

Statistical model of solids

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1971 J. Phys. A: Gen. Phys. 4 467

(<http://iopscience.iop.org/0022-3689/4/4/009>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 171.66.16.73

The article was downloaded on 02/06/2010 at 04:34

Please note that [terms and conditions apply](#).

Statistical model of solids

N. K. MARTINOV and N. A. NIKOLOV

Department of Physics, University of Sofia, Sofia, Bulgaria

MS. received 26th May 1970, in final form 8th January 1971

Abstract. A plasma model of solids is proposed. It is shown that, in the presence of a local dynamic equilibrium in a steady-state electronic-ionic plasma, a spatially periodic selfconsistent potential can exist leading to a periodic structure in the solid-state plasma. Calculations for the period of the crystal structure of a number of metals with cubic (face-centered) and hexagonal symmetry are performed. The work function of some metals with cubic (face-centered) symmetry is also calculated. The results obtained are compared with the corresponding experimental data.

The well known models, describing the structure of an electronic gas in solids, are usually based on a preliminary assumption of the arrangement of their atoms or ions. In this sense, the behaviour of the electronic gas is determined by the availability of the periodic potential given in advance. In the present work an attempt is made to show that in fact the periodic potential can be induced by the selfconsistent Coulomb interaction of the two components of the electronic-ionic gas in solids.

As in our two previous papers (Martinov *et al.* 1969, Martinov and Nikolov 1971) dealing with the problem of the steady-state spatial structure of a gas plasma, the model discussed presently will again be based on the assumption of a local equilibrium of the field and statistical factors (Vlasov 1966). This means that the spatial distributions of the two components of the electronic-ionic gas are determined by the selfconsistent potential of the system which, in turn, is determined by the distributions of the electrons and ions themselves. The velocity distributions of the particles are assumed to be of the Maxwell type; the system is in thermodynamic equilibrium and the Fermi temperature will formally be used as the average temperature of the electronic gas.

The steady state of the electronic-ionic gas in the present model will be determined by the following equations—equations for a local dynamic equilibrium, equations of state and field equations:

$$\begin{aligned} \frac{1}{\rho_1(\mathbf{r}(e\tau))} \nabla p_1(\mathbf{r}(e\tau)) + \nabla \{e\varphi(\mathbf{r}(e\tau))\} &= 0 \\ \frac{1}{\rho_2(\mathbf{r}(e\tau))} \nabla p_2(\mathbf{r}(e\tau)) - \nabla \{e\varphi(\mathbf{r}(e\tau))\} &= 0 \quad (1) \\ \Delta\varphi(\mathbf{r}(e\tau)) &= -4\pi e\rho_1(\mathbf{r}(e\tau)) + 4\pi e\rho_2(\mathbf{r}(e\tau)) \\ p_1(\mathbf{r}(e\tau)) &= \theta\rho_1(\mathbf{r}(e\tau)) \quad p_2(\mathbf{r}(e\tau)) = \theta\rho_2(\mathbf{r}(e\tau)) \end{aligned}$$

where subscripts 1 and 2 refer to the ions and the electrons respectively; $\rho_i(\mathbf{r}(e\tau))$ are the spatial distributions of the particles (the probable ones), $\varphi(\mathbf{r}(e\tau))$ is the probable self-consistent potential, θ is the average Fermi temperature ($\theta = \frac{2}{3}\mathcal{E}_f$) and e is the elementary electronic charge. The above system refers to singly charged positive ions.

We shall look for spatially periodic solutions to equations (1) under the following boundary conditions:

$$\begin{aligned} \varphi(\tau(e\tau) = 0) &= \varphi(0) & \rho_1(\tau(e\tau) = 0) &= \rho_1(0) \\ \varphi(x = L, 0, 0) &= \varphi(0) & \rho_2(\tau(e\tau) = 0) &= \rho_2(0) \end{aligned} \quad (2)$$

where L is the size of the system along the OX -axis.

As shown by Martinov and Nikolov (1971), the above system possesses steady-state spatially periodic solutions for $\varphi(\tau(e\tau))$ and $\rho_i(\tau(e\tau))$ of the type:

$$\begin{aligned} \varphi(\tau(e\tau)) &= \frac{\theta}{e}\chi - \frac{\theta}{e} \text{Intan}^2 \left(\frac{\pi}{D}(x+y+z) + \tan^{-1} e^{x/2} \right) + \varphi(0) \\ \rho_1(\tau(e\tau)) &= \rho(0) \tan^2 \left(\frac{\pi}{D}(x+y+z) + \tan^{-1} e^{x/2} \right) \\ \rho_2(\tau(e\tau)) &= \rho(0) \cot^2 \left(\frac{\pi}{D}(x+y+z) + \tan^{-1} e^{x/2} \right) \end{aligned} \quad (3)$$

where

$$\begin{aligned} D &= \pi\sqrt{3} \left(\frac{\theta}{2\pi e^2 \rho(0)} \right)^{1/2} \\ \rho(0) &= \{\rho_1(0) \rho_2(0)\}^{1/2} \\ \chi &= \ln \left(\frac{\rho_1(0)}{\rho_2(0)} \right)^{1/2} \end{aligned} \quad (4)$$

Here the quantity D is the spatial period of both the selfconsistent potential and the distributions of the electrons and the ions, that is, D determines the parameter of the unit lattice cell in the case of an fcc crystal structure. The calculated period D in the model proposed is considered as the distance between those points in the coordinate space in which the localization probability is maximal. From (4) one can see that the spatial dimension is approximately ten times greater than the respective Debye radius of screening.

Besides the solutions (3) referring to the case of an fcc lattice, equations (1) allow periodic solutions describing an orthogonalized hexagonal symmetry, that is, with a selfconsistent potential of the form

$$\varphi(\tau) \sim \text{Intan}^2 \left(\frac{\pi}{a}x + \frac{\pi}{a\sqrt{3}}y + \frac{\pi}{c}z + \tan^{-1} e^{x/2} \right). \quad (5)$$

Here a and c are the parameters of the hexagonal crystal lattice related to the spatial period D in the following way (Kittel 1956):

$$\begin{aligned} a &= 0.725 D \\ b &= a\sqrt{3} \\ c &= 1.186 D \end{aligned} \quad (6)$$

where the value 1.633, characteristic of the hexagonal symmetry, is assumed for the ratio c/a .

As can be seen from equations (4) and (6), the lattice parameters for fcc and hexagonal symmetry are determined solely by the mean Fermi temperature ($\frac{3}{8}\mathcal{E}_f$).

Table 1

fcc	$a(\text{\AA})$	$D(\text{\AA})$	$A(\text{eV})$	$A(\text{eV})$
	exp	theor	exp	theor
Al	4.04	4.25	4.20	3.86
Au	4.07	4.30	4.71	3.82
Ca	5.56	5.00	3.20	2.07
La $_{\beta}$	5.29	4.92	3.30	2.30
Cu	3.60	4.13	4.48	4.85
Pd	3.88	4.20	4.98	4.18
Pt	3.91	4.21	5.36	4.12
Pb	4.94	4.72	4.04	2.59
Ag	4.07	4.32	4.70	3.82
Sr	6.05	5.22	2.74	1.73
Ce	5.14	4.84	2.88	2.44

Table 2

hex	$a(\text{\AA})$	$c(\text{\AA})$	$a(\text{\AA})$	$c(\text{\AA})$
	exp	exp	theor	theor
Be	2.27	3.59	2.68	4.38
Gd	3.62	5.75	3.48	5.68
Cd	2.97	5.61	3.29	5.37
Co	2.51	4.07	2.88	4.70
Mg	3.20	5.20	3.27	5.33
Te	3.45	5.51	3.39	5.53
Ti	2.95	4.73	3.13	5.12
Zn	2.66	4.94	3.06	5.00
Ni	2.60	4.15	2.90	4.74
Os	2.73	4.58	3.01	4.92
Cz $_{\beta}$	2.72	4.42	2.94	4.80
La $_{\alpha}$	3.75	6.06	4.32	7.05

Tables 1 and 2 present the experimentally measured lattice parameters (Landolt-Börnstein 1955), as well as those theoretically calculated by us, for a number of metals of the fcc and hexagonal symmetry respectively.

Bearing in mind the second boundary condition for the potential and equation (3), it can easily be seen that $\varphi(0, y, z) = \varphi(L, y, z)$ if the size of the system along the OX axis consists of an integral number of spatial periods, that is, $L = lD$ ($l = 1, 2, \dots$). Similar considerations apply for the other two directions, which must also consist of an integral number of corresponding spatial periods.

Equations (3) make it possible to calculate the electronic work function. For this purpose the selfconsistent potential must be suitably cut off only at the points where it tends to infinity and where the electronic density is infinite. The cut-off will be made in a region of the order of magnitude of the classical electronic radius τ_0 , so that in these regions the probable electronic density will now possess a maximal but finite value. Having in mind the expression for the selfconsistent potential $\varphi(\tau)$, and assuming that the mean density of the ions is equal to that of the electrons ($\rho_1(0) = \rho_2(0) = \rho(0)$), one obtains for the potential energy of the electrons on the bottom of the potential well:

$$e\varphi = -\theta \ln \tan^2 \left(\frac{\pi \tau_0 (e\tau)}{D} \right). \quad (7)$$

The work function A of the electrons is determined by their mean potential energy and the averaging is performed in the potential well of the electrons. Figure 1 represents the shape of the electronic potential well. The theoretical calculations for A for metals of an fcc crystal structure, together with the experimentally measured ones (Landolt-Börnstein 1955), are given in the last two columns of table 1.

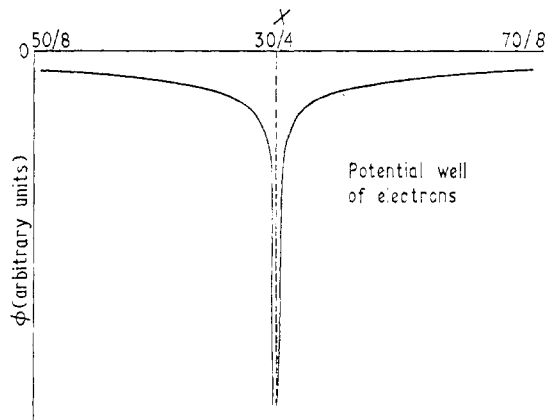


Figure 1.

The problems of the localization and the spatial periodic structure of the solid-state particles can be solved correctly only by means of quantum-mechanical considerations. The difficulties arising from such a treatment are well known. That is why the present work proposes a considerably simpler, although not yet sufficiently developed, model in which hydrodynamics is used for an account of the strong interactions between the particles; the quantities $\rho_1(\tau(e\tau))$ are the particles' probability distribution functions.

It is interesting to mention that Zachariev *et al.* (1971) have shown that the most favourable thermodynamic state—the one of minimum internal energy—of an electronic-ionic gas will be attained provided (i) the field equation is of the form $\Delta\varphi = \text{const} \times \sinh \varphi$ and (ii) the particle distributions satisfy $\rho_1(\tau(e\tau)) \rho_2(\tau(e\tau)) = \text{const}$.

It may be seen that both conditions hold good in our model. Moreover, the above mentioned work shows that the state of an electronic-ionic gas with a homogeneous distribution of the particles and $\varphi = 0$ is of higher energy than the periodic state considered here.

References

- KITTEL, C., 1965, *Introduction to Solid State Physics* (New York: Wiley).
 LANDOLT-BÖRNSTEIN, 1955, *Zahlwerte und Funktionen, Kristalls*, 4 (Berlin: Springer-Verlag).
 MARTINOV, N., NIKOLOV, A., and NIKOLOV, N., 1969, *Rep. 9th Int. Conf. on Phenomena in Ionized Gases, Buharest*.
 MARTINOV, N., and NIKOLOV, N., 1971, *J. Phys. A: Gen. Phys.*, **4**, 464–6.
 VLASOV, A. A., 1966, *Statistical Distribution Functions* (Moscow: Nauka).
 ZACHARIEV, I., *et al.*, 1971, to be published in *Zh. eksp. teor. Fiz.*