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Model of High Temperature Heat Transfer in Metals

By E. S. Filippov
National Research Technological University, Russian Federation

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Model of High Temperature Heat Transfer in Metals

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Abstract- Based on the analysis of the atomic – ionic radii and volume characteristics new the approach (exchange – fluctuation) is considered under band blurring. It is shown that atomic space between atomic and ionic radii is divided into the ready Kλ cells (where K - nearest neighbours, λ = h/mc). The heat energy transfer in this space is represented in the model of fluxes, exchanging by the electron density in the ±Kλ mode.

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I. Introduction

Despite greate progress in physic of metals the high temperature formation nature of heat transfere remains inexplicable. Main reason is band structure degradate. Because a nontraditional approach was chosen: instead of impulse (p=hk, its value and direction) the electron density distribution (its probability) was analyzed in the coordination (pozition) space between ionic cores, using atomic (r_a) and ionic (r_i) radius on the one hand and using values λ_F and Z (a valency) of condition electrons on the other hand [1,2].

II. Initial Data

Main assumption is as follows: electron density fluctuanions appear, when the density of probability is distributed in the pozition space between ionic cores (in coordinated space) at the pseudo – potential approximation. Differences in states of separate electrons can be described as mean value of all posible fluctuation, using a half - width distribution of probability per r at the level of the maximum electron density fluctuation. This level has been distinguished by ultimate possible fluctuations of potencial energies appear at $r_i \approx R_c$ and r_a (Its min. and max.), while one half these values is a mean ultimate fluctuation (It is $1/2\ (r_a + R_c)$). Based on conception of free electrons and approximation of non-screen Coulomb interaction we are obtained:

$$U(r) = (e^2/4\pi\varepsilon_0)\ Z/K[1/2(\ r_a + R_c)]$$

Where K is number of nearest neighbors, $R_c \approx r_i$ (where r_i – crystal-chemical ionic radius, R_c – a radius of atomic core in metals), Z/K - the density of the charge, $1/2(\ r_a + R_c) = R$ is the mean value between of ultimate fluctuations by R_c and r_a, U(r) is the bond energy [1,2]. If R is considered as a main

Author: National Research Technological University " MISA", Moscow, Russia. e-mail: philippoves@ya.ru

dimensional feature, then a chain of R interactions with co-ordinated (pozitions) space and the number nearest neighbors (K) can be obtained:

1) as an orbital: $1/2(r_a + R_c) = R$;
2) as a volume spheare in pseudo- potential field: $4/3\pi(r_a^3 - r_i^3)/K = R^3$ and also: $4/3\pi R^3 = 4/3\pi r_i^3 + r_s^3 Z$, when $r_s = 1{,}92\ \lambda_F/2\pi$;
3) as a surfase: $4\pi R^2 (K\lambda) = (r_a^3 - r_i^3)\ Z^{1/3}$ (where $\lambda = h/mc = 0{,}0242$Å);
4) as a characteristic of melting: $V_l - V_0 = R^3$ (where V_l and V_0 are volumes of liquid state at T_{melt} and at 0K [1,2];
5) as the characteristic SAP (statistical atomic packing, having $K_{SAP} = 1/12(1+2+\ldots+12) = 6{,}5$ [2]): $4/3\pi[(\sigma/2)^3 - r_i^3]/K_{SAP} = R^3$ (where σ – the diameter of hard sphere in number decidings of Eq. Percus-Yevick and hence it follows: $\sigma/2 - r_i = R - R_c$);
6) at last, on the other hand the value R can be obtained from characteristics of conduction electrons, using wave lengths $\lambda_F/2\pi$: $2\pi R = 2\pi R_c + n(\lambda_F/2\pi)$, where $2\pi R_c = 2\pi r_i + \lambda_F/2\pi$ and where n =1,2. Here, this standing wave formation at $R_c - r_i$ as self-closing orbital appears considering $\lambda_F/2\pi$ (a cicle of radius r comprises a whole number of de-Broglie wave lengths: $2\pi r = n\lambda$).

Conclusion: Coordinated (pozition) spase between ions can be represented by the value R, using all variants: as an orbital, as spheres and surfase in the fluctuation approximation. There is a reson – the best use of a space principle admiting the band structure degrades at high temperature. Consequently, there are grounds to the analisis of the high temperature processes, which has been represented by number nearest neighbors (K) and shortest distances (r_a,r_i) by using the parametr R. Here the value R is a coordinate per r of maximum probability at the electron density distribution between r_a and R_c in pseudo-potencial approximation. From here we can conclude the following: main progress is determined of the value R. This parameter is formed by dimensial rations in the coordinate space, where main role is consisted in the definition of the ionic core as function $\lambda_F/2\pi$ (its formed of a standing wave by self -closed orbital: $2\pi R_c = 2\pi r_i + \lambda_F/2\pi$). Here we can answer on question: why are we considered all rations by means of R: it is determined by the energy bond; it is represented by all variants: as a continual, as contactial spheres and a surface of a sphere into exchengeal intereaction on $\lambda = h/mc$, using both line-space values (r_a, r_i, R_c) and physical values (λ,λ_F,Z).

III. Model of the Fluctuanion- Exchange of Heat Transfer in Solid and Liquid States

The identified melting characteristics of the model R, R_c, r_a and r_i associated with the electron density fluctuanion in the coordinate space can be applied to the heat transfer model within the following assumptions: The heat energy flux is associated with the electron – photon interaction and, respectively, with $\lambda = h/mc$; and there is empirical fact: $R_c - r_i = K\lambda$ ffiλ , as result of which the coordinate atomic space has an excess $+K\lambda$ or a deficit $- K\lambda$ in the interaction mode (photon + electron $\rightarrow\lambda$) between the emitter and absorber

Ref
2. E. S. Filippov, Izv. Vyssh. Uchebn. Zaved. Chern. Metallurg., №5, 3-6 (2009).

photons [3]. The size of such an exchange – fluctuation cell must be limited to the value of λ_F :

$$R_c = r_i + K\lambda/Z \quad \text{and} \quad 2\pi R_c = 2\pi r_i + \lambda_F/2\pi \tag{1}$$

Hence: $$k_F = 1/2\pi[1/(K\lambda/Z\text{ffin}\lambda)] \tag{2}$$

Where at $n = 0,1,2$ there is a complete correspondence between $K\lambda/Z$ and k_F for the alkali and alkali-earth metals – Pb,Al,In….Justification of the $K\lambda$ value also follows from mentioned relation: $r_a^3 - r_i^3 \approx 4\pi R^2 (K\lambda)$, where the geometric volume in pseudo-potential approximation is coincided with the physical volume.

A mirror reflection – $K\lambda$ should correspond to the fluctuation level + $K\lambda$ (similar to the 2λ- model in the formation of the hcp- structure, where according to [1], the elongation by 2λ along the [a] – axis corresponds to the compression by 2λ along [c]- axis). Hence, in equilibrium – vibrational mode $(R - K\lambda) \leftrightarrow (R + K\lambda)$, we have the equality of fluxes (photon+ electron→λ) of the emitter and detector. This equality of fluxes we write by the following equations using the parametr R corresponding to the maximum level of the electron density fluctuation and determined as 1/2 ($R_c + r_a$) :

$$R + K\lambda = r_a - K\lambda/Z \tag{3}$$

$$R - K\lambda = R_c + K\lambda/Z \tag{4}$$

$$R_c = r_i + K\lambda/Z \tag{5}$$

Here, we take into account the number of valence electrons Z per photon absorption under the $K\lambda$ exchange interaction in the range from r_a to r_i.

Equations (3-5) are fulfilled accurate to (1,2) λ for 14 of metals under study: alkali and alkiline earth, Pb,Al,In,Cd and Zn.

For hexagonal structure (6+6) Cd and Zn, we find (Å/atom):

$$\text{For Cd} \qquad r_a^{max} - r_a^{min} = 0{,}152 \approx K\lambda;$$

$$\text{For Zn} \qquad r_a^{max} - r_a^{min} = 0{,}140 \approx K\lambda,$$

where $K\lambda = 6\lambda = 0{,}145$ and r_a^{max} and r_a^{min} are determined from the lattice parameters [a] and [c].

These data allow us to conclude that the value of $K\lambda$ corresponds to the maximum level of probability for the exchange interaction of conduction electrons of K atoms according to the scheme: electron + photon →λ . Combining Eqs.(3-5) and using the relation for determined R, we get:

$$R - R_c = K\lambda(1/Z + 1); \quad R - r_i = K\lambda(2/Z + 1); \quad r_a - R_c = 2K\lambda(1/Z + 1); \quad r_a - R = K\lambda(1 + 1/Z); \; R_c - r_i = K\lambda/Z. \tag{6}$$

These data confirm by the balans of line correlation between r_a, r_i and $K\lambda$:

$$r_a = r_i + K\lambda(1/Z + 1) + K\lambda(1/Z + 1) + K\lambda \text{ ffi } n\lambda, \tag{7}$$

where $n = 0,1,2$ for 14 metals.

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Thus, it can be assumed that the atomic space between r_a and r_i is divided into the ready Kλ cells, whose number could not be less than the maximum possible fluctuations of the electron density in the coordinate space. This number must be discret for Kλ. Therefore, the heat energy transfer (the change in the intensity of the atomic-vibrational mode) in this space is represented in the model of two fluxes exchanging by fluctuations of the electron density in the ffiKλ mode.

Along the radius R corresponding to the maximum of the electron density, two fluctuation fluxes before R and after R are separated and regulated: heating – cooling (here, R is determined by the bond energy). Heating mode is the fluctuation flux from the atomic periphery r_a to the ionic core R_c. Cooling mode – vice versa. The equilibrium state is the compensation of the electron density fluctuations (ffiKλ).

IV. Liquid State

A liquid aggregate state precisely fits into this model scheme of heat transfer, since according to [1,2] and Eqs. (3-6), we have:

$$\sigma/2 \; - \; r_i \; = \; r_a - R_c \; = \; 2\,K\lambda\,(1/Z + 1), \tag{8}$$

where σ/2 is a semi-diameter of the hard sphere (Percus-Yevick).

For the statistical packing of atoms (SAP), where the average statistical number of nearest neigbors is $K_{SAP} = 6{,}5$ we obtain:

$$\sigma/2 \; = \; R \; + \; K_{SAP}\,\lambda \tag{9}$$

Equation (9) is fulfilled with an accuracy of 1-3% for the 14 of the studied metals.

These data for the liquid state confirm the initially assumed model of heat transfer via the exchange fluctuation quantities Kλ between atomic spheres being in the thermal vibrational mode.

V. Analisis of Volume Correlations at the Exchange- Fluctuation Model of Heat Transfer

Here we have follows initial data: $K\lambda/Z = R_c - r_i$; $K\lambda(1/Z + 1) = \Delta R \equiv r_a - R \equiv R - R_c$ from Eqs.(3-7) and also for the coefficient packing $k_p = 0{,}68 - 0{,}74$:

$$k_p = V_a \,/\, (V_a + V_{void}) = r_a^{\,3} \,/\, (r_a^{\,3} + R^3) \text{ and also: } k_p = R^3 \,/\, (R^3 + R_c^{\,3}), \tag{10}$$

Hence it follows:

$$R^3 \,/\, r_a^{\,3} \; = \; R_c^{\,3} \,/\, R^3 \tag{11}$$

where values R and R_c are determined as: $2\pi R_c = 2\pi r_i + \lambda_F/2\pi$ and $2\pi R = 2\pi R_c + n\,\lambda_F/2\pi$ and $n = 1{,}2$. Here, we must mark that its new discovery correlation ($V_{voids} = R^3$) is connecting link between values R^3 and $R_c^{\,3}$ and by two principles: the uncertainty and the best use of the space- interatomic voids.

Main assuption is as follows: atomic sphere (r_a = const.) is transformated into a sphere, having variable radii but in definit limits: $r_a - r_i$ or $R - r_a$, $R - r_i$

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for which it is determined average value $(r_a - r_i)/2$, $(R - r_i)/2$ ets. However, atomic volume and the interatomic voids are remained by nonchangeable and also the coefficient packing (k_p). Besides, we have the ground for the approach to the problem of high temperature heat transfer into coordinate space, using the volume in different forms:

$$4\pi R^2 K\lambda = (r_a^3 - r_i^3) Z^{1/3}; \quad (12)$$

$$4\pi R_c^2 K\lambda = R^3 Z^{1/3}.$$

Equations (12) is fulfilled with an accuracy of $Z^{1/3}$ according to [1,2].

The value $K\lambda$ is the binding unit of two forms of atomic-ionic volumes in fact.

Here we must consider the balance of volumes. The physical volume should correspond to the geometrical volume. Here a radius can not has fixed orbital. It is average value in according to the principle uncertainty:

$\Delta V_{emitter} = 4\pi[1/2(r_a + r_i)]^2 K\lambda$; $\Delta V_{absortion} = 4\pi[1/2(r_a + r_i)]^2 K\lambda/Z$ and other relations.

$$\Delta V_{emitter} + \Delta V_{absorption} = r_a^3/k_p, \; r_a^3, \; R^3, \; R^3/k_p$$

Thus we have the ground for the combination of double form the volume, assuming that the coordinate space from r_a to r_i is divided into the ready $K\lambda$ cells. Consequantly, proceeding from these states and Eq.(12), we may write four balance relations for heat transfer by using assumption of ready $K\lambda$- cells into the coordinate space:

1) $4\pi[1/2(r_a + r_i)]^2 K\lambda (1/Z + 1) = r_a^3/k_p = r_a^3 + R^3$ (where $R^3 = V_{voids}$); (13)

2) $4\pi[1/2(r_a + r_i) - K\lambda/Z]^2 K\lambda/Z = R^3$; (14)

3) $4\pi[1/2(R + r_i)]^2 K\lambda (1/Z + 1) = r_a^3$; (15)

4) $4\pi r_i^2 K\lambda (1/Z + 1) = R^3/k_p = R^3 + R_c^3$ (where $R_c^3 = V_{voids}$). (16)

Eqs.(13-16) are fulfilled with an accuracy of ffi4% in average or the 14 of metals.

Here geometrical volume is a continual, it is without $4/3\pi$, assuming that interatomic space can has different forms in according to the principle uncertanty.

Hence it follows that the mechanism heat transfer may to present by the substitution R^3 in Eq.(13) on the same value R^3 from Eq.(14). Hovewer the value R^3 in Eq.(13) is the volume of interatomic voids and the value R^3 in Eq.(14) is the characteristic of the transfer $K\lambda$ in the direct of opposite situation ($-K\lambda$) instead of ($+K\lambda$) in Eq.(13). Besaides the value R^3 in Eq.(13) may substitude by the value R^3 from Eq.(16), using Eq.(11). Here we have the substitution R^3/r_a^3 into R_c^3/R^3. This chain of substitutions is allowed by the transference the volume of voids from r_i to r_a and vs and by heat transference of cells ($K\lambda$) at variable radii which may form from r_a to r_i. Here the principle uncertainty is formed by variable radii: $\Delta r = r_a - r_i$ and other and the principle of the best use of a space is determined by the coefficient of the packing (k_p).

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These mutual substitutions R^3 and r_a^3 in Eqs.(13-16) are the model of equilibrium process between the heating and the cooling. Hence, it may assume that heat transference of cells (ffiKλ) is connected with the transference of volumes voids from r_a to r_i and ves.

VI. Conclusion

The maximum possible value of the electron density fluctuation is theoretically determined as ffi Kλ and the heat transfer process is modeled as a λ exchange between the detector fluctuation and the fluctuation of the emitter of the photon – electron interaction. The main conclusion is: the atomic coordinate space corresponds to the maximum possible fluctuations of electron density for the exchange of + Kλ (emitted) by -Kλ (absorbed) in the photon – electron interaction. This space is discrete for placing Kλ or it quatized by Kλ. On the whole, the analysis of high- temperature processeses in coordinate space using the linear (R_c, R…) and volumetric (R^3, $4\pi R^2$…) characteristics reveals the processes of heat transference, the structure formation and phase transitions, which still did not have a simple explanation [1,2]

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