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Modeling of a vector: Fermi in metals under high temperature

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Abstract
It is shown that atomic space between atomic and ionic radii may be divided on the ready exchange-fluctuation cells Kλ/z, where K is nearest neighbors, λ = h/mc, z is valence. On this basis values of vector Fermi is established for 21 metals using model 1/ k_F in proportion Kλ/z ± nλ (where n is 0,1,2,3) in limits approximate of value λ = photon + electron. It is shown also a calculation of the thermal blurring k_F (potential permit) and it's a connect with high temperature phase transformation bcc ↔ hcp in such limits n λ.

Keywords: atomic and ionic radii, electron density, nearest neighbors, vector –Fermi

Introduction

High temperature has a limit in theoretical investigations, so as it is impossible to apply the modern theoretical analysis using the band theory of the perfect crystal. Because nontraditional approach was chosen - electron density distribution (its probability) in the coordination space between ionic core, using ionic and atomic radii (r_a, r_i) in pseoudo – potential approximation.

Here we considered ultimate possible fluctuations of potential energies appear at R_C and r_a (radii ionic core and atom) and a mean ultimate average fluctuation 1/2 (R_C + r_a) = K at z/K – density of the charge, where z is valence, K is number nearest neighbors and we are obtained bond energy U (r) = ($e^2/4\pi\varepsilon_0$) z/KR. If R is considered as a main dimension feature, then a chain of R-interaction with coordinated space can be obtained. So parameter R is formed by dimension rations in the coordinate space, where main role is consisted in the definition of the ionic core as function $\lambda_F/2\pi$, a namely: 2 πR = $2\pi R_C$ + n (λF/2π) and accordingly: $2\pi R_C = 2\pi r_i + \lambda_F/2\pi$, where r_i is crystal-chemical radius [1, 2].

This standing wave can be formed at R_C - r_i as self- closing orbital appears considering $\lambda_F/2\pi$ (a circle of a radius r comprises a whole number of de – Broglie wave lengths: 2πr = nλ). There are empirical fact: R_C - r_i = Kλ (where λ = h/mc) as result exchange by fluctuations at heat transfer in interaction photon + electron = λ between an emitter and an absorber photons.

With account of the value 1/z as a restriction of an absorber of photons we are obtained the chain relations, where the value ± Kλ/z may approximate as cells of the fluctuation exchange in heat transfer:

+ R + Kλ = r_a - Kλ/z; R - Kλ = R_C + Kλ/z; R_C = r_i + Kλ/z

These data are established the balance of line correlation between r_a, r_i and Kλ: r_a = r_i + Kλ (1/z + 1) + Kλ (1/z + 1) + Kλ/z ± nλ, where n =0, 1, 2. Hence, may assume that the atomic space between r_a and r_i is divided into the ready Kλ cells.

Hence, the general question should to arise: where the essential role of a vector – Fermi in model of exchange-fluctuation cells Kλ/z. An attempt to answer on this question is aim of given research.

Results

It is considered correspondence of a continuum particles in sphere - Fermi (it is characterized Fermi – vector k_F) with an exchange – fluctuation atomic space (it is an excess (+ Kλ) or a deficit (- Kλ) of the electron density) in the model a photon + an electron =λ between an emitter and an absorber photons [1, 2].

It is realized by using follows assumptions: 1) The atomic space is divided on cells Kλ/z with increase (+Kλ/z) and decrease (- Kλ/z) of the electron density, where the value z (valence) is the restriction of the absorber of photons and 2) The size of such an exchange – fluctuation cell must be limited by the value λ_F or k_F. Therefore we can write in the linear approxima tion for the size of a cell: ΔR_{min} = R_C - r_i = Kλ/z (where r_i – the crystal-chemical radius, R_C is the radius of ionic core in pseudo-potential approach) and for it's of the limit: 2π (RC - r_i) = $\lambda_F/2\pi$, where the value $\lambda_F/2\pi$ has been determined self-closing orbital (it is: 2πr = nλ) with the formation of a standing wave. In accordance to these correlations we can write:

k_F = 1/2 π [1/(Kλ/z ± nλ)], Where the number ± n = 0, 1, 2, 3 is the determant k_F, actually.

The calculation value k_F^{mod} has been coincided with experimental k_F as average value between two possible values as it shown for Sr (n = 0, n = +1) and for Al (n = - 1, n = + 1) and other metals in Tabl. In $(A)^{-1}$.

For Sr (z = 2)

$(k_F)_0$ = 1/2π[1/(Kλ/z + 0λ)];

$(k_F)_{+1}$ = 1/2π [1/ (Kλ/z + 1λ)];

$(KF)^{mod}$ = $[(k_F)_0 + (k_F)_{+1}]/2$

For AL (z=3)

$(k_F)_{+1}$ = 1/2π [1/ (Kλ/z + 1λ)];

$(k_F)_{-1}$ = 1/2π [1/ (Kλ/z - 1λ)];

$(KF)^{mod}$ = $[(k_F)_{+1} + (k_F)_{-1}]/2$.

Table 1

Me	Li	Na	K	Rb	Cs	Be	Mg	Ca
k_F	1,11	0,92	0,75	0,70	0,61	1,93	1,34	1.11
k_F^{mod}	1,05	0,93	075	0,71	0,62	1,96	1,31	1,07
+/- n	-2	- 3 / +3	0/ +2	0/+3	+3	-0/-1	-1	+2 / -1

Table 2

Sr	Ba	Pb	Al	In	Cu	Ag, Au	Zn	Zn	Cd	Cd
	0,98	1,57	1,75	1,51	1,36	1,20	1,57	1,57	1,40	1,40
1,02	0,95	1,56	1,76	1,50	1,35	1,20	1,56	1,55	1,37	1,46
-1/+3	+3	-3/+1	+1/-1	0/+1	0/-2	0/-1	-3/+1	-2/+2	-1/-2	-3/+3

Conclusion

The calculating value k_F^{mod} can be formed from two parts. This is a response on the thermal blurring (potential– permit for the thermal fluctuate) of Fermi surface, where (+n) is lengthening of k_F, and (-n) is shorten of k_F and a finish $k_F^{mod} = k_F$ on the boundar y of the dividing particles before and after Fermi surface. Besides the number (n) has to be with (+) and with (-) in equal parts and themselves values (n) have to be from 1 to 3 in equal parts also, a namely: n = 0, n = 1, n = 2 and n = 3 have to be: 6,11,7,10 times, accordingly, as it follows from data in Tabl. This relations is indication of the equal-probability character of the number (n).

All values (as a permit for the thermal fluctuate) have tendency to decrease for metals having the spherical Fermi surface or nearly to it. For the hexagonally packed (6+6=12) layered Cd and Zn we have two approaches for determination k_F in the according with its compound structure.

Besides for metals Cu, Ag, Au we must note deflection from the considering approach as it is for other metals. The reason has been in a degradation of a value R_C, so as a value $r_a - r_i$ has been coincided with Kλ (where r_a is atomic radius). According to [1, 2] we have: $r_a = r_i + 2K (1/z + 1) + K\lambda/z$. Hence we can write: $r_a - r_i = K\lambda/z = 12.0, 024 = 0, 29$ Å. For Cu and Ag: $r_a - r_i = 0, 32 \div 0, 28$ Å, then it is corresponded to Kλ = 0, 29 Å. For Au: $r_a - r_i = 0,045$ Å.

Therefore we have double of the value Kλ/z. This significant result has been calculated through (K/2) λ. Thus a modeling k_F for noble metals confirm adequate character of correspondence of exchange- fluctuation cell to vector-Fermi.

An accuracy in calculation k_F (Tabl.) is basis for conclusion: a vector k_F is a regulator of a value an exchange-fluctuation cell from 0λ to ± 3λ under high temperature in model: a photon + an electron = λ.

Unlike the above discussed k_F metals with hcp structure have a lattice compressed along the [c] axis at [c]/[a] ‹ 1,633 (where 1,633 correspondence to the close sphere packing). Minimal magnitude of compression should be within λ = h/mc. Compressing an atomic sphere by λ from above and below along the [c] axis, we obtain Δ[c] = [c] - 2λ (flattening along the [c] axis). Contrary, the alongation Δ [a] + 2λ along the [a] axis by λ from both sides corresponds to this value of Δ[c] in accordance the total volume for 12 neighbors.

If this simple model of the formation of a structure hcp is valid, then it should be defined by experimental data [c] and [a]. Adequate this modeling we carried out following way: the alongation Δ [a] and compression Δ[c] can be redused to an ideal ratio [c]/ [a] = 1,633 of a cubic close sphere packing. This requires determining an inverse ratio ([c] + 2λ) / ([a] - 2λ), where [c] and [a] are experimental data. Analysis of 14 metals (from be to Gd) showed that the mean value of inverse ratio coincides with the ideal ratio 1,633 using 2λ model. In this respect, indicative is the minimum value of [c]/ [a] = 1,623 for Mg, where Δ[c] and Δ [a] turned out to be equal to 1λ, instead 2λ, as it is for other 14 metals [3].

The structure Mg: in a layered close packing ABAB….layer [c] - λ alternates with a layer [a] + λ. From the analysis of the inverse ratio, we have for the layer (A): ([c] + λ) / [a] = 1,631, for the layer (B): [c] / ([a] - λ) = 1,635, and an averedge value of 1,633 between layers, as for the sphere packing. Besides metals Y, Dy and Ho have Δ[c] and Δ [a] equal 4λ, but not 2λ.

Conclusion

The phase transformation hcp ↔ bcc has been accompanied by the change of dimension lattice on the value nλ which is coincided with the value nλ of blurring of a vector – Fermi. However a distortion of a lattice (a compressing and a flattening) have the thermal nature. Hence we can assume that the value nλ of a blurring at the vector- Fermi has thermal a nature also in aspect - potential permit.

It is obvious a value nλ have complete ground to analysis of high temperature researches.

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