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Asphericity in the Fermi surface and Fermi energy of $Li_{1-x}B_x$ (B = Na, K, Rb and Cs) substitutional alloys

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Abstract

A detailed investigation into asphericity in the Fermi surface (FS) and Fermi energy (FE) of $Li_{1-x}B_x$ (B = Na, K, Rb and Cs) substitutional alloys are reported for the first time. The FE computed under pseudo-alloy-atom (PAA) model consideration is found higher than the FE computed under phase mixture (Mix) consideration. The non-linear relation for $E_F(x) = a_0 + a_1x + a_2x^2$ is predicted for all the substantial binaries. The exchange and correlation effects are found to suppress the value of FE. The alloying behavior of Na, K, Rb and Cs with Li generates the asphericity in the FS like bcc metals. For $Li_{1-x}B_x$, the asphericity in the FS of the binary decreases with increase in x, except $Li_{1-x}Cs_x$. In $Li_{1-x}Cs_x$, the asphericity in the FS of the binary increases with increase in x. The $Li_{1-x}Cs_x$ solid solution shows maximum Fermi surface distortion (FSD) in comparison to $Li_{1-x}B_x$ (B = Na, K and Rb) systems. Present study also concludes that the impact of local-field correction function on the asphericity in the FS is maximum at [1 0 0] point and minimum at [1 1 1] point. Among the high symmetry directions, the maximum asphericity in the FS is obtained at [1 1 0] point.

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Keywords: Fermi surface; Fermi energy; Lithium based binary alloys; Pseudopotential; Exchange and correlation effects

1. Introduction

Lithium, the lightest metal with a simple electronic configuration and a broad range of practical applications, has naturally been the subject of both the theoretical and experimental investigations [1]. In contrast to other alkali metals, it has no p-electrons in the core. Hence it becomes interesting to see the alloying behaviour of other alkali metals with lithium. On alloying the alkali metals into other alkali metals, the atomic matrix elements in the pure state are affected by lattice distortion and charging effects [2,3]. So it is an interesting field of studying the shape of the Fermi surface (FS) in the $Li_{1-x}B_x$ (B = Na, K, Rb and Cs) substitutional solid solutions. The Fermi surface distortion (FSD) among the pure alkali metals increases as one move from Na to Cs. So detailed study of the asphericity in the FS of $Li_{1-x}B_x$ will provide the understanding of alloying with respect to concentration x of other alkalis in lithium. Various studies on the Li–Na, Li–Mg and Li–Al alloys are reported in the literature [4–8] but not a single report is found on Fermi energy (FE) and FSD of $Li_{1-x}B_x$ (B = Na, K, Rb and Cs). Hence in the present work, we have focused our interest on the $Li_{1-x}B_x$ solid solutions and studied the asphericity in the FS and FE. The second order perturbation theory and PAA model potential are used to compute FE and FSD [2,3,9–14].

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2. Method of computation

In the second-order perturbation theory, using pseudo-alloy-atom model, the Fermi energy E_F is computed by the relation [2,3,9–11]

$$E_F(\mathrm{PAA}) = \frac{\hbar^2}{2m}(k_F^0)^2 - \frac{m}{2\hbar^2 k_F^0}\sum_{q\neq 0}\frac{|V_{\mathrm{PAA}}(q)|^2}{q}\ln\left|\frac{2k_F^0+q}{2k_F^0-q}\right| \quad (1)$$

Table 1
Constants and parameters used in the present work

Metal	Z	r_s (Å)	Lattice constants a (Å)	k_F (Å^{-1})	Ω_0 (Å^3)	r_c (Å)	ρ (gm/cm^3)	Atomic mass M (10^{-24} g)
Li	1	1.8717	3.8010	1.0253	27.4707	0.7696	0.5406	11.608
Na	1	2.0801	4.2242	0.9226	37.7108	1.0706	1.0196	38.453
K	1	2.5728	5.2240	0.7488	71.3319	1.3954	0.9176	65.46
Rb	1	2.7500	5.5839	0.6979	87.1127	1.3869	1.7883	142.96
Cs	1	2.9766	6.0438	0.6448	110.4653	1.9000	2.0124	222.307

Table 2
Fermi energy ($-E_F$ in 10^{-12} erg) for Li based binary alloys

x	$-E_F$ in (10^{-12} erg) using different local-field correction functions									
	H		T		IU		F		S	
	PAA	Mix	PAA	Mix	PAA	Mix	PAA	Mix	PAA	Mix
$Li_{1-x}Na_x$										
0.1	6.2232	6.3311	5.7997	5.9127	5.9822	6.0925	5.9847	6.0948	6.0470	6.1572
0.2	6.0082	6.1784	5.6247	5.7982	5.7916	5.9626	5.7936	5.9644	5.8490	6.0208
0.3	5.8267	6.0257	5.4870	5.6837	5.6364	5.8326	5.6380	5.8339	5.6861	5.8844
0.4	5.6695	5.8730	5.3750	5.5693	5.5063	5.7026	5.5073	5.7035	5.5482	5.7480
0.5	5.5298	5.7203	5.2800	5.4548	5.3933	5.5726	5.3936	5.5731	5.4276	5.6116
0.6	5.4027	5.5675	5.1956	5.3403	5.2914	5.4427	5.2912	5.4426	5.3187	5.4752
0.7	5.2842	5.4148	5.1167	5.2258	5.1963	5.3127	5.1955	5.3122	5.2172	5.3388
0.8	5.1717	5.2621	5.0399	5.1113	5.1046	5.1827	5.1033	5.1817	5.1199	5.2024
0.9	5.0630	5.1094	4.9624	4.9969	5.0140	5.0528	5.0123	5.0513	5.0246	5.0660
$Li_{1-x}K_x$										
0.1	5.6574	6.1452	5.2386	5.7194	5.4208	5.9029	5.4238	5.9052	5.4844	5.9683
0.2	5.0781	5.8065	4.7031	5.4116	4.8692	5.5833	4.8718	5.5851	4.9243	5.6429
0.3	4.6420	5.4678	4.3093	5.1038	4.4595	5.2637	4.4616	5.2650	4.5066	5.3175
0.4	4.2972	5.1291	4.0028	4.7960	4.1384	4.9441	4.1397	4.9450	4.1782	4.9922
0.5	4.0146	4.7904	3.7541	4.4882	3.8765	4.6246	3.8771	4.6249	3.9100	4.6668
0.6	3.7768	4.4517	3.5458	4.1804	3.6566	4.3050	3.6566	4.3048	3.6847	4.3415
0.7	3.5726	4.1130	3.3672	3.8729	3.4679	3.9854	3.4672	3.9847	3.4914	4.0161
0.8	3.3946	3.7744	3.2112	3.5648	3.3031	3.6658	3.3018	3.6646	3.3226	3.6908
0.9	3.2373	3.4357	3.0731	3.2571	3.1572	3.3462	3.1555	3.3445	3.1734	3.3654
$Li_{1-x}Rb_x$										
0.1	5.4445	6.1047	5.0345	5.6791	5.2137	5.8628	5.2170	5.8650	5.2759	5.9280
0.2	4.7710	5.7256	4.4123	5.3311	4.5728	5.5030	4.5756	5.5048	4.6252	5.5623
0.3	4.2872	5.3464	3.9746	4.9830	4.1178	5.1433	4.1200	5.1445	4.1614	5.1967
0.4	3.9162	4.9673	3.6427	4.6349	3.7711	4.7835	3.7724	4.7843	3.8072	4.8311
0.5	3.6190	4.5882	3.3780	4.2869	3.4938	4.4238	3.4944	4.4240	3.5238	4.4654
0.6	3.3734	4.2090	3.1591	3.9388	3.2645	4.0640	3.2644	4.0638	3.2895	4.0998
0.7	3.1656	3.8299	2.9735	3.5908	3.0702	3.7043	3.0694	3.7035	3.0910	3.7342
0.8	2.9867	3.4508	2.8129	3.2427	2.9024	3.3445	2.9011	3.3432	2.9198	3.3685
0.9	2.8305	3.0716	2.6719	2.8946	2.7554	2.9848	2.7535	2.9830	2.7700	3.0029
$Li_{1-x}Cs_x$										
0.1	5.1089	6.0307	4.6805	5.5723	4.8684	5.7716	4.8723	5.7743	4.9336	5.8403
0.2	4.2851	5.5776	3.8803	5.1175	4.0620	5.3207	4.0662	5.3233	4.1215	5.3869
0.3	3.7185	5.1245	3.3269	4.6626	3.5062	4.8699	3.5103	4.8722	3.5616	4.9336
0.4	3.2961	4.6714	2.9088	4.2078	3.0891	4.4190	3.0930	4.4212	3.1416	4.4802
0.5	2.9642	4.2183	2.5740	3.7529	2.7583	3.9681	2.7619	3.9702	2.8088	4.0269
0.6	2.6936	3.7652	2.2947	3.2981	2.4855	3.5172	2.4887	3.5192	2.5346	3.5736
0.7	2.4667	3.3121	2.0544	2.8432	2.2537	3.0663	2.2566	3.0682	2.3019	3.1202
0.8	2.2722	2.8590	1.8426	2.3884	2.0522	2.6155	2.0547	2.6172	2.0998	2.6669
0.9	2.1027	2.4059	1.6523	1.9335	1.8739	2.1646	1.8759	2.1662	1.9210	2.2135