

Fermi Surface Distortion of Transition Metals using Pseudopotential

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(Received December 22, 2011)

Abstract: Recently, we have proposed transition metal pseudopotential which is found to be good working in predicting almost all the lattice mechanical properties. In the present communication using present pseudopotential we have examined Fermi surface distortion of noble metals. Our results are well compared with recently published theoretical results. Present study confirms the use of pseudopotential in examining electronic properties of transition metals.

Keywords: Transition metals, Pseudopotential, Fermi surface distortion.

1. Introduction

The Fermi surface is a surface of Fermi energy in the wave number space. The Fermi surface (FS) concept enables us to visualize the relative fullness or occupation of the allowed empty lattice band geometry in K-space (wave-number space). The concept of FS helps in the theoretical determination of the electronic properties of a solid; it may be a metal, semiconductor or insulator. In fact, the purpose of the FS construction is to know about the details of the motion of an itinerant electron in three dimensions.

Transition metals have attracted continuous attention of physicist and chemists because of their unusual electronic and structural properties. These have their origin in the determinant influence of d-electrons on the electronic structure. In noble metals, narrow d-bands are filled and lie below

the Fermi energy. This group of metals often exhibits pronounced phonon anomalies as a result of complex FS geometries in conjunction with strong electron phonon coupling, whose consistent description still provides a challenge for theoretical approaches. For transition metals, one has to consider the fact that the tightly bound d-electrons hybridize with the nearly free electron resulting in a partially filled d-bands, crossing the Fermi energy. The melting temperature study shows that in case of noble metals d-bands are not seriously affected in melting. The applicability of local model pseudopotential to d-band metals is along standing problem and it still remains a problem of interest. For transition metals, unlike what happens for simple metals, there are not yet a large number of local model potentials which could account for a broad spectrum of properties of metals. In the present communication, we have used our pseudopotential¹ to calculate asphericity of FS of noble metals along the three symmetry directions

The paper is organized as follows. Section-2 Sketches all theories which are relevant to calculate FS distortion and pseudopotential. Results with necessary discussions are presented in section-3.

2. Theory

We construct the transition metal pseudopotential and arrive at the following form¹:

$$(2.1) \quad V_{ion}(q) = \frac{1}{\Omega_0} \left[-\frac{8\pi z^*}{q^2} \cos qR_c + \frac{\beta}{[1 + (qR_d)^2]^4} \right].$$

The pseudopotential has three parameters: (1) core radius- R_c (2) R_d and (3) β . The core radius was computed using relation $R_c = 0.51R_a Z^{*-1/3}$. R_d was taken equal to R_a -radius of Wigner seitz sphere. The remaining parameters α_β and γ_β appearing in Born-Mayer term $[\alpha_\beta \exp(-\gamma_\beta R)]$ and parameter β in equation (2.1) were fixed from zero pressure condition and overall fit with the experimental phonon dispersion curves. The computed parameters are shown in Table-1. Using present pseudopotential we have computed a large number of lattice mechanical properties for Cu, Ag, Au, Pd, Pt and Ni¹. It should be noted that comprehensive unified studies of several metals with pseudopotential theory are surprisingly rare²⁻⁴. A simple model that correlates a wide spread of properties for many metals is highly desirable. The distortion in spherical (free electron) Fermi surface can be studied using following two methods^{5,6}.

According to Schneider and Stall ⁵ the wave vector k_F can be defined as

$$(2.2) \quad k_F = k_{F^0} [1 + \Delta(\theta)],$$

where, θ is the angle between k_F and Q and k_{F^0} is the free electron Fermi wave number. Using second order perturbation theory and expanding k_F in the powers of $\Delta(\theta)$, they obtained following expressions for the change in k_F .

$$(2.3) \quad \frac{\Delta k_F}{k_{F^0}} = \sum_{pairs} Q \frac{|V(Q)|^2}{E_{F^0}} \left[\frac{1}{\frac{\hbar^2 Q^2}{2m} - 4 E_{F^0} \cos^2 \theta_{KQ}} - C(Q) \right],$$

where

$$(2.4) \quad C(Q) = \frac{m}{2\hbar^2 k_{F^0} Q} \ln \left| \frac{Q + 2k_F}{Q - 2k_F} \right|.$$

The function $C(Q)$ is estimated from the conclusion that distortion should not alter the volume element enclosed by the FS.

The Fermi energy is determined by requiring that the total number of conduction electrons is equal to the number of electrons is equal to the number of electron states with energy equal to or less than the Fermi energy. Using this fact, Wallace ⁶ has obtained an expression for Fermi vector k_F in second order in pseudopotential.

$$(2.5) \quad |k_F| = k_{F^0} - \frac{m}{\hbar^2 k_{F^0}} \sum_Q |V(Q)|^2 \left[\frac{1}{(E_{k_{K^0}} - E_{k_{F^0}} + Q)} + \frac{m}{2\hbar^2 Q k_{F^0}} \ln \left| \frac{Q + 2k_F}{Q - 2k_F} \right| \right],$$

where k_{F^0} is zeroth-order value of Fermi-vector. The dependence of $|k_F|$ on the direction of $\vec{k}_F$ is contained in the dependence of the right hand side on the direction of $\vec{k}_{F^0}$, through the energy denominators. The result of equation (2.5) is most interesting. It gives the FS correct to second order, in the pseudopotential, for arbitrary positions of the ions and hence can be used to calculate the fluctuations in the FS due to motion of ions⁶. The Fermi vectors $\vec{k}_F$ and $\vec{k}_{F^0}$ lie in the same direction since both these approaches are

equivalent, the numerical results obtained from using equations (2.3) and (2.5) are identical. In the present work, we have verified this fact.

3. Results and Discussions

The variation of Fermi surface from free electron-sphere at major symmetry points as calculated presently has been shown in Table-2. The Fermi surface of Cu as obtained presently is fairly spherical one. This result is in agreement with theoretical results ⁷ and differs from the experimental observations ⁸. It is also interesting to compare our results with theoretical results for Ag and Au ⁷ who observed reasonable distortion of Fermi surface at L point. It is observed that there have been limited attempts to calculate asphericity of FS of noble metals using pseudopotential. The asphericity calculations are carried out using crystal potential may be very close to the experimental results in one direction only, but not in the other two directions. In such case calculation of FS using pseudopotential can be regard as a sensitive test of the pseudopotential form factor. As far as pseudopotential calculations are concerned, it appears that the study of FS distortion still remains an interesting problem. An accurate clue might give a definite relation between the radial distortion of a nearly spherical surface and the fourier component of the effective lattice potential. Finally, we concluded that the presently used model is capable for studying static, dynamic and electronic properties of transition metals.

Table.1: Pseudopotential Parameters for Noble Metals (In Atomic Units)

Metal	Pseudopotential parameters		Born-Mayer Parameters		Vashistha-Singwi parameters	
	R_c	β	α_β	γ_β	A	B
Cu	1.2834	-6.468	125.0	2.151	0.9344	0.3082
Ag	1.4346	-4.061	94.0	1.89	0.9803	0.3042
Au	1.4683	-3.2258	136.0	1.80	0.9795	0.3043

Table 2: Distortion of Fermi Surface at Some Symmetry Points for Noble Metals

Symmetry points	$Cu(k_{F^0} = 0.7626)$			$Ag(k_{F^0} = 0.6895)$			$Au(k_{F^0} = 0.6950)$		
	k_F	Δk_F (10^{-2})	$\frac{\Delta k_F}{k_{F^0}} \times 100$	k_F	Δk_F (10^{-2})	$\frac{\Delta k_F}{k_{F^0}} \times 100$	k_F	$\Delta k_F = k_F$ (10^{-2})	$\frac{\Delta k_F}{k_{F^0}} \times 100$
X	0.7599	-2.67	0.3510	0.6858	-.357	0.5177	0.6897	-.529	0.76
W	0.7597	-2.85	0.3745	0.6855	-.398	0.5721	0.6889	-.600	0.86
K	0.7602	-2.37	0.3110	0.6861	-.340	0.5940	0.6895	-.548	0.78
L	0.7773	1.47	1.932	0.7131	2.36	3.423	0.7485	5.35	7.70
U	0.7600	-2.55	0.3355	0.6859	-3.54	0.513	0.6895	-.548	0.78

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