Shock Waves and High-Strain-Rate Phenomena in Metals

CONCEPTS AND APPLICATIONS

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THOMAS-FERMI APPROXIMATION

FOR SHOCK-WAVE STRUCTURE IN METALS

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The stationary shock wave structure in metals considered as cold plasma with degenerated electron gas is studied using the same approach as for the collisionless hot plasma. The shock wave parameters are derived from the cold ion-fluid equations, Poisson equation and Thomas-Fermi equation for electron density. The experiments to show the effects of the present approach are also discussed.

I. INTRODUCTION.

A number of attempts were undertaken lately to describe shock wave process in metals basing on microscopic conceptions. The investigation of the lattice dynamics (1), (2), application of the molecular dynamics method to determine the transition time of the compressed lattice into a new equilibrium state (3), etc., are related to these.

These calculations, based on nearest-neighbor interaction, are of interest for understanding space-time scales of the lattice rearrangement by shocks. Yet the assumptions concerning the nearest neighbor interaction and spheric symmetry of potentials between ions are fairly rough. They contradict some experimental data pertaining even to static properties of metals. Thus, the Cauchy relation, following from them, does not apply for a number of metals (4). Besides, the shock wave process analysis without taking into account the transition dynamics from undisturbed substance to the state behind the shock on atomic scale can distort the process image.

No more than 10^3 particles can be put under investigation by molecular dynamics methods using current computers (5). This provides for up to ten atomic layers in the three-dimensional case. It follows that no solution can be obtained under the circumstances as to the stationary shock, transition characteristics to the final state, etc. Different model conceptions should be developed, therefore, in order to understand microscale processes in metal, permitting to single out characteristics of the phenomena studied, which are manifested in extreme cases.

II. ANALYSIS.

A metal model is well known, based on the Thomas-Fermi approximation (6), the so called "jelly" model. It does not take into account many real characteristics and is a compressed metal model with elastic forces developed only due to the electron gas, while the ion arrangement, electron interaction, etc., are neglected. This simplest model yields accurate values for sound velocities in alcaline metals (6) and elucidates a number of other parameters.

Its application in the study of the shock processes in alkaline metals (Li, Na, etc.) seems to be of some interest. The ion volume of alkaline metals is about 10% of the total volume. Thus the direct ion collisions can be neglected in the first approximation. The electric field produced by ion density disturbance gives rise to ion motion. The electron gas in metals is degenerated at the temperature of $T<T_F$. The degeneracy temperature T_F is ~ 5.10^4K under normal conditions and increases as $n_e^{2/3}$ with electron density n_e increase.

As a result of the degeneracy, the electron velocity $V_F \sim 10^8$ cm/sec, thus being well above sound velocity $C_0 \approx 5 \cdot 10^5$ cm/sec.

The electron distribution in energy is fairly independent of temperature at $T<<T_F$. Hence, the electron gas is assumed to be cold (T_e = 0K) at shock compression. As $V_F>>C_0$, the electron distribution in the potential, produced by the shock with propagation velocity about C_0, could be assumed equilibrium one and the Thomas-Fermi approximation could be used (6).

Thermal ion motion can be also neglected, and the ion temperature in the shock compression process is assumed to remain zero T_i=0K. This is possible due to insignificant thermal ion pressure at moderate pressures of shock compression (1 Mbar).

The model where $T_e=T_i$=0K and the electron gas is degenerated is similar to the collisionless plasma case with cold ions T_i=0K and hot electrons $T_e>>T_i$ (7). Hence, the ion motion equations are similar to those for ions in the classic hot plasma (8), and in lieu of the Boltzman formula use is made of the Thomas-Fermi formula (6).

$$\frac{\partial \vec{v}}{\partial t} + (\vec{v}\nabla)\vec{v} = -\frac{e}{M}\nabla\phi \qquad [1]$$

$$\frac{\partial n}{\partial t} + \nabla(n\vec{v}) = 0 \qquad [2]$$

$$\Delta\phi = 4\pi e(n_e - n) \qquad [3]$$

$$n_e = n_{eo}\left(\frac{e\phi}{\mu_o} + 1\right)^{3/2} \qquad [4]$$

Here ν,n,M - velocity, density and mass of ions, ϕ - electrostatic potential, n_e - density of the electron gas, e - electron charge, μ - Fermi energy, m - electron mass, $\hbar$ - the Planck constant[1].

$$\mu_o = \frac{\hbar^2}{2m}(3\pi^2 n_{eo})^{2/3}$$

It should be noted that a number of important metal properties such as the periodic structure of ion arrangement, ion-electron interaction (9) as well as dissipative terms of the motion equation are neglected in our analysis. The system of equations [1] - [4] will not, therefore, describe stationary shocks. Even so we adopt the above approach, as it is a conventional one for collisionless plasma (8). The dissipative terms will be discussed later, and they will be inserted in the transformed equations [1]-[4].

It will also be seen that linearization of equations [1]-[4] in the quasi-neutrality approximation results in the following value for the ion-sound wave velocity

$$C_o = \sqrt{\frac{m}{3M}}\, V_F$$

This value coincides with the phase velocity of long-wave phonons, obtained with the help of the dielectric formalism (6), and is quite consistent with the experimental data for the sound velocity in alkaline metals.

Let's consider a stationary one-dimensional case in order to clear up peculiarities of ion motion, described by the system of equations [1]-[4]. All variables then depend only on (x-Dt), where D is the disturbance propagation velocity. In the system, progressing at the velocity D, we have (taking into account that ν =D if ϕ=0, $n=n_o$):

$$\nu^2 + \frac{2e}{M}\phi = D^2 \qquad [5]$$

$$n = n_{eo}\, D\left(D^2 - \frac{2e\phi}{M}\right)^{-1/2} \qquad [6]$$

1 $\hbar = h/2\pi$

By substituting the value n from [6] into Eq. [3] and integrating the latter one time, we get expression for the potential

$$\frac{1}{2}\phi'^2 = 4\pi n_{eo}\{\frac{2}{5}\ \mu_o\ (\frac{e\phi}{\mu_o} + 1)^{5/2} + MD(D^2 - \frac{2e}{M}\phi)^{1/2}\} + A \qquad [7]$$

Assuming that

$$A = -4\pi n_{eo}(\frac{2}{5}\mu_o + MD^2)$$

$\phi' \to 0$, if $\phi \to 0$. It will be seen that in our case analogously to that with collisionless hot plasma (8) there is despite the nonlinearity of equations [1]-[4] a solitary stationary pulse (similar to the particles motion in the potential field), propagated at the velocity D.

Thus even in the absence of dissipation, the system [1]-[4] has stationary solutions. The solitary pulse velocity could be related to the maximum value of the potential in the wave, for $\phi'=0$ at $\phi=\phi_m$. D is determined from Eq. [7]:

$$D^2 = \frac{\mu_o}{5M}\,[(\frac{e\phi_m}{\mu_o} + 1)^{5/2} - 1]^2 \cdot [\frac{e\phi_m}{\mu_o} + 1)^{5/2} - 1 - \frac{5}{2}\frac{e\phi_m}{\mu_o}]^{-1} \qquad [8]$$

If $e\phi_m \ll \mu_o$ then expanding it as a series in $e\phi/\mu_o$ we have:

$$D = C_o + \frac{2}{3}\,(\frac{e\phi_m}{\mu_o})\,C_o \qquad [9]$$

It follows that with $e\phi_m \ll \mu_o$ the velocity of the solitary pulse is close to that of sound C_o and maximum potential value can be derived from [8] or [9]. The medium returns into initial state after the wave had passed.

In case of medium dissipation being taken into account the soliton solution is transformed, under adequate boundary conditions, into the shock one with the final state differing from the initial one.

The potential value behind the shock can be determined, taking dissipation into account, with the help of the mechanical analogy (8). The Poisson equation [3] should be written to this purpose with allowance for [5], [6] in the same approximation $e\phi/\mu_o \ll 1$:

$$\phi'' \approx 4\pi n_{eo}\,\frac{\partial}{\partial\phi}\,\{\frac{4e^3\phi^3}{9M^2C_o^4} - \frac{2e^2\phi^2(D-C_o)}{MC_o^3}\} = \frac{\partial W}{\partial\phi} \qquad [10]$$

Then the steady value of the potential behind the shock will correspond, with the dissipation available, to the point where the effective potential energy W in Eq. [10] is at its minimum. Hence:

$$e\phi_k = \left(\frac{D - C_o}{C_o}\right) \mu_o \qquad [11]$$

Thus the value of the potential ϕ_m in the first oscillation is 1.5 more than the value of the potential behind the shock, if only damping is low enough. For metals $\phi_m \approx 0.5V$ at the shock pressure of ~ 10 GPa. The order of the electric field in a shock can be found provided the half-width of the solution, where $\phi=\phi_m$ is obtained, is determined. The potential profile and solution width Δ can be determined by integrating [7]. The right-hand expression should be developed in $e\phi/\mu_o$ up to the third order inclusive prior to integration (see also conclusion below). The solution width:

$$\Delta = 2 \lambda \left(\frac{C_o}{U}\right)^{1/2}$$

Here U equals approximately to the particle velocity behind the shock. The electric field intensity in the shock is then equal approximately to:

$$E \approx \frac{\phi_m}{\Delta} \sim \frac{\mu_o U^{3/2}}{e\lambda C_o^{3/2}} \sim 10^7 \div 10^6 \text{ V/cm}$$

Such a value of the electric field might result in the situation with $T_e > T_i$ (10) and should be taken into consideration when analyzing the deformation mechanism by strong shocks.

The present field value is at the same time the maximum one for shock compression of metals (provided that $e\phi/\mu_o \ll 1$) for it was obtained ignoring the dissipation effect resulting in additional shock front widening.

In the classic plasma there is an upper limit for the solution velocity D_m above which non-linear effects can not be compensated for by dispersion only (8). In our case, it can be seen from [6] that:

$$\frac{MD^2}{2} > e\phi$$

for every ϕ.

Maximum value for D_m can be derived from the equality

$$e\phi_m = \frac{MD_m^2}{2}$$

with $\phi=\phi_m$; $\phi'=0$ and using [7] we can find

$$(\frac{1}{3}y + 1)^{5/2} = \frac{5}{3}y + 1; \quad y = (\frac{D_m}{C_o})^2$$

This equation has the only physical root y=3,4, where from $D_m \approx 1.85 C_o$. This corresponds to shock pressure of 1.6 Mbar for Cu, 80 kbar for Na and 900 kbar for Al.

It should be noted, that non-linearity of equations [1]-[4] results in lesser slope of shock adiabat in the D-U coordinates than it does in experiments, as it will be shown below. So, if all non-linear terms, relating to the ion interaction, are taken into account, the value of D_m should diminish. There is no stationary solution with $D>D_m$. Crossing D_m in the classic plasma represents transition from the laminar flow structure to the turbulent one (8). The residual properties of shock-loaded metals might be observed in the metals in the vicinity of D_m. Thus, a marked increase in point defects concentration can be observed in case of shock velocity exceeding the value D_m provided the shock profile is essentially determined by non-linearity and dispersion, and not by dissipation. It is also possible in this case that electric effects can be observed in the vicinity of $D=D_m$ at loading of the bimetalic contracts.

In order to study the flow structures in the $D<D_m$ region in more detail and to simplify introduction of the dissipative terms we shall transform the equations [1]-[4] into an equation for ν only in the following approximations:

$$\frac{\lambda}{L} = \xi << 1; \quad \frac{\delta n_e}{n_o} = \frac{n_e - n_o}{n_o} = \gamma << 1; \quad \lambda^2 = \frac{\mu_o}{6\pi n e^2}$$

where L - the characteristic length of the changing ion parameters; λ - the Debye length.

The difference between n_e and n is of the order of $n_o \xi^2 \gamma$. Indeed:

$$n_e - n = \frac{\Delta\phi}{4\pi e} = \frac{\mu_o}{4\pi e^2 n_o^{2/3}} \Delta n_e^{2/3} \sim \frac{\mu_o}{6\pi e^2 n_o} \frac{\delta n_e}{L^2} \sim n_o \xi^2 \gamma$$

Hence, in order to determine the kind of dependence of $\partial\phi/\partial x$ upon n the equations [3], [4] are solved by the successive approximations method, assuming in the zero approximation that $n_e = n$ (11). From [4] we can find:

$$\Delta\phi = \frac{\mu_o}{e n_o^{2/3}} \Delta n^{2/3}$$

In the next approximation:

$$e \frac{\partial \phi}{\partial x} = \frac{MC_o^2}{n_o^{2/3}} \cdot \frac{\nabla n}{n^{1/3}} + \frac{C_o^2 \lambda^2 M}{n_o} \nabla (\Delta n) \qquad [12]$$

In the equation [12] the least order term on $\xi(\sim \frac{\mu_o}{L} \xi^2 \gamma)$ is taken into account. The finite amplitude wave will progressively steepen up without this term, and condition $\xi \ll 1$ will not be satisfied. Using equations [12], [1], [2] we get the velocity equation:

$$\frac{\partial \nu}{\partial t} + \frac{4}{3} \nu \frac{\partial \nu}{\partial Z} + \beta \frac{\partial^3 \nu}{\partial Z^3} = 0; \quad \beta = \frac{\lambda^2 C_o}{2} \qquad [13]$$

The non-linear term of the least order on velocity is taken into account in equation [13] and passing to the coordinate system, moving with the sound velocity C_o, $x = Z + C_o t$ is realized. It should be noted, that the derivation of this equation is based on neglecting terms $\sim \gamma^3$ as well as terms of higher order as compared with $\gamma \xi^2$, i.e., on condition $\gamma^2 \ll \xi^2$.

The dispersion relation for the equation obtained looks in the linear approximation as follows:

$$\frac{w}{k} = C_o - \beta k^2; \; \beta = \frac{\lambda^2 C_o}{2}$$

Here k = the wave vector.

The dispersion relation for shocks in a one-dimensional lattice with nearest-neighbor interaction taken into account concerning particles with interatomic separation d is (4):

$$\frac{w}{k} = C_o - \beta_1 k^2; \; \beta_1 = \frac{a^2 C_o}{48}$$

Hence, the correction of the ion-sound wave phase velocity due to dispersion, related to the deviation from quasi-neutrality at the given k, is more than by an order of magnitude in excess of the correction related to the geometric dispersion. Therefore, it is justified to neglect ordered ion arrangement. As the dispersion term is the linear one the both dispersion mechanisms can be taken into account assuming that:

$$\beta = \beta + \beta_1$$

The kind of solution for equation [13] depends upon initial conditions (11), and solitary pulses (8,11) are, in particular, its solutions.

$$\nu = \nu_0 \ \mathrm{sech}^2\{(\frac{\nu_0}{g\beta})^{1/2} (Z - \frac{4}{9} V_0 t)\}$$

Their characteristic width Δ equals:

$$\Delta \approx 2\lambda \ \frac{C_0}{\nu_0} \sim 10^{-6} \div 10^{-7} \text{ cm}; \quad \nu_0 \sim 10^4 \text{ cm/c}$$

Equation [13] can describe shocks, provided the dissipative term is introduced into it. In the simplest case it can be considered as a conventional viscous term. Thus, for wave lengths much in excess of λ and for small wave amplitudes ($\gamma \ll 1$) an attempt can be undertaken to describe in the Thomas-Fermi approximation the shock in metal by the following equation:

$$\frac{\partial \nu}{\partial t} + \frac{4}{3} \ \frac{\partial \nu}{\partial Z} + \beta \frac{\partial^3 \nu}{\partial Z^3} - \beta \frac{\partial^2 \nu}{\partial Z^2} = 0 \qquad [14]$$

This is the Cortweg-de-Vries-Burgers equation (KdVB). The KdVB equation for the stationary shock, moving at the velocity C, can be integrated over Z, taking into account the boundary conditions with $x=\infty$, $\nu'=\nu''=0$; $\nu=\nu_k$, where ν_k is the velocity jump in the shock.

$$\beta \cdot \frac{d^2\nu}{dZ^2} - \beta \cdot \frac{d\nu}{dZ} = C\nu - \frac{2}{3}\nu^2 = -\frac{dW}{dZ} \qquad [15]$$

According to the mechanical analogy (8), this equation could be interpreted as non-linear oscillator equation ($Z \to t, \nu \to x$; W - the potential energy), starting its motion with $\nu=0$ and stopping with $\nu=\nu_k$. The damping oscillations are described in the equation. The final value $\nu_k = \frac{3}{2}$ C, and the first peak value ν does not exceed 9/4 C. The shock adiabat in the rest system looks as follows:

$$D = C_0 + \frac{2}{3} \cdot \nu_k$$

This shock adiabat differs from the experimental ones, where the second term equals (0.9 to 1.4) ν_k. The discrepancy results from omitting some of the non-linear terms, due to ion interaction. In case of the insignificant dissipation the shock front profile is close to the solution form (12). As a rule, dissipation is more effective in damping the high frequency spectral components. Hence, taking it into account should result in widening of the stationary shock front, and the solution width Δ predetermines the order of magnitude for the minimum shock front width in the $D<D_m$ region.

The stationary shock has the oscillating structure with characteristic wave length ~ Δ if:

$$\beta < \beta_m = \left(\frac{8}{3} \cdot \beta \cdot \nu\right)^{1/2}$$

where ν is the velocity jump at crossing the shock front and it has the monotonic profile if $\beta > \beta_m$ (11).

The viscosity value ν_m at $\nu=5\cdot10^4$ cm/s is equal to $\beta_m=10^{-2}$ to 10^{-3} cm^2/s, thus coinciding with the order of magnitude for the fluid metals viscosity. The oscillating structure of the shock is not, then, excluded in these substances. The viscosity value β in metals is determined by a number of mechanisms, which play a different part in different temperature, frequency, and amplitude ranges of the shocks (4). The viscosity 10^5 cm^2/s obtained in the oblique collision experiments with plates (13) can not be used to describe the shock front structure, for the scale and the mechanism of the phenomenon determinative of the velocity distribution in the contact zone differs from the dissipation mechanism in the shock.

Viscosity of the order of magnitude $10^{-4}cm^2/s$ is introduced into the motion equation for dislocation (14). This phenomenon is of the same scale as the characteristic oscillation width Δ in the shock front. The hypersound damping represents a process close to that under consideration. The frequency range up to $10GH_z$ is investigated at present, corresponding to the sound wave length of $2\cdot10^{-6}$ cm, i.e., of the same order of magnitude as Δ. Having experimental data concerning the supersound decay factor α at the frequency w the viscosity value β can be found from the following formula (15):

$$\alpha = \frac{\beta \cdot w^2}{2 \cdot C_o^3}$$

The value α for Z_n at the 150 MH_z frequency equals 1 $\frac{d\beta}{\mu s}$ (15). Hence, $\beta \approx 6\cdot10^{-2}cm/s$. This value β is of the order of magnitude of β_m, quoted above. Therefore, possibility of the oscillating shock front structure in the typical metals under normal conditions ahead of the shock is not altogether excluded. Decay of the large amplitude waves due to the non-linear effects could be described by viscosity factors, differing from those found for the supersound (15).

Estimates of the viscosity factors by orders of magnitude do not suffice for solving the problem of the possibility of oscillating structure emergency. It does not emerge from the step-like initial disturbances (12) even in the non-stationary section of the wave development at $\beta \approx 2\beta_m$ already. A final conclusion on the existence of the oscillating shock structure can be made only with reliable data on the dissipation mechanism being available. The KdVB equation for dielectric monocrystal was investigated in (2). The dissipation was found to induce the monotonic shock profile under normal temperatures.

The dispersion phenomenon in metals and related shock peculiarities are experimentally manifested in the following cases:

1. Dispersion alongside with dissipation prevents shock steepening up due to the non-linearity. It specifies shock front width with $D<D_m$. At $D>D_m$ dispersion alone can not prevent steepening up of the shock and the shock front width will be determined by only non-linearity and dissipation competition. It follows that in the vicinity of $D \approx D_m$ sharp diminution of the shock front width is possible and, as a consequence of this, increase in defects concentration.

2. The flyer plate impacting the metal surface, substance in the vicinity of the shocked surface will be loaded in such a manner that pressure growth time will be different from the stationary shock·pressure growth time. The ion velocity in the first oscillation on the non-stationary section for the KdVB equation can by a factor of 2 exceed the particle velocity behind the shock (12), while on the stationary section this excess is 1.5 times. The final states behind the shock, can be identical in this case if the flyer plate is thick enough. Therefore, metallic microstructure in the near-impact area can be seen to differ from that in the depth. It is interesting to compare the residual effect of the contact detonation shock compression to the same effects of flyer plate shock loading with the same Hugoniot parameters, for solution of [14] depends on the initial disturbance steepness (11). Dependency of the residual properties on the pressure profile in the shock is discussed in (16).

3. The emergence of the shock wave with oscillating structure, whose space scale is $\Delta \sim 10^{-6}$ to 10^{-7} cm on the free metal surface should be accompanied by destruction of its surface layers on the interatomic scale and mass ejection from the free surface.

4. The ion-sound oscillation excitation behind the shock will result in higher effective temperature of phonons, propagating normal to the shock front. As a consequence, this should be reflected in the phonon drag effect in this direction. This, in its turn, may cause abornally high electric signals at bimetallic contacts loading (10), (17).

5. The electric field magnitude in the shock 10^7, 10^6 V/cm suffices for electron gas heating up. This fact could be of importance for the electron temperature profile in the shock, at least, for low temperatures ahead of the

shock front (10). The electric field of this order of magnitude should be taken into consideration also on investigating mechanisms of the atomic lattice rearrangement and defect generation in the shock.

III. SUMMARY

The paper shows that effects related to the deviation from the quasi-neutrality and not those related to the periodicity of ion arrangement are the main contribution in the ion-sound dispersion in metals in the Thomas-Fermi approximation. Taking into account non-linear terms makes possible the existence of solitary pulses (solutions) and, if dissipation is manifested, of stationary oscillating shock structure. The model discussed permits one to obtain estimates of minimum shock front width, magnitude of oscillating parameters; and is predictive of some characteristics of shock compression of metals.

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