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Superheating of solid metal prior to electric explosion of wires at fast energy deposition

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Abstract

We develop the concept which distinguishes the initial stages of the fast (nanosecond) electric explosion of wires: the superheating of the solid conductor, its spontaneous (spinodal) decay and the successive formation of the non-ideal plasma column. We use the molecular dynamics simulation approach to simulate homogeneous nucleation from a stationary state and at a constant heating rate. We study the parameters of the spinodal, the dependence of the melting temperature on the heating rate and the character of the decay. We consider the subsequent evolution of the fluid column and the axial plasma uniformity. We compare the results with the experimental data on nanosecond wire explosions.

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1. Introduction

The electric explosion of wires is in the focus of the non-ideal (strongly coupled) plasma community, since it is one of the applications of non-ideal plasma [1–6] and also an important means of non-ideal plasma generation [7–9]. The initial stage of the explosion depends on the energy deposition rate and defines the subsequent development of the process. It has been suggested that the conductor could be superheated to the spinodal of metastable solid by the isochoric energy deposition at the fast electric explosion of wires [10]. This hypothesis [10] has been inspired by the experimental findings [3] and correlates with subsequent studies [2, 4, 5]. The existence of the metastable superheated solid has been noted both in the theory and experiments [11–15].

The molecular dynamics (MD) method has been used to simulate superheated crystals and study their properties [16–21]. Both the Lennard–Jones and the uniform soft-sphere

pair potential $U = \epsilon(\sigma/r)^n$ were chosen. The latter potential was used earlier for the Monte Carlo simulation of melting [22], glasses and liquids [23]. In the case of such a potential, dimensionless system properties $T^* = k_BT/\epsilon$, $Z = P(V,T)V/(Nk_BT)$, $C^*_{ab} = C_{ab}V/(Nk_BT)$, $J^* = ((m\sigma^2/\epsilon)^{1/2}\sigma^3 J)/(\rho\sigma^3/m)^{(8+n)/6}$ depend only on a single parameter $X = 2^{-1/2}(\rho\sigma^3/m)(\epsilon/k_BT)^{3/n} \sim \rho T^{-3/n}$ [24], where P is pressure, V is volume, T is temperature, C_{ab} is the elasticity module, J is the homogeneous nucleation rate, ρ is the density and m is the atom mass. The set of isotherms on the P–V plane is reduced to the single dependence of $ZX \sim P$ on $(1/X) \sim V$. The melting and spinodal curves on the same plane are reduced to two points.

The MD simulation of the soft-sphere model is used in section 2 of this paper to study melting of the superheated defect-free crystal without an open surface. We study systems of N particles with periodic boundary conditions arranged initially in fcc lattice sites. We use ϵ, σ, m and $(m\sigma^2/\epsilon)^{1/2}$ as units of energy, distance, mass and time in simulation. The equation of state and elasticity modules are calculated. Both the spontaneous homogeneous nucleation in the superheated crystal and the melting under stationary heating are investigated. We obtain the results for the lifetime, the scatter of the lifetime values and the dependence of the melting temperature on the heating rate.

In section 3, the simulation results are compared with experimental data for the equation of state of metal under high pressure and the lifetime of superheated wire. The scenario of spontaneous decay, subsequent expansion and stratification of the fluid column, excitation of non-equilibrium plasma oscillations are briefly considered. The most extensive experimental studies [4, 5] of the initial stage of the ultrafast wire explosion are used for the comparison with the theory.

2. Superheating of solid: MD simulation

The first type of simulation is carried out to obtain the equation of state, the elasticity module, the nucleation rate and the spinodal. The MD simulation consists of the calculation of the evolution of the configuration $\{\vec{r}(t) = \vec{r}(t)_1, \ldots, \vec{r}(t)_N, \vec{v}(t) = \vec{v}(t)_1, \ldots \vec{v}(t)_N\}$ of the many-particle system in the phase space, where $\vec{r}_i$ and $\vec{v}_i$ are the coordinate and velocity vectors of the ith particle. In this case the initial ensemble of M configurations $\left([\{\vec{r}(0), \vec{v}(0)\}_k]_{k=1}^M\right)_{T,\rho}$ that correspond to the certain values of $T = 1/(2N)\left(\sum_{i=1}^N \vec{v}_i^2\right) > T_m$ (T_m is equilibrium melting temperature) and ρ is prepared in the following way. The system is heated by the gradual velocity rescaling up to the desired value of T and then equilibrated. To prevent melting, before the necessary degree of metastability $(T - T_m)/T_m$ is reached, the spherical restrictions on particle motion are applied around each lattice site (artificial reflective spheres whose radii are equal to half of the nearest-neighbour distance). The set of M independent phase-points from the equilibrium MD trajectory with temperature T forms the initial ensemble.

A bundle of trajectories $\left([\{\vec{r}(t), \vec{v}(t)\}_k]_{k=1}^M\right)_{T,\rho}$ is calculated from such an ensemble of initial configurations. The *NVE* ensemble without restrictions on the motion of particles is simulated in this case. On each trajectory of the bundle, the isochoric melting transition occurs as soon as the liquid nucleus of the critical size is formed spontaneously. The fluctuational formation of the critical nucleus is observed in the animation of the structural evolution in the MD cell. This corresponds to the characteristic step on temperature–time (T–t) dependence. The period τ before its formation is the lifetime of the metastable ordered structure (see figure 1(a)). The upper and lower runs in figure 1(a) correspond to two trajectories in the same bundle. Both runs of figure 1(a) correspond to the melting transition 1 in figure 1(b). Transition 2 in figure 1(b) corresponds to another bundle of MD runs with different temperature

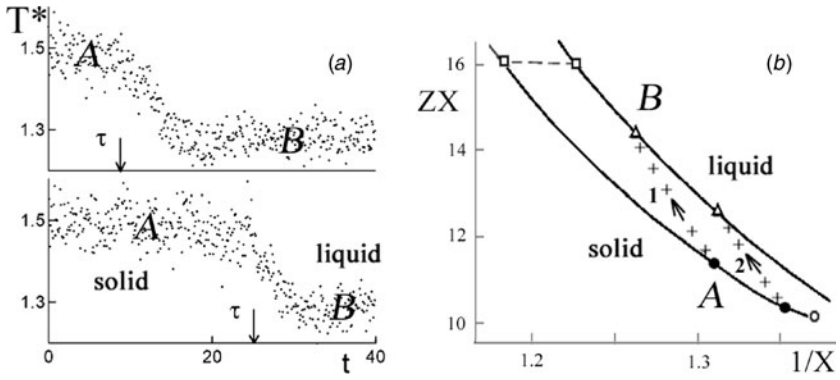

Figure 1. Melting of the superheated crystal on the T–t (a) and P–V (b) planes: (a) fluctuations of the instantaneous temperature T along two MD runs (the values of the lifetime τ for two different MD runs from one ensemble are indicated by arrows); (b) the dimensionless $P(V)$ isotherm for metastable solid (●), stable liquid (△), the equilibrium melting phase transition (□) and the spinodal (○) points, two examples of the melting decay (+).

and/or density. The character and duration of the melting of the superheated crystal can also be deduced from figures 1(a) and (b).

From the distribution of lifetimes $\left([\tau_k]_{k=1}^{M}\right)_{T,\rho}$ we can derive the value of the most probable lifetime $\tau^*_{T,\rho} = 1/M \sum_{k=1}^{M} \tau_k$ and the rate of the homogeneous nucleation $J(T;\rho) = (\tau^*_{T,\rho} N/\rho)^{-1}$ (the average number of critical nuclei of the new phase appearing in the unit of time per unit of volume). The general type of the homogeneous nucleation rate dependence on temperature is $J(T) = J_0 \exp(-W/k_B T)$, where activation energy $W \sim {T_m}^2/(T - T_m)^2$. The MD data for various values of T are fitted by this dependence. Since the soft-sphere potential is a uniform one, the unique function $J^*(1/X)$ can be obtained (figure 2(d)).

The determination of the $J(T)$ dependence allows us to evaluate the corresponding kinetic limit [25] of crystal stability (figure 2(d)) determined by the maximum value of nucleation rate $J_{\max} = \omega/V_c$, where ω is the average frequency of lattice vibrations, and V_c is the volume of the critical nucleus. The thermodynamic $(\partial P/\partial V)_T = (\partial ZX/\partial(1/X)) = 0$ and mechanic $C^*_{44} \to 0$ limits of stability are also estimated. It is evident that the limits of stability cannot be exactly achieved in the MD simulations. The extrapolation procedures are performed in figures 2(b) and (c). The values of P and C_{44} are calculated for the stationary part A of MD runs in figure 1(a). The results show that all three criteria give close limits which do not contradict each other and define the spinodal of the superheated solid in the model considered. The consistency of various criteria of stability is discussed [25–28]. Melting and spinodal X points for different potential softness n^{-1} fit a smooth curve which is consistent with the OCP point $n = 1$ from [29].

The previous results are related to the case of the spontaneous melting of the metastable solid when nucleation is observed from a stationary state. Another situation is also simulated via MD to see how heating conditions influence the process of melting. The second type of simulation is carried out to determine the dependence of the melting temperature on the heating rate.

Initially the temperature of the system is equal to T_m. Then the temperature is gradually increased with a certain heating rate $\dot{T} \equiv \mathrm{d}T/\mathrm{d}t = \text{const}$ by the appropriate velocity rescaling. The parameters of the heating method are chosen so that the system is in equilibrium at temperature $T(t)$ at each moment t. The moment of melting corresponds

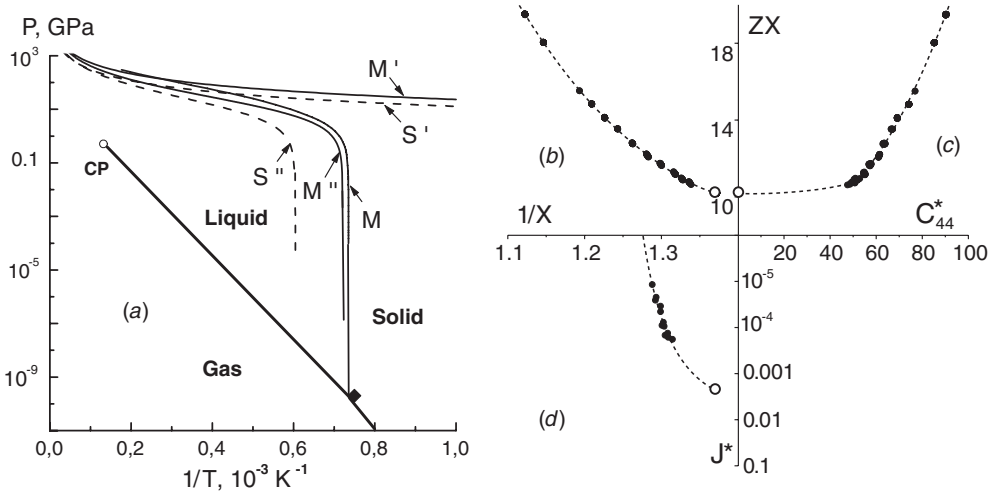

Figure 2. Limits of stability for copper and the soft spheres ($n = 12$): (a) copper phase diagram where M is the experimental melting curve, M' and S' are soft-sphere melting and spinodal curves, and M'' and S'' are soft-sphere melting and spinodal curves corrected for electron cohesion contribution (CP is the critical point); (b) thermodynamic limit; (c) mechanic limit; (d) kinetic limit for soft spheres.

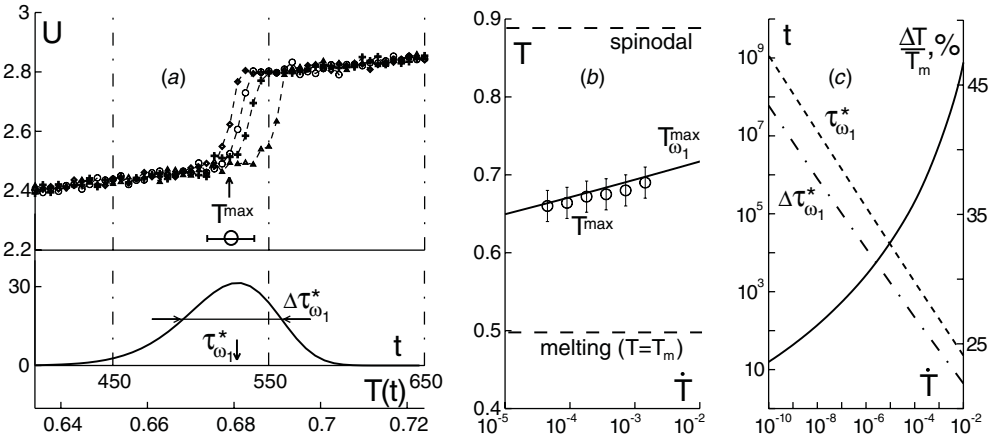

Figure 3. (a) The dependence of the average potential energy of particles U on temperature T and time t during the heating with constant rate ($\dot{T} = \text{const}$). The probability density of the first critical nucleus formation $\omega_1(T(t))$ calculated from the data on $J(T)$ from the independent calculations (see figure 2(d)) according to (1). The lifetime $\tau^*_{\omega_1} = (T^{\max}_{\omega_1} - T_m)/\dot{T}$ and the scatter time $\Delta\tau^*_{\omega_1}$. (b) The dependence of the melting temperature $T^{\max}$ on the heating rate $\dot{T}$: results of the direct MD simulation of the heating (○), dependence of $T^{\max}_{\omega_1}$ (——). (c) The dependencies of lifetime $\tau^*_{\omega_1}$ (- - -), scatter time $\Delta\tau^*_{\omega_1}$ (—·—·—) and the superheating ($\Delta T = T^{\max}_{\omega_1} - T_m$, ——) on the heating rate $\dot{T}$ calculated via (1).

to the jump on the dependence of the averaged potential energy of particles $U(T(t)) = 1/N\left(\sum_{i<j}\phi(|\vec{r}_i(t) - \vec{r}_j(t)|)\right)$ on time/temperature (see figures 3(a) and (b)).

For a fixed value $\dot{T}$ a bundle of MD trajectories $\left([\{\vec{r}(t), \vec{v}(t)\}_k]_{k=1}^{M}\right)_{T_m,\rho,\dot{T}}$ is calculated. The crystal structure in the MD cell melts at a certain moment τ_k along the kth trajectory.

This means the formation of the first critical nucleus of the liquid phase and its growth (until the whole MD cell is disordered). The corresponding value of the temperature is $T_k^{\max} = T_m + \tau_k \dot{T}$. The set $\left([\tau_k]_{k=1}^{M}\right)_{T_m,\rho,\dot{T}}$ gives the average value of the lifetime $\tau^*(\dot{T};\rho) = 1/M \sum_{k=1}^{M} \tau_k$ and its dispersion $\Delta\tau^*(\dot{T};\rho)$, i.e. the time scattering (figure 3(*a*)). The average value of temperature that can be reached with the certain heating rate is $T^{\max}(\dot{T}) = 1\Big/M \sum_{k=1}^{M} T_k^{\max}$.

The dependence $T^{\max}(\dot{T})$ can be also evaluated from the known dependence $J(T)$ in the framework of the general theory of the homogeneous nucleation in a non-isothermal process [30]. The probability density ω_1 of the appearance of the first critical nucleus in the volume $V = N/\rho$ under the heating $\dot{T} = \text{const}$ at the moment t is given by

$$\omega_1(T(t);\dot{T},V) = \frac{J(T(t))V}{\dot{T}} \exp\left(-\frac{J(T(t))V}{\dot{T}\,\mathrm{d}\ln J/\mathrm{d}T}\right). \tag{1}$$

If we assume that the crystal melts after the first critical nucleus has appeared, the maximum of $\omega_1(T(t))$ corresponds to the most probable melting temperature $T_{\omega_1}^{\max}$ and the average lifetime $\tau_{\omega_1}^*$. The scattering $\Delta\tau_{\omega_1}^*$ may be estimated as the FWHM of $\omega_1(T(t))$, figure 3(*a*). The results give the values of $T^{\max}(\dot{T})$ that are in very good agreement with $T_{\omega_1}^{\max}(\dot{T})$, figure 3(*b*). Since the latter dependence is obtained from the independent data $J(T)$, the consistency of the results is the evidence of the appropriate usage of (1) to describe nucleation and melting in the situation considered.

3. Superheating of metal and plasma column formation at wire explosion

The values of ϵ, σ and n for metals are taken from [31] to compare simulation and experimental results. The soft-sphere model is a simplified model of a metal under high pressures and temperatures. This model was tested in thermodynamical calculations [31] mostly for liquid metals. The comparison for solid metal is presented in figure 2(*a*) where the copper phase diagram is shown. Both the melting curve M' and the spinodal curve S' are obtained using the results of MD simulation for the soft-sphere system. The curve M' corresponds to the experimental curve M for high pressures, therefore we can expect that the soft-sphere spinodal S' is also reliable in this region. The correction for the electron cohesion is needed for lower pressures. Amendments according to the model [31] adjust the melting curve M'' close to the curve M. So the curve S'' gives the reasonable location of the solid copper spinodal.

Now we proceed to the comparison of the simulation lifetimes of the superheated solid with the experimental findings for the fast energy deposition.

According to [4] there is no change in the wire diameter during the initial process of increasing the temperature of the wire. The wire radius remains constant even when the energy deposited exceeds the sublimation energy. Then all the properties of the discharge change abruptly and the wire begins to expand linearly. Notice that the current increases by an order of magnitude in the transition point. So the magnetic field [32] is relatively low when the wire radius remains constant and the wire starts to expand despite the remarkable increase of the magnetic field. We suggest that this transition is interpreted as an abrupt change of the mechanic properties of the wire, i.e. as a spontaneous decay of the solid wire. The rigidity of the solid compensates for the possible difference between the internal pressure and the magnetic force before the transition.

The expansion of the wire was simulated by the magnetohydrodynamic (MHD) code in [6]. There is a reasonable agreement between experimental and computed rates of expansion points to the fluid state of the wire after the transition since fluid properties are used in the simulation. But the results of the MHD simulation [6] of wire explosions are not in complete agreement with experiment. The expansion of the wire in simulation begins about 5 ns before

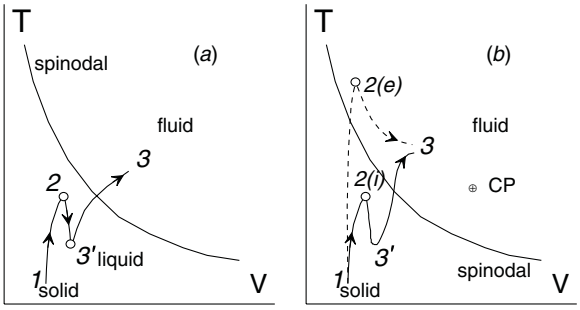

Figure 4. Schematic representation of the quasi-equilibrium (*a*) and non-equilibrium (*b*) scenarios of the initial stage of the fast electric explosion of wires.

the voltage collapse, however experiments show that these two phenomena are completely synchronized.

The equation of state used in the MHD model considered did not include the region of metastable solid. It is likely that taking into account the possibility of solid superheating can increase the time interval before the beginning of the wire expansion and improve results of MHD simulation. Using equation (1) we estimate the duration of the solid metal existence in the superheated state before the spontaneous spinodal decay to be about several nanoseconds. The heating rates in experiments are several orders of magnitude slower than it would be possible to simulate in MD runs. So we derive our estimations extrapolating the simulation data. The results obtained are in agreement with the introduced interpretation of the findings [4, 5].

Slow and fast explosion regimes are distinguished in [5]. The wire begins to expand as was noted above at the fast exploding. The wire disintegration is observed sometimes in the relatively slow explosion, when only some small parts of the wire disappear in the shadowgrams, whereas the other parts of the wire retain their initial diameter. These facts correlate with the results of our simulation that the scatter of lifetimes of superheated solid increases with the decrease of the heating rate.

For sufficiently high superheating, the rate of the heterogeneous nucleation (on defects, interfaces, etc.) [33] is much smaller than the rate of the homogeneous nucleation [25]. Hence the latter is the dominant melting mechanism. We assume that it may be valid for the experiments under consideration.

The experimental time resolution of the wire radius break at the moment of transition is less than 2 ns. It can be compared with the simulation of the spontaneous decay of the superheated wire. It is clear from figures 1(*a*) and 3(*a*) that the MD simulation gives the picture of the decay as well. We are able to obtain the duration of about 1 ns or less for the dimensional variables.

Two different scenarios of the superheating of solid metal prior to electric explosion of wires at fast energy deposition could be suggested. At the first scenario (figure 4(*a*)) the electron temperature equals the lattice temperature and solid superheating 1–2 finishes by the spontaneous spinodal decay 2–3′ and decrease of temperature according to figure 1(*a*). At the second scenario (figure 4(*b*)) lattice superheating 1–2(i) and non-equilibrium overheating of electron subsystem 1–2(e) [34] finish by a spinodal decay of the lattice 2–3′ as in figure 4(*a*) and subsequent equilibration 3′–3 of electrons and ions in non-ideal plasma formed. Relaxation times for such processes achieves the nanosecond range in the experimental findings [35, 36].

According to the experimental results [2–5] wires can accumulate energy several times larger than the sublimation energy at the fast initial heating stage of electric explosion before the decomposition. The soft-sphere model gives no more than one energy of sublimation. Preliminary estimates double superheating for the Lennard–Jones potential accounting for the attraction, cf figure 2(*a*). Non-equilibrium overheating of electrons is an additional factor in the second scenario. A similar problem of high-energy deposition arises in the physics of a vacuum arc cathode spot [37]. The problem needs additional study both experimentally and theoretically.

The possibility of immediate decomposition of overheated solid metal to plasma state is indirectly confirmed by the experiments on fast electric explosion of thin wires made in [6]. Namely, the appearance of alternating light and dark layers along the conductor (transverse stratification) was observed. This phenomenon is the characteristic feature of the most electric explosions of wires on their plasma stage. As shown in [38, 39], this is caused by the development of so-called overheat instability. The latter results from a decreasing dependence of electrical conductivity on temperature at the transition of solid metal to other phase states. The initiation of this instability is caused by an initial weak longitudinal non-uniformity of the conductor cross-section. The strata wavelength l observed is selected by the 'bottle-neck' mode of the magnetic-hydrodynamic instability which is driven by the competition of the surface tension and the magnetic pressure [40]. The value of l can be evaluated by the following equation, $l = 4\pi r((12\pi\sigma)/(rH^2))^{1/4}$, where r is the initial radius of the wire, σ is the surface tension coefficient, and H is the magnetic field created by the current. The rough estimate gives $l \approx 40$ μm which is comparable to the experimentally observed values.

It was shown in [39] that the transverse strata existence can result in strong electric fields between hot and cold layers. This can lead to the appearance of runaway-electron beams, which in turn excite plasma turbulence. The latter is accompanied by even more energy consumption by the electron subsystem. The consideration of this and further stages of the wire explosion is beyond the frames of the present paper. The competing processes of the instability development, which might be opposite to the equilibration 2–3, are not shown in figure 4(*b*).

4. Conclusion

The initial process of the ultrafast electric explosion of the wire is divided into successive stages: superheating of the solid wire, its spontaneous decay, fluid column formation and stratification, excitation of superthermal plasma oscillations in non-ideal plasma formed.

It is shown that the lifetime of the superheated metal is about 10 ns, therefore wire superheating is really possible during the ultrafast wire explosion. The spontaneous decay is accomplished for the time of about 1 ns or less. The stratum size is estimated for the non-ideal plasma column formed.

More theoretical and experimental work is needed to support the suggestion introduced in this paper.

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