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Asphericity in the Fermi Surface of d and f-Shell Metals

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Abstract

Recently proposed pseudopotential has been used to calculate asphericity in the Fermi surface of d and f-shell metals along the three symmetry directions [100], [110] and [111]. The parameter of the potential has been determined by zero pressure condition and the exchange and correlation function due to Taylor has been incorporated. The present results are in good agreement with experimental findings for Cu, Ag, Au and Pd; while for other d and f- shell metals we could not found sufficient theoretical as well as experimental data for the asphericity in the Fermi Surface in order to workout a quantitative comparison. It, therefore, seems difficult to give concrete remark about the present results. We conclude that the calculations of asphericity in the Fermi Surface based on pseudopotential theory can be regarded as a sensitive test for the proper assessment of the pseudopotential form factor. A successful application to the asphericity in the Fermi Surface confirms the ability of model potential for predicting wide range of physical properties of transition metals.

Key Words: Pseudopotential, Asphericity in the Fermi Surface, exchange and correlation effects.
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1. Introduction

The Fermi Surface (FS) of a pure metal show a small but definite departure from a free electron sphere and the study of its asphericity thus provides a direct test of band theory predictions. Several electronic properties of metals are determined from variation in the shape of the FS. The FS concept enables one to visualize the relative fullness or occupation of the allowed empty lattice band geometrically in **q**-space (wave-number space). Such Fermi surface concepts help in the theoretical determination of the electronic properties of a solid, as a metal, semiconductor or insulator. In fact, the purpose of the FS construction is to know about the detail of the motion of an itinerant electron in three dimensions.

In our previous work [1, 2], a simple model potential for transition metal was proposed in which a single parameter was obtained through the zero-pressure condition. This model was successfully exploited for the calculation of a large number of physical properties of some d and f-shell metals. The results were in reasonable agreement with experiment and also show consistent improvement with other theoretical findings. We have also explored the same potential [1, 2] for the thermodynamic calculations [3] of liquid d and f-shell metals, successfully. This confirms the ability and strength of our model potential for the investigation of wide class of various properties in the d and f-shell metals. In the present paper we have calculated asphericity of FS to testify the ability of proposed potential.

2. Theory

The FS is a surface of Fermi-energy E_F in wave-number space and is defined by

$$\varepsilon(k) = E_F. \tag{1}$$

The FS provides us all the electron states that can play any part in the ordinary transport properties of the metal. For a metal at absolute zero temperature, all the states inside the FS are filled while those outside are empty. Thus the FS is a mathematical construction related to the dynamical properties of the conduction electrons in a metal. In a free electron gas the FS is a sphere.

It is a well-established fact that the FS of a real metal shows a small but definite departure from the perfectly spherical shape of the free electron gas. The asphericity of the FS provides us a sensitive test of certain results derived from electronic energy bands. Several electronic properties of metals are determined from variation in the shape of the FS.

The distortion in the spherical shape of the free electronic Fermi surface is the case of simple metals [4] and noble metals [5] may be given by the expression [4, 5]

$$k_F \; = \; k_F^0 \; \left[\, 1 \; + \; \Delta \, (\theta_{kq}) \, \right] \tag{2}$$

Here, $\Delta(\theta_{kq})$ is the dilation to the free electron Fermi wave number, k_F^0 and θ_{kq} are the angle between direction k and reciprocal lattice vector q. The Fermi energy E_F on the basis of perturbation approach up to the second order may be written as [4, 5]

$$E_F \; = \; \frac{\hbar^2}{2\,m} \, (\, k_F^0 \,)^2 \; - \; \sum_{q \; pairs} C \, (\, q \,) \;\; W^2 \, (\, q \,) \tag{3}$$

where $W(q)$ is the screened ion pseudopotential form factor [1, 2]. The function $C(q)$ is given as [4, 5]

$$C \, (\, q \,) \; = \; \frac{m}{2 \, \hbar^2 \; k_F^0 \, q} \; ln \; \left| \; \frac{2 \, k_F^0 \; + \; q}{2 \, k_F^0 \; - \; q} \; \right| \tag{4}$$

This function is estimated from the conclusion that the distortion should not alter the volume element enclosed by the FS.

The expression representing the distortion in the FS from the spherical shape, after neglecting higher powers of $\Delta\ (\theta_{kq})$ is given as [4, 5]

$$\Delta k = \frac{\Delta k_F}{k_F^0} = \sum_{q-pairs} \frac{W^2(q)}{E_F^0} \left[\frac{1}{\frac{\hbar^2}{2m} q^2 - 4 E_F^0 cos^2 \theta_{kq}} - C(q) \right] \tag{5}$$

where E_F^0 is the free electron Fermi energy. Another method for computing the distortion in the FS has been suggested by Wallace [6]. Both the methods are found to give similar results.

3. Results and Discussion

The equations (1)–(5) were used to study the asphericity of the FS for some fcc metals: Cu, Ag, Au, Au, Ni, Pd, Pt, Rh, Ir, La, Yb, Ce and Th. The variation of FS from free electron sphere at major symmetry direction are shown in Figures 1, 2 and 3 and numerical values at major symmetry points are shown in Tables 1, 2 and 3. The Fermi surface of Cu as obtained presently is fairly spherical one with the experimental findings [7] while for Ag and Au our result differs from the experimental observations at necks and belly [7], particularly at L point we get quit reasonable distortion of FS and for Pd our results are extremely good with the experimental findings of Vuillemin [8]. Since experimental as well as theoretical results for rest of the metals are not available, it seems difficult to give concrete remark about the present results.

Table 1. Distortion of Fermi surface at some symmetry points.

Symmetry points	Cu (k_F^0=0.82568)			Ag (k_F^0=0.72739)		
	k_F	$\Delta k_F = k_F - k_F^0$ $in 10^{-2}$	$\frac{\Delta k_F}{k_F^0}\%$	k_F	$\Delta k_F = k_F - k_F^0$ $in 10^{-2}$	$\frac{\Delta k_F}{k_F^0}\%$
X	0.824298	-0.1382	0.1674	0.729814	0.2421	0.3328
W	0.825481	-0.0198	0.0204	0.727479	0.0086	0.0118
K	0.826442	0.0762	0.0922	0.727048	-0.0344	0.0473
L	0.810662	-1.5018	1.8188	0.719280	-0.8112	1.1152
U	0.825289	-0.0390	0.0473	0.728215	0.0822	0.1130
Symmetry points	Au (k_F^0=0.802458)			Ni (k_F^0=0.845042)		
	k_F	$\Delta k_F = k_F - k_F^0$ $in 10^{-2}$	$\frac{\Delta k_F}{k_F^0}\%$	k_F	$\Delta k_F = k_F - k_F^0$ $in 10^{-2}$	$\frac{\Delta k_F}{k_F^0}\%$
X	0.888305	8.5847	10.6980	0.842787	-0.2254	0.2668
W	0.808427	0.5969	0.7438	0.844707	-0.0335	0.0396
K	0.810039	0.7581	0.9447	0.846310	0.1268	0.1500
L	0.787359	-1.5098	1.8815	0.819199	-2.5842	3.0581
U	0.816984	1.4526	1.8102	0.844413	-0.0628	0.0744

Table 2. Distortion of Fermi surface at some symmetry points.

Symmetry points	Pd (k_F^0=0.764753)			Pt (k_F^0=0.758938)		
	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$
X	0.75828	0.1075	0.1405	0.760251	0.1312	0.1730
W	0.764816	0.0063	0.0082	0.759014	0.0075	0.0100
K	0.764523	-0.0230	0.0300	0.758656	-0.0282	0.0371
L	0.764367	-0.386	0.504	0.0758348	-0.0589	0.0777
U	0.765101	0.0348	0.0455	0.759365	0.0427	0.0562
Symmetry points	Rh (k_F^0=0.782769)			Ir (k_F^0=0.774764)		
	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$
X	0.783137	0.0368	0.0470	0.77542	0.0677	0.0874
W	0.782779	0.0009	0.0012	0.774800	0.0035	0.0045
K	0.782748	-0.0021	0.0027	0.774642	-0.0122	0.0157
L	0.780993	-0.1776	0.2269	0.773931	-0.0833	0.1075
U	0.782893	0.0123	0.0157	0.774985	0.0220	0.0284

Table 3. Distortion of Fermi surface at some symmetry points.

Symmetry points	La (k_F^0=0.616929)			Yb (k_F^0=0.642779)		
	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$
X	1.060212	44.3283	71.85	1.027200	38.4421	59.80
W	0.707785	9.0856	14.72	0.718074	7.5294	11.71
K	0.768008	15.1078	24.48	0.767267	12.4487	19.36
L	0.496287	-12.064	19.55	0.540643	-10.213	15.88
U	0.754804	13.7874	22.34	0.758689	11.5909	18.03
Symmetry points	Ce (k_F^0=0.634156)			Th (k_F^0=0.643820)		
	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$	k_F	$\Delta\, k_F = k_F - k_F^0$ $in10^{-2}$	$\frac{\Delta\, k_F}{k_F^0}\%$
X	1.007722	37.3565	58.90	0.957711	31.3890	48.75
W	0.703568	6.9412	10.94	0.695561	5.1740	8.03
K	0.748112	11.3955	17.96	0.727283	8.3462	12.96
L	0.537575	-9.6581	15.22	0.567347	-7.6472	11.87
U	0.74865	10.8708	17.14	0.728276	8.4456	13.11

4. Conclusion

It is interesting to point out here that in spite of relative simple application of pseudopotential formulation in the study of metallic properties, there have been limited attempts to calculate asphericity of FS of different metals. Usually, the asphericity calculated using certain crystal potential may be very close to the experimental

results in one direction only, but not in the other two directions. Therefore, testing of various pseudopotentials proposed so far with the same approximation in the asphericity in FS of metals might give additional information.

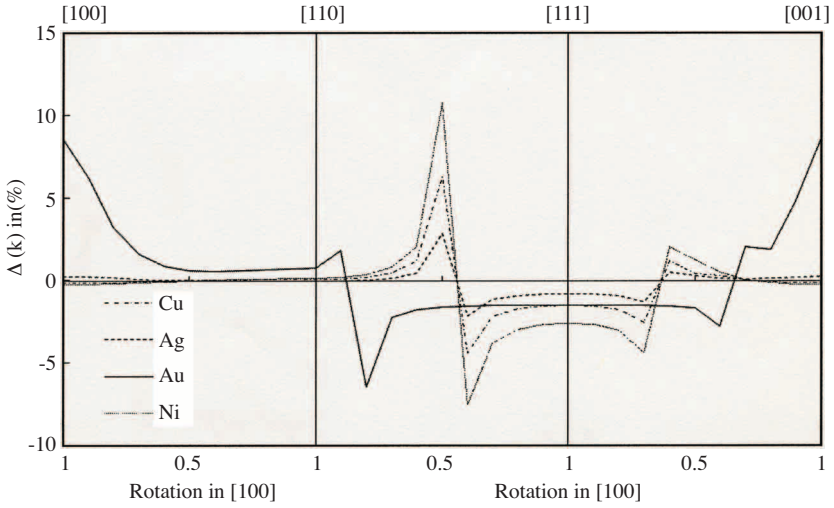

Figure 1. Asphericity in the Fermi Surface of Cu, Ag, Au and Ni.

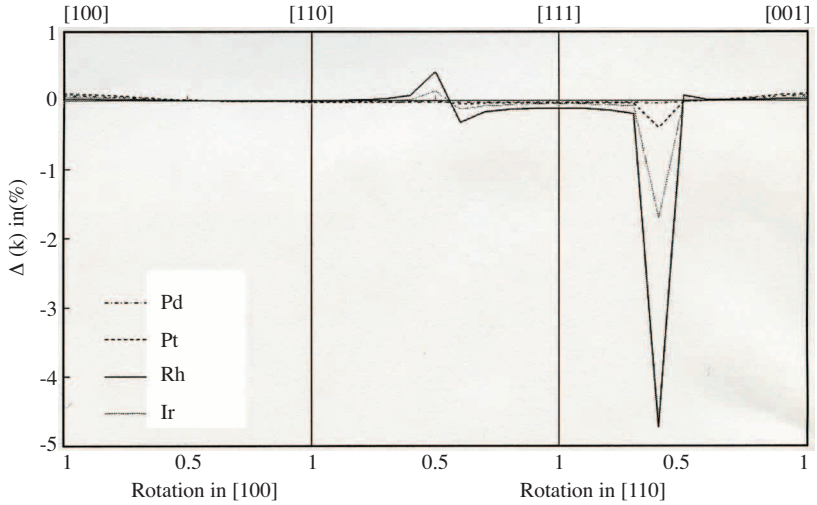

Figure 2. Asphericity in the Fermi Surface of Pd, Pt, Rh and Ir.

We conclude that the calculations of asphericity in FS based on pseudopotential theory can be regarded as a sensitive test for the proper assessment of the pseudopotential form factor. A successful application to the asphericity in the FS confirms the ability of model potential for predicting wide range of physical properties of simple, non-simple, transition and Lanthanide metals in solid [1, 2] as well as in the liquid phase [3].

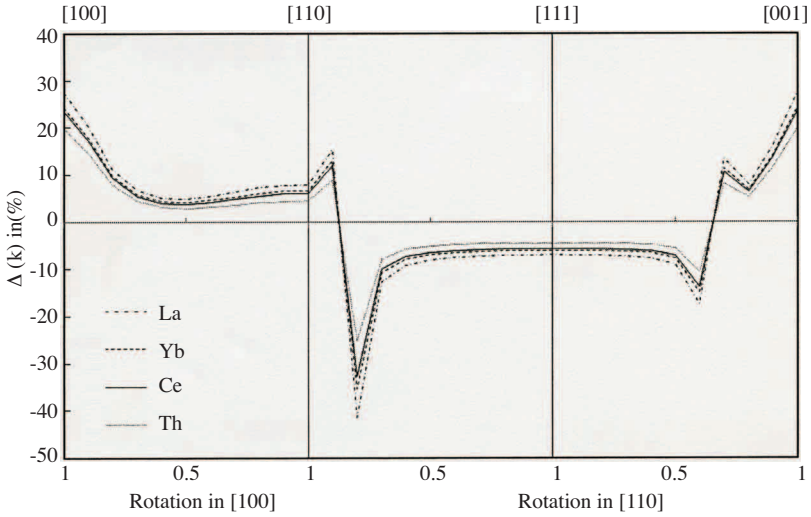

Figure 3. Asphericity in the Fermi Surface of La, Yb, Ce and Th.

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