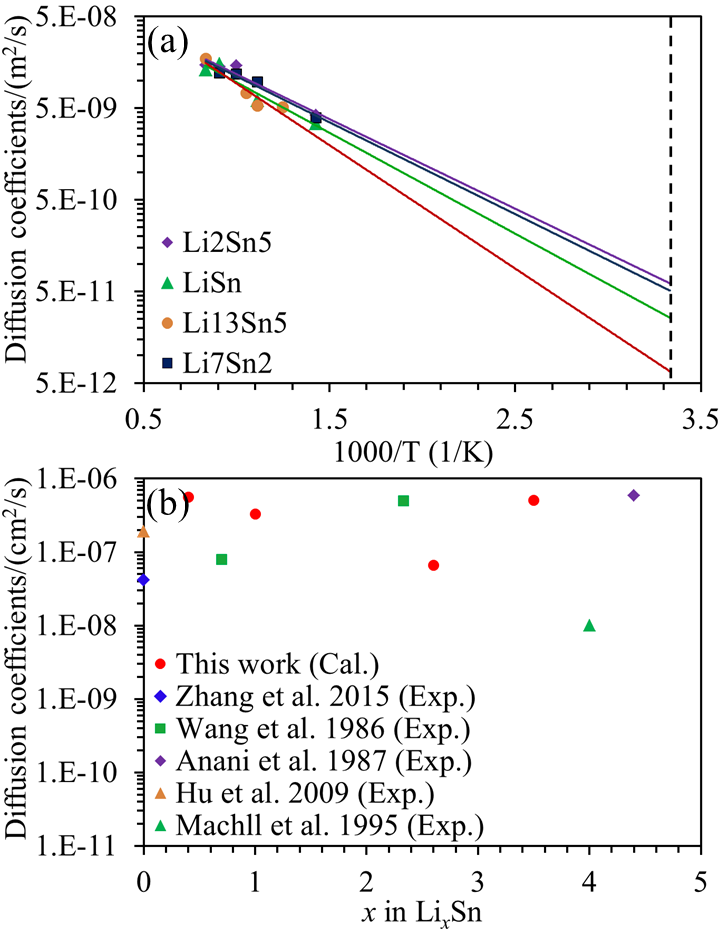
J.J. Shi et al. Figure 1



J.J. Shi et al. Figure 2



J.J. Shi et al. Figure 3



J.J. Shi et al. Figure 4