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Soliton solutions of logarithmic wave equation and their application for polycrystalline metals

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Abstract. Wave equations with logarithmic nonlinearity are applied to Korteweg-type materials which can undergo liquid-solid or liquid-gas phase transitions. One of predictions of the theory is a periodical pattern for inhomogeneities of density, which can occur in the form of bubbles or cells. Such inhomogeneities are described by soliton and solitary wave solutions of the logarithmic wave equation in the vicinity of a liquid-solid phase transition. During the solidification process, these inhomogeneities become centers of nucleation of grains. Previous works were dealing with generic natural silicate materials in geophysics, such as magmas in volcanic conduits, where the (approximately) periodical flows and structures were observed. Here we report an experimental evidence of a large-scale periodicity in structure of grains in the structural steel S235/A570 Grade 36, copper C-Cu/C14200, stainless steel X10CrNiTi18-10/AISI 321, and aluminium-magnesium alloy 5083/5056.

1. Introduction

Wave equations with logarithmic nonlinearity find fruitful applications in different branches of physics - from nuclear physics and condensed-matter theory to particle physics, theory of physical vacuum and quantum gravity, to mention just a few literature landmarks [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17]. Such a universality can be explained by the fact that one can derive the logarithmic nonlinearity for a large class of the strongly-interacting manybody systems in which interaction energies predominate kinetic ones, using simple statisticalmechanics arguments and Madelung hydrodynamical presentation [17]. Examples of such systems include the Korteweg-type materials which can undergo liquid-solid or liquid-gas phase transitions [8, 18, 19]. In these materials, capillarity and surface tension play a substantial role, which makes them useful for modeling various flows with non-negligible surface and interface effects [20, 21].

One of theory's predictions are large-scale periodical inhomogeneities of density and microhardness, bubbles, cells or grains, caused by existence of multiple soliton and Gaussianshaped solitary wave solutions for an underlying logarithmic wave equation in the vicinity of a liquid-solid phase transition. Recently, a study of these solutions' application was done for generic natural silicate materials in geophysics [19], such as magmas in volcanic conduits, where

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the (approximately) periodical flows and structures were known to occur [18]. In this paper, we report an experimental evidence of above-mentioned periodicity in a grain structure of nonalloy structural steel S235/A570 Grade 36, copper C-Cu/C14200, stainless steel X10CrNiTi18-10/AISI 321, and aluminium-magnesium alloy 5083/5056.

2. Formalism

Let us use the fluid approximation of continuum mechanics and introduce the fluid wavefunction which encodes main properties of a flow. This function can be written in a Madelung form [22]

$$\Psi = \sqrt{\rho} \exp\left(iS\right),\tag{1}$$

where $\rho = \rho(\mathbf{x}, t)$ is a fluid density, and $S = S(\mathbf{x}, t)$ is a phase which is related to the fluid velocity $\mathbf{u} = \nabla S$ (we assume the irrotational flow for simplicity). This wavefunction should not be confused with particle wavefunctions in quantum mechanics, but rather it is a complex-valued function which stores macroscopic information about our fluid, such as the density and velocity of a fluid parcel [12, 22].

Nevertheless, some mathematical similarities between these categories of functions do exist and will be used in what follows. In particular, function Ψ obeys a normalization condition

$$\int_{V} |\Psi|^2 \mathrm{d}V = \int_{V} \rho \,\mathrm{d}V = M,\tag{2}$$

where M and V are the total mass and volume of the fluid. This poses restrictions upon fluid wave functions which are similar to a quantum-mechanical case: the set of all normalizable fluid wave functions must constitute a Hilbert space, such as L^2 .

Let us assume that such a fluid is in an isothermal state for which the characteristic kinetic energies of its particles are smaller than interaction potentials energies between them. This can happens not only at low temperatures but also in high-density or effectively low-dimensional system, because it is the ratio of kinetic and potential energies which matters.

If this ratio is small then, following a line of reasoning of works [17, 19], one can find out that the equation, which controls the dynamics of a function Ψ , contains the logarithmic nonlinearity:

$$i\partial_t \Psi = \left[-\frac{\mathcal{D}}{2} \nabla^2 - b \ln\left(|\Psi|^2 / \rho_0\right) \right] \Psi,\tag{3}$$

where b, ρ_0 and \mathcal{D} are real-valued parameters. One can show that $b \sim T$ where T is an absolute temperature and notation "~" means "a linear function of". This equation must be supplemented with the above-mentioned normalization condition.

It should be noted that, for the same set of boundary conditions, eq. (3) allows multiple (eigen)solutions which correspond to excited states in the Hilbert space of the problem. This means that the Korteweg-type fluid can "choose" one of these solutions spontaneously and thus undergo spontaneous phase transitions. However, the ground state is a preferable one as it corresponds to a minimum of the wave-mechanical energy. This and other low-energy states will be discussed in the next section.

Furthermore, substituting eq. (1) into eq. (3), one can recover the hydrodynamic laws for mass and momentum conservation for a two-phase compressible inviscid fluid with internal capillarity which flow is irrotational and isothermal:

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \tag{4}$$

$$\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \frac{1}{\rho} \nabla \cdot \mathbb{T} = 0, \tag{5}$$

with the stress tensor \mathbb{T} of the Korteweg form with capillarity effects [20], which is used to model fluid mixtures with phase changes and diffuse interfaces [21]:

$$\mathbb{T} = -\frac{\mathcal{D}}{4\rho} \nabla \rho \otimes \nabla \rho - \tilde{p} \mathbb{I}, \tag{6}$$

where \mathbb{I} is the identity matrix, $\tilde{p} = p(\rho) - \frac{1}{4}\mathcal{D}\nabla^2\rho = -b\rho - \frac{1}{4}\mathcal{D}\nabla^2\rho$ is a capillary pressure, and $p(\rho) = -b\rho$ is a barotropic equation of state for the fluid pressure p [8, 18].

Thus, eq. (3) is as a matter of fact a short form of writing two equations of hydrodynamics. This makes it useful for studies, especially because a large amount information about logarithmic wave equations has been revealed in different branches of physics and mathematics.

3. Phase structure and solutions

Depending on whether the nonlinear coupling b is positive or negative, the Korteweg-type material can be in different phases. Since this coupling is related to temperature, these phases correspond to the material above and below a certain critical temperature.

Cellular phase. If the nonlinear coupling is positive, then the field-theoretical potential density, given by

$$\mathcal{V}(|\Psi|^2) = -b|\Psi|^2 \left[\ln\left(|\Psi|^2/\rho_0\right) - 1 \right] + \mathcal{V}_0,\tag{7}$$

has an upside-down Mexican-hat shape, with local degenerate maxima at $|\Psi| = |\Psi_e| \equiv \sqrt{\rho_0}$ [19]. In this case, one solitary wave solution of eq. (3) can be found analytically [1, 2]. It has the form of a Gaussian parcel

$$\Psi_g^{(+)}(\mathbf{x},t) = \pm \sqrt{\rho_g^{(+)}(\mathbf{x})} \exp\left(-i\omega_g^{(+)}t\right),\tag{8}$$

$$\rho_g^{(+)}(\mathbf{x}) = \tilde{\rho} \exp\left[-\frac{(\mathbf{x} - \mathbf{x}_0)^2}{\ell^2}\right],\tag{9}$$

$$\omega_g^{(+)} = b \left[\bar{d} - \ln \left(\frac{\tilde{\rho}}{\rho_0} \right) \right], \tag{10}$$

where d is the number of spatial dimensions of the fluid, and

$$\tilde{\rho} = M/\tilde{V}, \ \tilde{V} = \pi^{\bar{d}/2}\ell^{\bar{d}}, \ \ell = \sqrt{|\mathcal{D}/(2b)|}$$
(11)

are the density peak value, effective volume and Gaussian width, respectively. One can show that the solution $\Psi_g^{(+)}$ has a lowest eigenvalue of the frequency, $\omega^{(+)}$, which makes it an analogue of a ground state in wave mechanics.

Therefore, in this phase, our material tends to fragment into clusters of density inhomogeneities with a Gaussian profile, referred here as cells. If this phase is a melt of some metal, then these inhomogeneities are more likely to become centers of crystalline nucleation when solidification begins.

Foam phase. If the nonlinear coupling is negative, then the field-theoretical potential density (7) has a conventional Mexican-hat shape, with a local maximum at $|\Psi| = 0$ and local degenerate minima at $|\Psi| = |\Psi_e|$; the latter correspond to a state with the lowest eigenvalue of frequency $\omega_g^{(-)} = 0$. This suggests that the model contains multiple topological sectors, and the topologically nontrivial solitons exists which interpolate between local minima.

Unfortunately, no topological solutions of eq. (3) can be found analytically in this phase, but numerical study reveals their existence. In Cartesian coordinates, this solution is a product of \bar{d} 1D kink solitons saturating the Bogomolny-Prasad-Sommerfield (BPS) bound,

$$\Psi_{s}^{(-)}(\mathbf{x},t) = \prod_{j=1}^{\bar{d}} \psi_{j}(x_{j},t),$$
(12)

and each of these 1D kinks have a nonzero topological charge,

$$Q = \rho_0^{-1/2} \left[\psi_j(x_j \to +\infty) - \psi(x_j \to -\infty) \right], \quad j = 1, ..., \bar{d},$$
(13)

where $\rho_0 = \rho_0^{1/\bar{d}}$. Numerical plots of these solutions and their densities can be found in figure 2 of ref. [19]. Despite this solution is not the lowest-frequency one, a nonzero topological charge enhances its stability against decay into a ground state Ψ_e . According to a value of charge Q, all non-singular finite-energy solutions can be cast into four topological sectors [10]. For two of these sectors, topological charge does not vanish, which ensures stability of corresponding BPS solitons.

Furthermore, the mass density of the soliton, $|\Psi_s^{(-)}|^2$, grows from its center of mass outwards, cf. figure 2 of ref. [19], therefore this solution can be viewed as a bubble with a characteristic size ℓ . In a single-solution setup this solution would extend for the whole space, but in the real material the multi-soliton picture must occur: kinks and antikinks would alternate and match each other at distances of an order ℓ . Therefore, a Korteweg material tends to form a foam-like structure in this phase. This process facilitates the release of previously dissolved gas. It can result in either boiling during the liquid-gas transition or in the formation of cavities in the bulk of the material, such as pores and blowholes caused by decreased hydrogen solubility or carbon monoxide production during solidification. Therefore, the above-mentioned phases can be used for modeling of both the liquid-gas transitions and the liquid-solid ones, depending on whether the temperature of the foam phase is larger or smaller than the temperature of the cellular phase.

4. Large-scale structure of metals

The crystalline structure appears in metals during a solidification process. In pure metals, this structure is merely a crystal lattice, which can be of a simple cube, body-centered cube and face-centered cube type. In real metals, due to various impurities and inhomogeneities, a much more complicated pattern arises. Throughout the melt, multiple centers of nucleation occur. Crystals begin to grow from those centers until the reach each other in the bulk. This is where interfaces develop marking borders of single-crystal domains grains, each of about a micrometre scale. Finally, the non-crystal polycrystalline structure occurs as a macroscopic large-scale pattern of adjacent grains.

The question arises: how orderly is this large-scale pattern? Is the size and mass of each grain a totally random value? Apart from purely academic interest, such questions have an immediate practical importance. Each grain's microscopic hardness depends on its size and density distribution therein. Therefore, if one controls sizes of grains, at least on average, one can control the macroscopic properties of the whole material, such as hardness, plasticity and mass. This is of utmost importance for industrial applications.

The conventional statistical mechanics of the nucleation process is extremely complicated, due to an obvious complexity of this process and large number of effects and acting agents involved, both physical and chemical. In most cases, one ends up applying the "commonwisdom" arguments: since the impurities and hence nucleation centers are randomly distributed in the molt bulk, one would expect that distances between those centers are going to be random too. Therefore, one would expect that the distribution of sizes of grains would be close to uniform, hence no periodic pattern in the large-scale structure in the polycrystalline metals can form.

A theory described in previous sections gives a different answer to this question, which is also a more specific one. If the melt can be described by a Korteweg-type system, at least in the leading-order approximation, then, according to our model, its density has a tendency to form a periodic pattern of repeating solitonic solutions (gaussons or kinks, depending on a phase).



Figure 1. Hardness profile (a) and distribution of grain sizes (b) for the structural steel S235/A570 Grade 36.

In other words, the density inhomogeneities emerge in a melt on a large scale which are not directly related to molecular bonding but they are a collective nonlinear phenomenon. During a solidification process, those points where density profile reaches extrema are more probable to become centers of nucleation. Therefore, an average size of a grain can not be a random value, but it must be close to a width ℓ of the solutions of a previous section, cf. formula (11).

5. Experiment

We consider a few most common polycrystalline metallic materials: non-alloy structural steel S235/A570 Grade 36, copper C-Cu/C14200, stainless steel X10CrNiTi18-10/AISI 321, and aluminium-magnesium alloy 5083/5056.

Microstructure of the steel S235/A570 consists of the ferrite and pearlite phases, with a 75 : 25 proportion, respectively. Ferrite grains have mainly an equiaxial structure, except a few stringer grains of an elongated shape. They have no particular spatial orientation, and their size varies around 20 μ m. Sizes of the pearlitic microconstituent grains for this steel vary between 5 and 45 μ m.

Microstructure of the copper specimen consists of approximately equiaxed grains of a size about 100 μ m. As in the previous material, a few stringer grains of an elongated shape are present. Inside grains one can find deformation twins.

Microstructure of the stainless steel is austenitic and consists of polyhedral grains of a size about 100 μ m. As in the copper specimen above, one can encounter deformation twins in this steel.

Microstructure of the aluminium alloy specimen consists of approximately equiaxed grains of a size about 30 μ m. A small amount of secondary ferric and silicon phases can be found both inside grains and on their borders.

The microhardness measurements of microstructure components were performed for abovementioned metals by using the Vickers hardness method. The load during the measurements was chosen according to a size of indentation in a specimen. The minimal load was chose to be either 0.025 or 0.05 N, depending on a grain's size. The points of load's application were in the following areas of a grain: grain's center, half-way to the grain's border, near the border, and on the border.

The profile of a microhardness throughout the structured steel's specimen is given in figure 1a. Since the hardness is related to a density of the material, its pattern immediately suggest a presence of a large-scale structure. The statistical analysis confirms that the average size of grains is not random: its distribution is far from being uniform but has a peak, cf. figure 1b. Other materials from those mentioned above demonstrate similar patterns to figure 1, and thus they are not listed here.

6. Conclusion

Wave equations with logarithmic nonlinearity are applied to Korteweg-type materials which can undergo liquid-solid or liquid-gas phase transitions. These materials have a two-phase structure where each phase is marked by a sign of the nonlinear coupling. Depending on whether the nonlinear coupling is positive or negative, solutions can have both trivial and non-trivial topology.

From a physical point of view, such solutions describe the inhomogeneities of density, which can occur in the form of bubbles or cells in the vicinity of liquid-solid phase transition. For instance, during the solidification process, these inhomogeneities become centers of nucleation of grains in the Korteweg-type material. One of theory's predictions is a large-scale periodical patterns, which is opposite to the randomness expectations based on plain statistical arguments. Due to numerous additional effects occurring during the solidification process, this periodicity gets distorted but not entirely destroyed.

Previous works were dealing with generic natural silicate materials in geophysics, such as magmas in volcanic conduits, where the (approximately) periodical flows and structures are known, see works [8, 18, 19] and references therein. We conducted experimental studies of structure of grains in structural steel S235/A570 Grade 36, copper C-Cu/C14200, stainless steel X10CrNiTi18-10/AISI 321, and aluminium-magnesium alloy 5083/5056. Based on results, we thus report an experimental evidence of the above-mentioned periodicity in these materials' structure. We show that an average size of grains in metals should be closely related to the average width of the soliton-type solutions ℓ .

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