Project name:

The physics of laser action on materials: theory, simulations and applications

1.3. Keywords (given no more than 15 terms)

creation of nanostructures and meta-surfaces, laser and plasmonics, ablation into liquid, droplet fragmentation, computer physics, semiconductors

1.4. Annotation of the project (no more than 2 pages; including, briefly, the relevance of solving the above scientific problem and scientific novelty)

Beams of particles and light generate innovative processing technologies. Electron flux, focused ion beam (FIB) and laser irradiation are new tools that increase manufacturing precision by many orders of magnitude compared to, say, the drill traditionally used in mechanical engineering. On the other hand, continuous lasers and powder targets for 3D printing make it easy to get around topological problems that are inevitable with conventional ways of creating complex three-dimensional objects, for example, lattice products or products with intricate internal geometry. This project addresses the fundamental problems that arise precisely in laser applications, since laser micro-structuring is much more economical than ablation by means of electrons or FIB.

In this case, the electron microscope and FIB are also used in the project, but as diagnostic equipment, when working with experimenters, see, for example, [1-3].

The promising and already used technologies, which are studied in this application, are based on the subtle control of the space-time distributions of the radiated laser energy. This operation is carried out in two ways. First, by exciting surface plasmon-polariton (SPP) modes [4]. And, secondly, through the use of complex beams [2,5] - here we speak of beam-forming phase plates and vortex effects in optics [5] or in x-rays [2].

We are talking about making holograms, meta-surfaces, metamaterials, i.e. materials with properties that are not found among natural substances [1]. The appearance of unusual characteristics is due to precise ordering, structuring at the micro- and at the nanolevel for the use of interference effects between light and SPP by electromagnetic (EM) fields [1]. Just for this precision is required.

Other important directions in our project. not yet investigated or insufficiently studied, are the ablation of metals and semiconductors into a liquid [6], laser fragmentation of liquid drops [7], ablation of refractory metals, and sintering/melting of powder targets [8].

The experience accumulated in the team allows in this application to take up these complex, necessary in practics problems.

We will discuss the relevance and novelty. The excitation of the SPP mode by electromagnetic (EM) laser radiation has been discussed for a long time [9]. In these works, a resonance is sought between the incoming flat EM wave and the corresponding SPP mode with equal frequency, represented in the spectrum of the SPP mode. The SPP mode spectrum is associated with a random initial roughness of the reflecting surface. Interference of the EM waves of a laser and PP polaritons undoubtedly influences the formation of laser induced periodic surface structures (LIPSS). To create LIPSS, a wide beam is used (many wavelengths fit in a spot on the surface) and multiple exposures. LIPSS grows gradually "out of nothing". The spatial period of LIPSS is poorly controlled.

In our proposed approach, an SPP mode is immediately created with a frequency required for interference with the laser. In our previous work, the Kretchmann configuration [4] was used for this. In the new project, the source of the SPP field is a localized spatial perturbation on the surface in the form of a protuberance-dome. The processes of formation of such a hillock by a single shot were studied in our previous works [10]. The EM wave of the second shot at or near the same point, firstly, generates a running SPP mode with the desired frequency and, secondly, interferes with this SPP mode, creating a standing wave. As a result of the action of a standing wave, instead of a protuberance, a complex pattern arises of the spatial interference imprinted in the material, which was observed by our colleagues [11]. We will create a physical model and explain how a standing wave is impressed, how to control the picture, what are the optimal conditions (focus, duration, intensity) - this is new compared to [4] and [11]. The urgency of the problem is connected with the problems of creating metamaterials.

Works on physical models and modeling of metal ablation into a liquid with the formation of nanoparticles are extremely in demand. The relevance of appropriate applications in electronics, catalysis, nanotechnology, biomedicine is described in detail in recent reviews [12]. Today there is no description of how nanoparticles are formed, and how they get into the liquid. Only the initial stage of the process [6] and the final stage with a bubble [13] are described. The part of the initial stage studied [6] is still very far from the formation of a bubble. Whereas the final stage relies on a rather simple approach with the Rayleigh-Plesset equation in spherical geometry [13]. This approach is in no way connected with ablation at the initial stage, which proceeds in a one-dimensional geometry — the diameter of the heating spot is of the order of fractions of a millimeter, and the thickness of the heating layer is of the order of 100 nm. In our project work, a theory and a computational methods will be created for all stages of the process, from the absorption of laser energy to the formation of a bubble and the transition of nanoparticles into a vapor-liquid mixture using water as an example. The approach will be based on the equations of state and interatomic potentials of the interaction of metals and water. The equations of state are used in hydrodynamic calculations, and the interaction potentials are used in molecular dynamics simulations.

Very difficult tasks are laser crushing of droplets. The laser action generates a highly unsteady three-dimensional multiscale flow in which it is important to take into account all factors from hot plasma to strength/destruction effects and capillary spattering [7,14]. We has created a code describing the fragmentation of the tin microdroplets, see [7] and the movie in the "SV.mp4" on

site http://laser.itp.ac.ru/RNF2019/index.html (comments in reference [7]). The physical model developed by us includes the EAM (embedded atom method) potential for the interaction of atoms of liquid tin. Tin drop fragmentation is an important part of a comprehensive program related to the creation of the lithographic machines of the future. In such machines, the length associated with the diffraction limit is sharply reduced, since vacuum ultraviolet with a photon energy of 90 eV and a wavelength of EM radiation of 13.5 nm is used. The task was developed jointly with the staff of the Institute of Spectroscopy RAS and JIHT RAS.

In the new project, the problem of the action of a hard X-ray laser beam (8 keV photon, pulse duration 30 fs) on a water drop will be solved. The corresponding experiments [14] were performed recently on a Coherent X-ray Imaging (CXI) device at a Stanford linac (Linac Coherent Light Source - LCLS). The calculations will use two-temperature hydrodynamics and a new modification of our multiprocessor SPH (Smoothed Particle Hydrodynamics) code [15], along with detailed information on the characteristics of water.

The problem of ablation of ruthenium will be solved. This is an important little-studied refractory metal, which is used in X-ray optics. The interatomic potential of ruthenium will be created, which is not just because of the need to fit it to a large surface tension and high melting point plus additional complexities of the crystallographic plan (hexagonal close-packed lattice is characterized by two parameters). The equation of state will be created taking into account the two-temperature effects. On this basis, two-temperature hydrodynamic and molecular dynamics calculations will be carried out. Work will be conducted in conjunction with the experiment. Action of ultrashort laser pulses with different wavelengths from optical to hard ultraviolet and hard x-rays at different angles of incidence will be considered.

Studies will be conducted on melting of powders of microparticles by a laser pulse. This is an important new topic that has been little studied in relation to the creation of physical models and codes for analyzing ongoing processes.

The improvement of the SPH code in the direction of the inclusion of phase transitions will be continued. This is a high-performance multiprocessor code that is used in the project in the problems of ablation into water, crushing of droplets, and thermo-hydrodynamics of powders. It is very important that the code has no space-time limitations, in contrast to molecular dynamics, limited by the space scale of the order of a micron and by times of the order of tens of nanoseconds. The SPH code named VMD3 (Voronoi Material Dynamic Domain Decomposition) developed in our team [15] is effective in describing fracture and fragmentation in multidimensional geometry.

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1.5. Expected results and their significance (the expected results and their scientific and social significance are indicated (assessment of the compliance of the planned results with the world level of research, the possibility of practical use of the planned results of the project in the economy and the social sphere))

A) Spatially distributed heating due to a combination of plasmon and laser EM fields.

The wide possibilities for creating complex spatial structures on the surface are associated with the interference of the plasmon and laser EM fields (motivation: making holograms and meta-surfaces). The plasmon wave is created by the same laser pulse on the spatial inhomogeneity of the flat surface of the target. Due to interference, a standing wave is formed. In the standing

wave, the heating maximums are in the antinodes (hot ridges). There are nodes between the ridges, there is no heating in nodes. We are interested in the amplitude of the laser action, which is sufficient to fully or partially melt the film. The pulse duration is less than the time of mechanical rebound of a thin film from the underlying dielectric substrate and less than the time of heat transfer from the antinodes into the nodes.

The formation of the dome by the first shot will be simulated. For this, the previously developed approach will be used, see references [10] to section 1.4 of the application and the movies "Au-220.gif", "Au-225.gif" and "Au-226.avi" on the site http://laser.itp.ac.ru/RNF2019/index.html. Near EM field of a standing wave associated with a laser, surface and dome will be calculated by numerical methods of electrodynamics. The heating of the film in the standing wave due to the absorption of the EM field of the standing wave in the skin layer of the film will be calculated. Both film movement and thermal processes in a moving film will be modeled by using molecular dynamics and SPH method. As a result, data will be obtained on the formation thresholds and on the characteristics of the spatial structure consisting of the dome and the standing wave imprint in the film and substrate. The results obtained will be compared with the results of experiments from reference [11] to section 1.4 and the new experiments of the Vladivostok group.

It will be understood what happens as a result of lighting the above structure with the third shot. For this, additional electrodynamic modeling will be performed.

Today in the world literature there is neither a description nor a solution to such a problem. This is due to the difficulties of creating a physical model and a numerical scheme that matches the electrodynamic calculation with thermal-hydro-physical modeling. From the decision of the problem there are significant benefits associated with the creation of technologies for meta-surfaces and holograms.

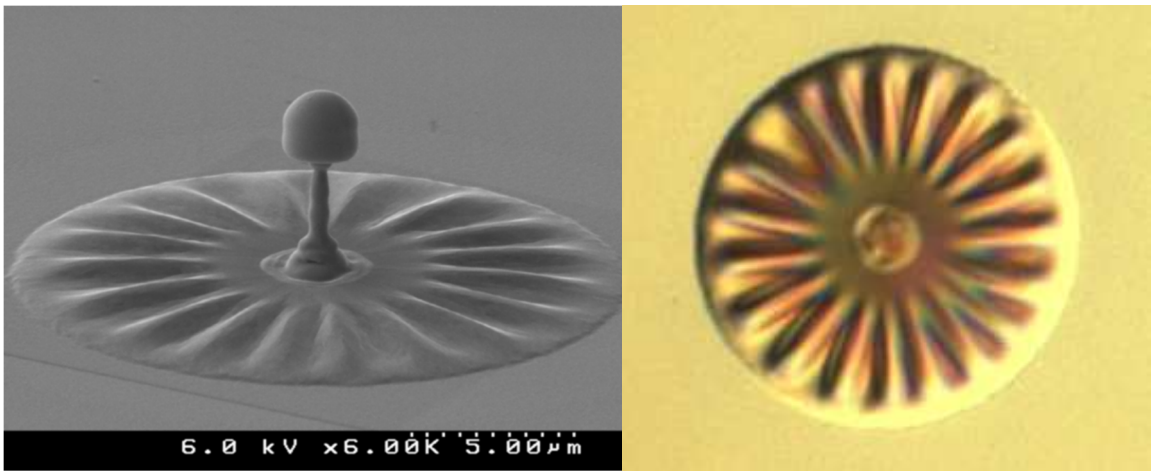

Fig. 1. Side and top view of the settled and frozen dome. Visible radial corrugation of the dome. Michael R. Armstrong Lawrence Livermore National Laboratory (private message), see also https://simes.stanford.edu/events/mike-armstrong-simes-seminar/ . Similar observations were made in the group of prof. B.N. Chichkova: Wortmann et al., Journal of Laser Applications V. 24, 042017 (2012); doi: 10.2351 / 1.4734048

The formation of radial goffering on the domes will be explained, see the example shown in fig. 1.

B) Action of vortex beams.

Relatively recently, the audience working in the field of laser applications was quite shocked by the work [5] (see literature to section 1.4; several Nature articles) on vortex beams with acute focusing (i.e., spot size on an irradiated target about the wavelength). Typical formations in the form of twisted spiral tips are shown in fig. 2.

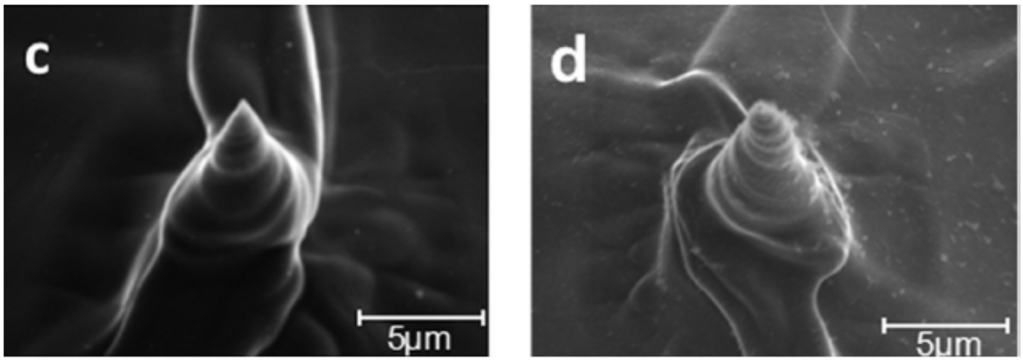

Fig. 2. Twisted pointed tops arising after the impact of the vortex bundle. The illustration is taken from the article by Toyoda et al., Nano Lett. (2012) DOI: 10.1021/nl301347j (200 references to this article), see [5] in section 1.4.

The authors of works from the group of prof. T. Omattsu associate the formation of chiral structures with the angular momentum brought by the photons of the vortex beam. Moreover, when creating such twisted tips, the authors use lasers with different pulse durations and different targets. But no quantitative calculations that would explain the origin of the structures are not available today. The project will create a theory, find an explanation for the phenomenon, solve this problem and carry out numerical calculations. The results will be compared with the experiments that are conducted in the FIAN in the department of prof. A.A. Ionin.

The work is practically significant. It represents a new variant of the fundamental problem related to the interaction of laser radiation with matter. Such a vortex treatment opens wide additional technological possibilities: filtering of molecules based on their chirality, the formation of chiral plasmon devices (illumination of the structure returns a vortex wave in reflected light), the creation of highly sensitive sensors, etc., see [5] in section 1.4.

C) The formation of nanoparticles during ablation into a liquid.

A very difficult problem on the ablation of a metal into a liquid will be solved. This problem is relevant due to its importance in many applications, see the reviews [12] in the list of references to section 1.4; International conferences are held on the problem; see this year's ANGEL conference website: http://angel-conference.org/en. Currently, there are only the very first

attempts to solve this problem, which is important for optimizing the very costly (in the financial term) technologies [12] of laser fabrication of nanoparticles. These attempts cover only either the initial (see [6] in section 1.4) or the final (see [13] in 1.4) stages of the processes taking place.

In the project, an exhaustive end-to-end solution will be obtained that covers the initial stage, follows the development of phenomena at several intermediate stages and continuously moves to the vaporization stage in the hot contact layer of the liquid with the appearance of the vapor bubble, its expansion, stop of expansion and the begining of the return movement leading to the compression of the bubble. The success of such work would greatly help the groups involved in the fabrication of nanoparticles. Calculations will first be performed for the case of water. Detailed information available in the literature on water properties will be used.

In addition to problems with a hard impulse X-ray and a drop of water, research on a drop of tin will be continued. It is necessary to replace the equation of state of Mi-Grüneisen, used in [7] (see the literature for § 1.4), with a tabular equation of state.

D) Laser fragmentation of liquid droplets and jets.

The problems of fragmentation of liquid microdroplets by laser action are very complex. Difficulties are associated with rich physics (from the interaction of radiation with the target matter and the creation of extreme conditions in temperature and pressure to capillary phenomena) and the sharply unsteady three-dimensional nature of flows. Moreover, the flow structure is hierarchical, covers several orders of magnitude in time and space: from fast to slow processes and on a spatial scale from the order of the size of a drop to the smallest fragments of fragmentation. We have a positive experience in solving the problem, see reference [7] in section 1.4.

The project will solve the problem of the impact of a thin cylindrical beam of hard X-rays on a microdroplet of water or a liquid jet. The beam diameter is 1 μm, the size of the droplet and the diameter of the jet are several tens of μm. Task setting is shown in fig. 3.

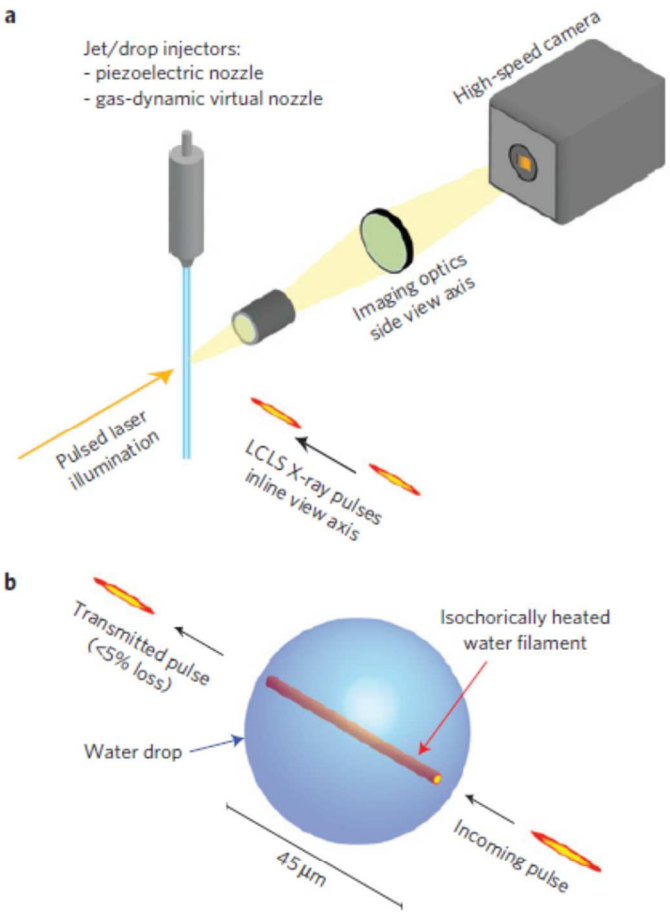

Figure 1 | Inducing liquid microexplosions with ultraintense X-ray pulses. **a**, Experimental design. Pulses from an X-ray free-electron laser, focused to a ~1 µm beam diameter, intercept water droplets (32 to 45 µm diameter) or water jets (2.75 to 30 µm diameter) flowing in a vacuum chamber. The subsequent phenomena are imaged optically, after a variable delay time, using a femtosecond laser for illumination. **b**, Schematic of the energy deposition process. A focused femtosecond X-ray pulse passes undeflected though the drops, and a small fraction of the pulse energy is absorbed in the drop, heating isochorically a micrometre-wide filament of water to average energy densities tens to hundreds of times higher than those needed to vaporize water.

Fig. 3. Figure illustrates the formulation of experiments. Taken from the first of the works in reference [14] in Section 1.4.

Typical data of the experiments conducted by the Stanford accelerator Linac Coherent Light Source are shown in fig. 4. Coherent X-ray Imaging (CXI) instrument was used.

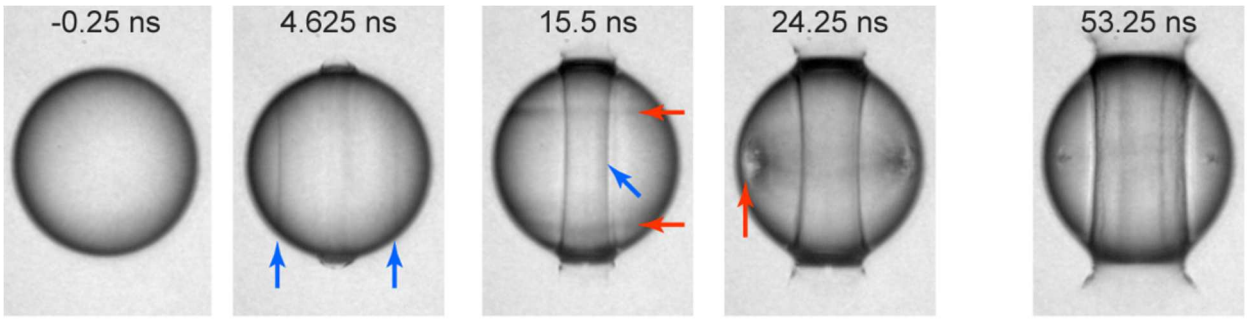

Figure 1. (a) Experimental design. A focused, ultraintense X-ray laser pulse deposits energy in microdrops of water, forming a high-pressure filament that launches a shock wave and forms a cavity inside a drop. These processes are investigated using time-resolved, bright-field optical imaging. (b) Images of 55 μm diameter water drops during the experiments. For each column in the array of images, the solid arrows indicate the location of the phenomena listed at the bottom of the column, in the same font color as the arrows. The shock waves are visible as straight lines; they are reflected from the surface of the drops into negative pressure waves that can lead to cavitation or spallation inside the drop. Spallation produces a void–liquid interface that reflects the illumination light and leads to the appearance of bright regions in the images.

Fig. 4. Figure taken from Stan et al., J. Phys. Chem. Lett. V. 7 (11), 2055–2062 (2016). The figure illustrates the pattern of dispersion and fragmentation of a liquid drop of water after ultrashort (30 fs) exposure to a thin hard X-ray cylindrical beam (8 keV) —the figure goes vertically along the central diameter. As a result of the ultrashort impact, an expanding column is formed, filled with low density hot plasma.

To solve the problem presented in Fig. 3 and 4, the complex of programs will be modified and new approaches will be added, both in physics and in the algorithms used. In physics, we are talking about the description of the interaction of the X-ray beam and in the description of two-temperature phenomena. There is extensive experience in the study of X-ray effects in a team [1]. Also applies to two-temperature models [2]. Subroutines with X-ray physics and two-temperature effects, as well as detailed information about the equation of state of water, will be inserted into the SPH algorithm.

E) Ablation of refractory metals.

The first in the application in the section on refractory substances is the example of ruthenium. This is an important structural material used in X-ray optics. Therefore, it is necessary to investigate its behavior in different modes of irradiation.

A potential of interatomic interaction of ruthenium will be created. An equation of state for ruthenium will be developed taking into account two-temperature effects. DFT (density functional theory) calculations will be carried out to develop the potential and to create the equation of state. They will be performed using quantum-mechanical computation packages (VASP, Elk, etc.). In such calculations, the cold ruthenium curve is determined. It is necessary for building the interatomic interaction potential using the stress matching algorithm. In DFT calculations, two-temperature effects will be defined. For this, a series of calculations will be performed on the electron temperature, in which the electron subsystem is excited to a given temperature in the hcp ruthenium crystal. As a result, electronic contributions to pressure and internal energy are determined, and the electronic heat capacity is found. These values are non-

trivial functions of density and temperature. They cannot be approximated by functions that correspond to the free Fermi gas.

Next, two-temperature hydrodynamic and molecular-dynamic calculations will be performed. Work will be conducted in conjunction with the experiment. Ultrashort action of lasers with different wavelengths from optical to hard ultraviolet and hard x-rays at different angles of incidence will be considered. Our team has begun preliminary work in this area [3].

F) Laser melting of powders.

The problem of melting powders using a laser beam is an important and complex. The importance of the problem is connected with modern technologies of three-dimensional printing of objects. With this approach, some difficult problems related to the manufacture of objectss of complex shape are removed, see section 1.4. Manufacturing of objects by melting powders is cheaper and technically easier than traditional methods associated with castings. On the other hand, research in this area is currently in its initial state. The mechanics of flowing media (soft matter) [4,5] is analyzed in connection with the process of filling the chamber with powder before melting. But the problem of melting actually remains unresolved.

While researchers are considering problems on the melting pool, they speak about thermocapillary convection caused by the temperature dependence of the surface tension coefficient (the Marangoni effect). In this case, the question of melting the powder itself remains unexplored. Here it is impossible to apply the statement as in the Stefan problem, since the medium is not homogeneous.

Our team has experience in solving problems of throwing powders with a shock wave and experience in analyzing of shock compression of porous media. But the melting problem stands alone. The pressure is relatively small, the shock compactification has no place. It needs to focus on thermodynamics and melting kinetics, on thermal effects, and then on the problem of melt recrystallization. A lot of work has been done on the problem of solidification of the liquid phase in our group.

The project will solve the problem of melting of a powder of metal microparticles with a laser pulse.

G) Computational physics, large-scale high-performance numerical simulation.

Computational techniques play the most important role in the execution of the project. We have powerful effective hydrodynamic and molecular dynamics codes. In the project, these codes will be improved and filled with new physics. The development of codes in itself is a practically important task. Next methods will be developed and applied:

(1) one-dimensional two-temperature hydrodynamic program in Lagrangian coordinates with complete physics (absorption, thermal conductivity, electron-ion exchange) and a tabular equation of state; for examples of application, see [6] in the list of references to § 1.4; the program will be used in relation to tasks A, B, C, D, E;

(2) multiprocessor high-performance program for molecular dynamics simulation with deep parallelization. At present, an important modification of the program has been developed, which includes the Monte Carlo block. This allows us to simulate the problem of melting and recrystallization of metals. As is known, in metals the electron thermal conductivity is much higher than the thermal conductivity associated with the thermal motion of ions.

A method has been developed for scaling calculation by capillary and thermal dimensionless parameters. Scaling in size and time relies on complete freedom in setting the coefficient of electron thermal conductivity κ in the Monte Carlo block, as well as on some freedom in varying the surface tension coefficient σ. A change in the coefficient κ has no effect on the characteristics of the substance modeled by the EAM (embedded atom method) of the interatomic potential. These characteristics include: compressibility, coefficient of thermal expansion, energy of formation of defects, melting point, and others; for the constructed EAM, these values with good accuracy correspond to the table values for this substance.

This is understandable, since the Monte Carlo block is external to the molecular dynamics program itself.

The surface tension is also adjustable in the direction of decreasing compared to the actual value approximately two times. V.V. Zhakhovsky developed EAM versions for one substance with different σ values. At the same time, the characteristics listed above (compressibility, etc.) remain in accordance with the table values. The pressure of saturated steam and the position of the critical point vary somewhat.

The scaling technique allows us to significantly expand the spatial-temporal limits of the application of molecular dynamics (MD). Usually, the upper limit for MD is sizes of the order of microns and times of the order of tens of nanoseconds. The MD code with a Monte-Carlo extension or without it will be applied when solving all the problems listed above, A – F.

(3) Improved material models will be developed for use in the SPH (Smoothed Particle Hydrodynamics) code.

This code will be used to solve problem C in the list above; C - ablation into fluid. Using the SPH code, we will remove restrictions on linear sizes and on the duration of the simulated time period; such limitations are inherent in molecular dynamics code.

New physical models for SPH calculations include tabular equations of state of materials with phase transformations and models of substance tensile strength in solid and liquid states in a wide range of temperatures and strain rates. A lot of hard work will be done to account for capillary effects in the SPH code.

The SPH code will be adapted to solve problem D; D is a splitting of a drop or jet of water by a narrow beam of hard x-rays from the American XFEL / LCLS (X-ray free electron laser / Linac Coherent Light Source) SLAC laser at Stanford.

By modifying the SPH code, the problem of laser heating and melting of mesoscopic objects — powders of microparticles (problem E in the list above) will be modeled.

(4) Use of packages of quantum-mechanical programs of the density functional theory and the simplex method for constructing the interatomic potential in ruthenium.

A new potential of the interatomic interaction of ruthenium will be developed using an approach combining the rolling polygon method (simplex method) with Monte Carlo with random walks. The parameters of the potential are determined from comparison with stresses (stress-matching), calculated in dependence on the density and orientation of the crystal at low temperature (cold curves) using the packages of quantum-mechanical programs of the density functional theory VASP, Elk, Abinit.

(5) Use of COMSOL Multiphysics © and LS-DYNA packages for calculating plasmon and laser electromagnetic fields and vortex electromagnetic beams in the problems A, B.

(6) As a major tool in our team, combinations of programs and hybrid approaches based on them are used. This allows in a reasonable time to describe the tasks that seem unsolvable at first glance.

This is how the problem of crushing a drop of tin by a laser stroke at the illuminated hemisphere of a spherical drop was solved; see [7] in the list of references to section 1.4. The fact is that the SPH code used in this problem cannot cover the laser absorption zone of the order of 100 nm and the entire radius of a drop of 50 μm. The size ratio is 500; if we even put 10 SPH particles per absorption zone, then the number of particles exceeds tens of billions.

This is an unaffordable number even for our SPH code, whose performance has been increased by many orders of magnitude compared to the usual (up to 105 particles) single-processor versions due to the use of an algorithm with deep parallelization and auto-balancing between compute nodes, see the description in [15] in the list of references to section 1.4. Normal loading for our multiprocessor version is tens of millions of particles.

Therefore, a hybrid approach was applied in which the absorption in the absorption zone, the formation of a compression wave and its propagation into the drop interior were calculated separately. And then the resulting field of hydrodynamic variables was transferred to the SPH code.

Another example of an effective hybrid approach is described in [10] in the list of references to section 1.4. A physical model was created that allowed us to use a combination of the Lagrangian two-temperature hydrodynamic program (1) and the MD-MC (molecular dynamics and Monte Carlo) program (2) to solve the problem of laser blistering of thin-film coatings. As a result, the practically very significant problem of laser formation of meta-surfaces (see [1] in section 1.4) was solved by creating arrays of micro-nano-caps.

Similar techniques will be applied when solving the above problems A-F.

H) Characteristics of silicon irradiated by laser

See form 4

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals

See form 4

Literature to 1.5

[1] *Previous publications of the team on X-ray sources*

A.Ya. Faenov, N.A. Inogamov, V.V. Zhakhovskii, V.A. Khokhlov, K. Nishihara, Y. Kato, M. Tanaka, T.A. Pikuz, M. Kishimoto, M. Ishino, M. Nishikino, T. Nakamura, Y. Fukuda, S.V. Bulanov, T. Kawachi, Low-threshold ablation of dielectrics irradiated by picosecond soft x-ray laser pulses, Appl. Phys. Lett. V. 94, 231107 (2009);

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N.A. Inogamov, V.V. Zhakhovsky, A.Y. Faenov, V.A. Khokhlov, V.V. Shepelev, I.Y. Skobelev, Y. Kato, M. Tanaka, T.A. Pikuz, M. Kishimoto, M. Ishino, M. Nishikino, Y. Fukuda, S.V. Bulanov, T. Kawachi, Y.V. Petrov, S.I. Anisimov, V.E. Fortov, Spallative ablation of dielectrics by x-ray laser, Appl. Phys. A V. 101(1), 87-96 (2010); arXiv:0912.3184 [physics.optics];

M. Ishino, A.Ya. Faenov, M. Tanaka, N. Hasegawa, M. Nishikino, S. Tamotsu, T.A. Pikuz, N.A. Inogamov, V.V. Zhakhovsky, I.Yu. Skobelev, V.E. Fortov, V.A. Khohlov, V.V. Shepelev, T. Ohba, T. Kaihori, Y. Ochi, T. Imazono, T. Kawachi, Nanoscale surface modifications and formation of conical structures at aluminum surface induced by single shot exposure of soft x-ray laser pulse, J. Appl. Phys., V. 109, 013504 (2011);

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M. Ishino, N. Hasegawa, M. Nishikino, T. Pikuz, I. Skobelev, A. Faenov, N. Inogamov, T. Kawachi, M. Yamagiwa, "Low electron temperature in ablating materials formed by picosecond soft x-ray laser pulses," Proc. SPIE 9589, X-Ray Lasers and Coherent X-Ray Sources: Development and Applications XI, 958904 (September 22, 2015);

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[2] *Previous work of the team on the physics of two-temperature phenomena (several selected publications in recent years)*

N.A. Inogamov, Yu.V. Petrov, V.V. Zhakhovsky, V.A. Khokhlov, B.J. Demaske, S.I. Ashitkov, K.V. Khishchenko, K.P. Migdal, M.B. Agranat, S.I. Anisimov, V.E. Fortov, I.I. Oleynik, Two-temperature thermodynamic and kinetic properties of transition metals irradiated by femtosecond lasers, Intern. Symp. High Power Laser Ablation 2012; AIP Conf. Proc. Vol. 1464, 593-608 (2012);

Yu.V. Petrov, N.A. Inogamov, K.P. Migdal, Thermal Conductivity and the Electron–Ion Heat Transfer Coefficient in Condensed Media with a Strongly Excited Electron Subsystem, JETP Lett., V. 97, 20–27 (2013);

Yu.V. Petrov, N.A. Inogamov, Elimination of the Mott Interband s–d Enhancement of the Electrical Resistance of Nickel and Platinum Owing to the Excitation of Electrons by Femtosecond Laser Pulses, JETP Letters, V. 98, 278–284 (2013);

K.P. Migdal, Yu.V. Petrov, and N.A. Inogamov, Kinetic coefficients for d-band metals in two-temperature states created by femtosecond laser irradiation, Fundamentals of Laser-Assisted Micro- and Nanotechnologies 2013, edited by Vadim P. Veiko, Tigran A. Vartanyan, Proc. of SPIE V. 9065, 906503 (2013);

D.K. Ilnitsky, V.A. Khokhlov, N.A. Inogamov, V.V. Zhakhovsky, Yu.V. Petrov, K.V. Khishchenko, K.P. Migdal, and S.I. Anisimov, Two-temperature hydrodynamics of laser-generated ultrashort shock waves in elasto-plastic solids, J. Phys.: Conf. Ser. V. 500, 032021 (2014);

Yu.V. Petrov, K.P. Migdal, N.A. Inogamov, V.V. Zhakhovsky, Two-temperature equation of state for aluminum and gold with electrons excited by an ultrashort laser pulse, Appl. Phys. B V. 119, 401--411 (2015);

Yu.V. Petrov, N.A. Inogamov, and K.P. Migdal, Two-temperature Heat Conductivity of Gold, PIERS Proceed. (ISSN 1559-9450), Prague, Czech Republic, July 6-9, 2015, pp. 2431-2435 (2015);

K.P. Migdal, D.K. Il'nitsky, Yu.V. Petrov, and N.A. Inogamov, Equations of state, energy transport and two-temperature hydrodynamic simulations for femtosecond laser irradiated copper and gold, J. Phys.: Conf. Series V. 653, 012086 (2015);

Yu. V. Petrov, N. A. Inogamov, S. I. Anisimov, K. P. Migdal, V. A. Khokhlov, and K. V. Khishchenko, Thermal conductivity of condensed gold in states with the strongly excited electron subsystem, J. Phys.: Conf. Series V. 653, 012087 (2015);

K.P. Migdal, Yu.V. Petrov, D.K. Il'nitsky, V.V. Zhakhovsky, N.A. Inogamov, K.V. Khishchenko, D.V. Knyazev, P.R. Levashov, Heat conductivity of copper in two-temperature state, Appl. Phys. A V. 122, 408 (5 pages) (2016);

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Petrov Y.V., Mokshin A.V., Galimzyanov B.N., Inogamov N.A. Electrical resistivity and thermal conductivity of liquid aluminum in the two-temperature state IOP Conf. Series: Journal of Physics: Conf. Series V. 946, 012096 (2018);

[3] https://www.usasymposium.com/hpla/agenda.php Simulations of Damage of Ru Thin Films Induced by Single-Shot fs EUV FEL Pulses, Mr. Igor Milov, MESA+ Institute for Nanotechnology, University of Twente;

V.A. Khokhlov, I. Milov, I.A. Makhotkin, V.V. Zhakhovsky, D.K. Ilnitsky, K.P. Migdal, V.V. Shepelev, Y.V. Petrov, and N.A. Inogamov, Dynamics of ruthenium mirror under action of soft x-ray or optical ultrashort laser pulse, Journal of Physics: Conf. Series, accepted

[4] H. Mindt, M. Megahed, N. Lavery, M. Holmes, S. Brown, Powder Bed Layer Characteristics: The Overseen First-Order Process Input, Metallurgical & Materials Transactions. Part A, V. 47, Issue 8, 3811-3822 (2016)

[5] Christoph Meier, Reimar Weissbach, Johannes Weinberg, Wolfgang A. Wall, A. John Hart, Modeling and Characterization of Cohesion in Fine Metal Powders with a Focus on Additive Manufacturing Process Simulations, arXiv:1804.06816v3 [cs.CE] 25 May 2018

1.7. Compliance of the professional level of the research team members with the project objectives

Inogamov Nail Alimovich. He has extensive experience in building physical models for the interaction of laser radiation with matter. His work on the study of ablation under the action of ultrashort laser pulses, its mechanisms and results have received worldwide recognition. Such well-known, often cited works include

Inogamov, N. A.; Zhakhovsky, V. V.; Khokhlov, V. A.; Petrov, Y. V. & Migdal, K. P. Solitary Nanostructures Produced by Ultrashort Laser Pulse. Nanoscale Research Letters, 2016, 11, 177[1-13]

Inogamov, N. A., Zhakhovsky, V. V., Ashitkov, S. I., Emirov, Yu. N., Faenov, A. Ya., Petrov, Yu. V., Khokhlov, V. A., Ishino, M., Demaske, B. J., Tanaka, M., Hasegawa, N., Nishikino, M., Tamotsu, S., Pikuz, T. A., Skobelev, I. Ya., Ohba, T., Kaihori, T., Ochi, Y., Imazono, T., Fukuda, Y., Kando, M., Kato, Y., Kawachi, T., Anisimov, S. I., Agranat, M. B., Oleynik, I. I. & Fortov, V. E. Surface Nanodeformations Caused by Ultrashort Laser Pulse, Engineering Failure Analysis, 47, 328-337 (2015)

N.A. Inogamov, Yu.V. Petrov, S.I. Anisimov, A.M. Oparin, N.V. Shaposhnikov, D. von der Linde, J. Meyer-ter-Vehn, Expansion of matter heated by an ultrashort laser pulse, JETP Lett., 69 (4), 310-316 (1999)

Petrov Yury Vasilyevich. Conducted important studies of the thermodynamic and kinetic properties of metals and dielectrics in the states arising under the action of laser radiation, as well as their optical characteristics. For the implementation of the project are of interest such works as

Yu.V. Petrov, K.P. Migdal, N.A. Inogamov, S.I. Anisimov, Transport Processes in a Metal with Hot Electrons Excited by a Laser Pulse, JETP Lett., 104(6), 431-439 (2016)

Yu. V. Petrov, N. A. Inogamov, S. I. Anisimov, K. P. Migdal, V. A. Khokhlov, K. V. Khishchenko. Thermal conductivity of condensed gold in states with the strongly excited electron subsystem Journal of Physics: Conference Series, 2015, v. 653, 012087

Yu.V. Petrov, N.A. Inogamov, K.P. Migdal, Thermal conductivity and the electron-ion heat transfer coefficient in condensed media with a strongly excited electron subsystem, JETP Lett., 97(1), 20-27 (2013)

Khokhlov Victor Alexandrovich. He created Lagrangian hydrodynamic codes, which are of great importance for solving problems under the project, both in independent use and in combination with molecular-dynamic modeling. These codes, which contain two-temperature thermodynamics in a wide range of electronic and ionic temperatures and densities and two-temperature transfer coefficients, have been tested when performing such significant works as

N.A. Inogamov, V.V. Zhakhovskii, V.A. Khokhlov, Dynamics of Gold Ablation into Water, JETP 127(1), 79-106 (2018)

N.A. Inogamov, V.A. Khokhlov, V.V. Zhakhovsky, Formation of a Single Microstructure and Ablation into a Transparent Insulator under Subnanosecond Laser Irradiation, JETP Lett., 2018, 108, 439–445 (Письма, 108(7), 470-477 (2018))

N.A. Inogamov, V.V. Zhakhovskii, V.A. Khokhlov, Jet formation in spallation of metal film from substrate under action of femtosecond laser pulse, JETP 120(1), 15-48 (2015)

Zhakhovsky Vasily Viktorovich. At a high global level, often ahead of him, performs work on molecular dynamic and hydrodynamic modeling of laser ablation problems. The use of parallel computing, a large number of particles reaching hundreds of millions, adequate potentials of their interactions form the basis of reliable molecular dynamics calculations. Well known are such as

B.J. Demaske, V.V. Zhakhovsky, N.A. Inogamov, I.I. Oleynik, Ultrashort shock waves in nickel induced by femtosecond laser pulses, Phys. Rev. B, 87(5), 054109 (2013) [9 pages]

V.V. Zhakhovsky, M.M. Budzevich, N.A. Inogamov, I.I. Oleynik, C.T. White, Two-Zone Elastic-Plastic Single Shock Waves in Solids, Phys. Rev. Lett. 107, 135502 (2011) [4 pages]

B.J. Demaske, V.V. Zhakhovsky, N.A. Inogamov, I.I. Oleynik, Ablation and spallation of gold films irradiated by ultrashort laser pulses, Phys. Rev. B 82, 064113 (2010) [5 pages]

Migdal Kirill Petrovich. It has experience, important for project tasks, using density functional theory. Using software packages based on it (VASP, Elk, Abinit), electronic energy zones of many metals, their thermodynamic functions (internal energy, heat capacity, pressure), conductivity, coefficient of electronic thermal conductivity including in the two-temperature state are obtained. This valuable experience for the implementation of the project is described in particular in the works

Migdal, K. P.; Petrov, Y. V.; Il'nitsky, D. K.; Zhakhovsky, V. V.; Inogamov, N. A.; Khishchenko, K. V.; Knyazev, D. V. & Levashov, P. R. Heat conductivity of copper in two-temperature state. Appl. Phys. A, 122, 408[1-5] (2016)

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Petrov, Y. V.; Migdal, K. P.; Knyazev, D. V.; Inogamov, N. A. & Levashov, P. R. Transport properties of copper with excited electron subsystem. J. Phys.: Conf. Ser., V. 774, No. 1, 012103[1-17] (2016)

Grigoriev Sergey Yurievich. He is a recognized specialist in the field of numerical hydrodynamic modeling. Required for the project specialist. Features important his experience in the application of the SPH code (Smoothed Particle Hydrodynamics) and the use of molecular dynamics. His high scientific level is evidenced by such works as

Dyachkov S. A., Parshikov A. N., Egorova M. S., Grigoryev, S. Y., Zhakhovsky V. V., Medin S. S., Explicit failure model for boron carbide ceramics under shock loading, J. Appl. Phys., 124(8), 085902 (2018)

Grigoryev, S. Y.; Dyachkov, S. A.; Khokhlov, V. A.; Zhakhovsky, V. V.; Parshikov, A. N. & Inogamov, N. A. Liquid tin droplet fragmentation by ultra-short laser pulse, J. Phys.: Conf. Ser., (2018), accepted

Dyachkov Sergey Alexandrovich. Prepared for the defense scheduled for December 2018, a thesis for the degree of Candidate of Physical and Mathematical Sciences "Quasiclassical model of thermodynamic properties of electrons taking into account the states of the discrete spectrum and its range of applicability". The work performed in the thesis is interesting for the study of the thermodynamic properties of materials in the course of the project. For the objectives of the project are important work SA. Dyachkova on molecular dynamics simulation and using the numerical SPH method:

S. A Dyachkov, A. N. Parshikov, V. V. Zhakhovsky, SPH simulation of boron carbide under shock compression with different failure models, J. Phys.: Conf. Ser., 815(1),012012 (2017)

Dyachkov S. A., Egorova M. S., Murzov S. A., Parshikov A. N. and Zhakhovsky V. V., Auto-balancing algorithm for parallel SPH simulation of materials in extremes, Lobachevskii J. Math. 38, 893–897 (2017)

Egorova Maria Sergeevna. While studying in graduate school is well mastered the numerical methods of hydrodynamics. In particular, her ability to work with the multidimensional hydrodynamic SPH code will be a significant contribution to the implementation of project tasks. The high level of preparation for these tasks can be judged by the work

M. S. Egorova, S. A. Dyachkov, A. N. Parshikov, V. V. Zhakhovsky, A. A. Serezhkin, I. S. Menshov, D. B. Rogozkin, S. E. Kuratov, Shock-induced ejecta from a layer of spherical particles. Part I: SPH meso-scale simulation, J. Phys.: Conf. Ser., 815(1), 012012 (2017)

Dyachkov S. A., Egorova M. S., Murzov S. A., Parshikov A. N. and Zhakhovsky V. V., Auto-balancing algorithm for parallel SPH simulation of materials in extremes, Lobachevskii J. Math. 38, 893–897 (2017)

Also see the work of Egorova et al. [15] in the list of references to § 1.4 (abstract).

Murzov Semyon Aleksandrovich. He studies in graduate school, during his studies he received a good training in numerical methods of hydrodynamics, molecular dynamics (MD) and SPH code, which will be used when performing work on the project. Masterfully owns the AtomEye package, which allows to build graphical images of atoms in three-dimensional space, which is important for illustrating and understanding the results that are obtained in MD simulations. Here are some of his works

S. A. Murzov, V. V. Zhakhovsky, Extinction and growth of cylindrical hotspots in AB model explosive: molecular dynamics studies, J. Phys.: Conf. Ser., 815(1), 012034 (2017)

Dyachkov S. A., Egorova M. S., Murzov S. A., Parshikov A. N. and Zhakhovsky V. V., Auto-balancing algorithm for parallel SPH simulation of materials in extremes, Lobachevskii J. Math. 38, 893–897 (2017)

S.I. Anisimov, V.V. Zhakhovsky, N.A. Inogamov, S.A. Murzov, V.A. Khokhlov, Formation and crystallisation of a liquid jet in a film exposed to a tightly focused laser beam **Quantum Electron., 47(6), 509-521 (2017)**

FORM 4

4.1. Scientific problem addressed by the project

Great prospects are associated with laser technology. But the prospecting works are mostly performed on the off-chance with using the trial-and-error procedure in experiments. We have to get out of this situation by creating the theoretical approaches, physical models, numerical methods aimed to provide explanations and solutions. This is the modern style that combines physics and development of new technology. In this style, it is possible to move quickly from an incomprehensible phenomenon or the most incredible idea to its practical implementation.

Let's give some examples.

Example 1. Yet recently, the formation of bumps on thin films during a tightly focused laser exposure with focusing on the diffraction limit did not have any clear explanations, no physical model, or computational techniques. But the phenomenon has been known from experiments for quite some time, from 2003-2004 [1]. The creation of a theory describing this process made it possible to understand the thermophysics and mechanics of the phenomena occurring in ultralow volumes during femto-pico-nano-second (fs-ps-ns) times with a hierarchical cascade of different-time processes [2]. As a result, there are now possibilities to control the cultivation of "bumps-domes-cones" (blistering thin-film coatings) of given sizes and shapes (say, with a tip on top).

This is important for tuning the nanoantennas, which can be considered as "bumps" [3]. Accordingly, it is possible to set the desired color of the surface (without the usage of any dyes) illuminated with white light, or to optimize the meta-surface of bump array working as a sensor [3].

Another important direction involves the use of bumps as generators of droplets flying exactly in a given direction in LIFT/LIBT laser printing devices (laser induced forward / backward transfer). The complete theory is created in [2]. Using such printing, complex mosaics are now created for microelectronics (chip formation) and medicine (artificial tissues of the body), as well as complex three-dimensional microstructures, see the works of the Israeli group from the Additive Manufacturing Lab, Orbotech Ltd. and the Hebrew University of Jerusalem [4] and groups from the University of Twente, Holland [5].

Example 2. Another important example is related to the explanation of Newton's interference rings with the growing number of rings [6] (today there are 300 to 600 references to this article in different citation systems; the phenomenon was discovered virtually by chance in the experiments by the group of Prof. Dietrich von der Linde from University of Duisburg-Essen). Thanks to the developed theory [7], now this phenomenon is well understood and it is used in an important diagnostic technique [8] to observe what is happening in the irradiation spot at ps-ns times. Moreover, with using a soft X-ray laser (λ = 13.9 nm) such Newton's rings are used for

tracking [9] the dynamics of inflating bubble in molten gold after a femtosecond optical pump (such irradiation has the character of a shock). Needless to say, the use of such short waves [9] for interference opens up new opportunities for improvement of the pump-probe technique.

Example 3. Thanks to the work on the project RSF 14-19-01599, in addition to the creation of the theory of dome formation [2,3] a theory of 3D fragmentation of tin droplets was developed and corresponding simulation was performed, see [7] in the list of references to p. 1.4. And again, the development was based on a hybrid model with the separation of the surface layer of primary heating by a laser pulse and further cumulation of the compression wave towards the center of the droplet. It occurs with significant deviations from spherical symmetry - for example, the pressure maximum is reached at some distance beyond the center with respect to the irradiated hemisphere.

Similar situation happens with paragraph B) of section 1.5 (ablation into a liquid). The work was started with support from the grant of the RSF 14-19-01599. Now they need to be continued with an emphasis on the equation of state and thermal conductivity of water; it is necessary to go from the initial stages to the formation of a bubble. Again, work is being done in a hybrid way, with a combination of molecular dynamics, SPH code, and two-temperature hydrodynamics programs. There is confidence that this fundamental and very important work for applications in the framework of the new RSF project will be completed. Namely, an end-to-end chain of processes from the initial stages with radiation absorption to the final stages with the evolution of a bubble in a liquid will be revealed and demonstrated to experimenters. This kind of research will greatly simplify and cheapen the manufacturing of nanoparticles by the laser method. The point is to get an opportunity for meaningful control of the processes, which opens doors to create nanoparticles with the required structure, for example, shell-core (core-shell particles).

We turn to the description of the problems of H and I.

H) The role of electron and phonon heat conduction processes in the evolution of the surface of a solid-state silicon target after ultrashort laser irradiation of moderate intensity.

Silicon is one of those materials for which the research on the possibility of treating its surface at the nanoscale and obtaining surface nanostructures of a given shape as a result of processes occurring after irradiation is of great relevance. When irradiated, as a rule, the primary surface is in the solid phase. Since solid silicon is a semiconductor, at temperatures about room temperature, the dominant contribution to thermal conductivity is determined by phonons and turns out to be at the same level with typical values for metals (150 W / m / K). With an increase in temperature, the orderliness of the silicon lattice decreases, as does the phonon lifetime, as a result of which the thermal conductivity of silicon at temperatures above 1000 K, but below the melting point, is of an order of magnitude less than at room temperature. The electronic

contribution to thermal conductivity becomes noticeable only after the melting of the silicon lattice, when the electronic spectrum becomes continuous in the region of the Fermi energy.

The picture described here reflects the qualitative behavior of the thermal conductivity of silicon with increasing temperature, which can be observed with ultrashort laser irradiation. When describing such an effect using the two-temperature hydrodynamics method, we will need not only a quantitative description of the total thermal conductivity depending on the temperature and density of silicon, but also its separation into contributions corresponding to electron and lattice/ion transfer. This task will be solved with the help of modern approaches to the calculations of flow-to-flow correlators within the framework of quantum and classical molecular dynamics (Kubo-Greenwood and Green-Kubo methods). In the first case, we are talking about determining the contribution of electrons to thermal conductivity, and in the second case, the lattice or ions, if we are talking about the molten state.

I) First-principle calculations of the electron-phonon interaction constant in two-temperature metals in comparison with the simulation data of electron-phonon relaxation by the method of an effective force field within the framework of molecular dynamics.

In conclusion of this section 4.1, we can say that there are a wide range of tasks and an important scientific direction related to the fundamental problems of laser exposure of materials. The claimed project covers a set of important tasks in this direction. Implementation of the project goals will help the experiment and accelerate the transition to required technologies.

In modern calculations of metal surface modification using ultrashort laser irradiation, one of the key parameters is the rate of electron-phonon heat transfer, which determines the characteristic time of electron-ion relaxation, as well as temperature profiles of electrons and ions, and their pressure in the irradiated surface layer. There are several methods for calculating this value, among which we can mention the Kaganov-Lifshits-Tanatarov method, adapted by the authors for two-zone metals (Petrov, Inogamov, Migdal, P. ZhETF, 97, 24, 2013), the Allen method (PB Allen, Phys. Rev.Lett, 1987) for single-band metals, extended to the arbitrary case by X. Wang et al (Phys. Rev. B 50, 8016, 1994). The second approach is based on the entire length from the moment of the formulation of the generalization, on the assumption of a weak change in the phonon characteristics with increasing electron temperature. This assumption is ideologically close to the popular hypothesis that the lattice characteristics during electronic heating do not change, which underlies the model of a two-temperature state. However, with the development of first-principle calculations, it has been shown that the density of phonon states will change with heating in metals such as gold or copper (V. Recoules et al, Phys. Rev. Lett, 96, 055503, 2006; D.V. Minakov, P.R. Levashov, Phys. Rev. B, 224102, 2015).

In the framework of the Allen-Downer method, there is a need to use an experimentally determined electron-phonon interaction constant, which is determined at low temperatures, corresponding to the superconducting state of the metal. It has not been tested to what extent

the use of such a numerical value in metals with high electron and ion temperatures can affect the result for the electron-phonon interaction rate. Such methods of first-principle calculations, like the frozen phonon method and the density functional perturbation theory, allow us to calculate the force constants for metals both in equilibrium and in the two-temperature state, which allows us to determine the electron-phonon interaction constant for this case as well. Thus, it is planned to check the validity of the method of calculation of electron-phonon heat transfer used in the literature.

In addition, it is proposed to conduct a direct simulation of the electron-phonon (electron-ion) heat exchange in a simplified model of the electron force field, which uses a semiclassical description of the valence electrons using localized Gaussian packets. In this case, it is possible to trace the characteristic scales of electron and phonon thermalization, i.e. the start time of the two-temperature stage, and also to estimate directly from the behavior of the electron and ion temperatures during the simulation, the rate of electron-phonon heat exchange.

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4.2. The scientific relevance and relevance of the solution of the designated problem

Relevance and timeliness of research on the problems listed in section 1.5 were discussed in the previous sections. Briefly summarize what has been said. The list of problems (from section 1.5) to be solved is as follows:

A) Spatially distributed heating due to a combination of plasmon and laser EM fields

B) Action of vortex beams

C) The formation of nanoparticles during ablation into a liquid

D) Laser fragmentation of liquid droplets and jets

E) Ablation of refractory metals

F) Laser melting of powders

G) Computational physics, large-scale high-performance numerical simulation

We describe the importance and relevance specifically, by points.

A) Spatially distributed heating due to a combination of plasmon and laser EM fields

The task is of great interest for electronics, plasmonics, for the creation of holograms, for the manufacture of meta-surfaces, see [1] and [4] in the references to 1.4. In plasmonics, several

international conferences are held annually. Recently in Sochi one of the following conferences took place: METANANO 2018: https://metanano.ifmo.ru/ which gathered about half a thousand participants and even more presentations (the work [4] from section 1.4 was presented at METANANO-2018). A keynote address was made by Andrei Geim, Nobel Prize winner in 2010.

The problem proposed by us is a fairly new, promising direction in plasmonics. We are talking about the conjugation of plasmonic problems, which have the character of applied electrodynamics, with the possibilities of modern physics of the interaction of intense electromagnetic radiation with matter. In this case, the role of heating/crystallization and mechanical effects, leading to the transformation of the target, become essential. This transformation will be used to form meta-surfaces.

The path of the combination of laser radiation and surface plasmon-polariton modes for the formation of holograms, meta-surfaces is much more economical than "cutting out" the relief of the meta-surface by the electron beam bombardment in a vacuum.

B) Action of vortex beams

What has been said above regarding applications of the combined laser-plasmon action also applies to the section on applications of vortex beams - this is the formation of meta-surfaces. In addition, there are a number of applications that are associated precisely with the chirality of the twists of the vertices. It is proposed to use arrays of solitary vortex vertices (vortex meta-surface) to create supersensitive sensors, filter molecules depending on their chirality (for example, purification of medicaments), to form chiral plasmon devices in which the illumination of the structure returns vortex wave in reflected light (which will replace phase plates), see [5] in section 1.4.

So a new variant of the fundamental problem arises, relating to the physics of the interaction of laser radiation with matter.

C) The formation of nanoparticles during ablation into a liquid

Laser formation of nanoparticles has several advantages compared with cheaper, but more multistage and "dirty" means of chemical synthesis. In addition, chemists have not been able to approach some of the structured nanoparticles. Detailed information is available in reviews, published a year ago, concerning the laser fabrication of nanoparticles in liquids (preparation of colloidal solutions of nanoparticles), see [12] to section 1.4. In fig. a diagram of applications of laser synthesis of colloids is shown.

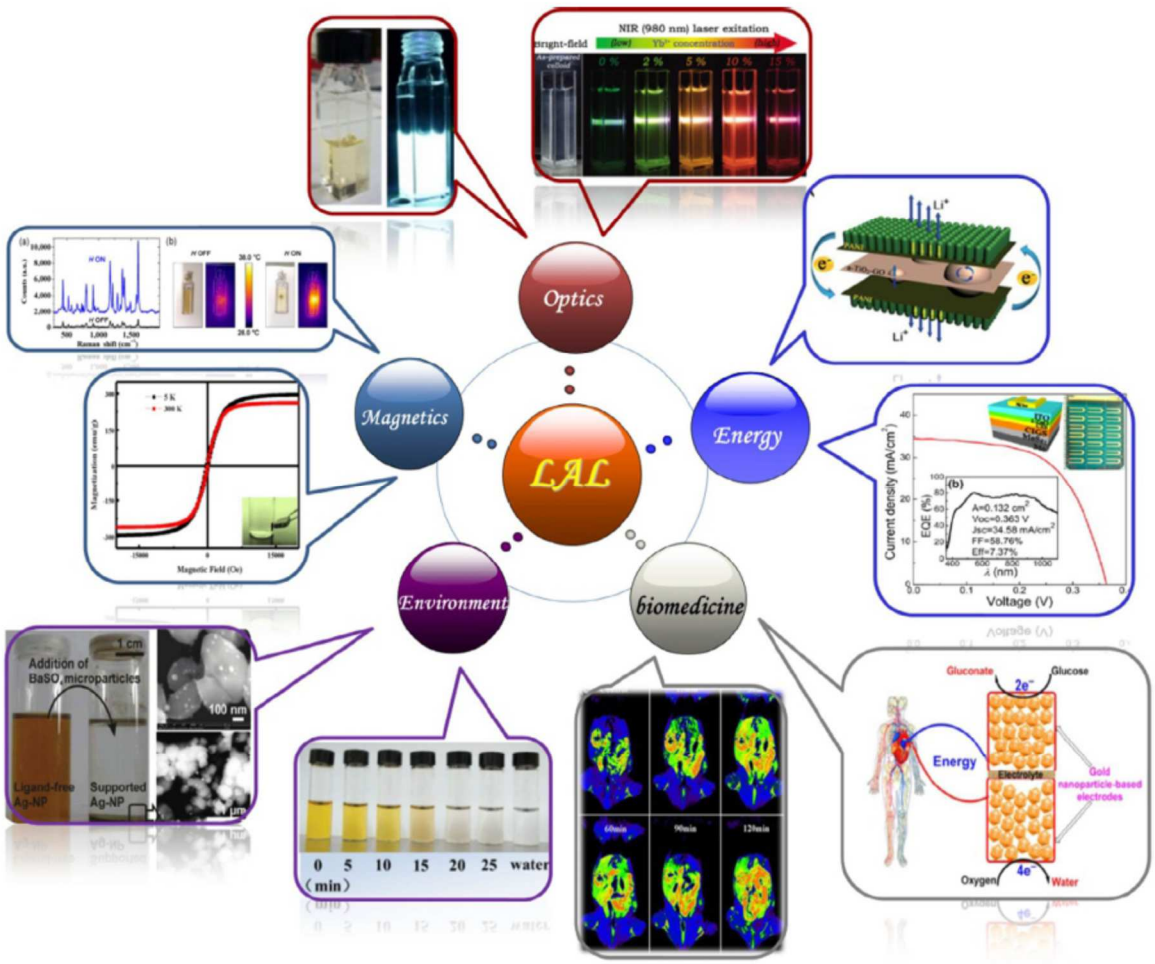

Fig. 4. The increasing and extensive applications based on LAL reported by the present literatures, including optics, magnetics, energy, environment as well as biomedicine.

Fig. 5. Laser synthesis applications from the article by Xiao et al., Progress in Materials Science 87, 140-220 (2017), see 2], in p. 1.4.

According to statistics collected in an article by Xiao et al., Progress in Materials Science 87, 140-220 (2017), see [12] in section 1.4, the number of publications on ablation in a fluid has increased exponentially over the past few years and exceeded 300 articles per year, and the number of citations reached 7,000 per year. This indicates the relevance and necessity of the subject.

D) Laser fragmentation of liquid droplets and jets

In the case of tin drops, applications are associated with projects for creating plasma sources of short-wave radiation: soft X-rays — vacuum ultraviolet, which form the basis of the next-generation photolithographic machines. Such machines will have a much higher resolution, since the diffraction limit, proportional to the wavelength, will sharply decrease. The project is engaged in such a giant, a leader in the production of machines for photolithography, as ASML, Holland. This is, so to speak, the production of means of production, as further these machines

are used in the microelectronic industry for the manufacture of integrated circuits, memory devices and microprocessors.

In the case of water droplets and jets and their irradiation with an ultrashort hard X-ray pulse from an American XFEL laser on an SLAC, the physics of x-ray interaction with a liquid medium is of interest, see comments in [14] to section 1.4 of the project.

E) Ablation of refractory metals

The physics of metal ablation is of independent interest. Today, gold, silver, aluminum are well studied in this respect. There are a number of publications on these metals, including many of the work of our team. Of refractory metals tantalum was analyzed in our theoretical work and in collaboration with experimenters from the laser plasma department under the guidance of M.B. Agranat at JIHT RAS.

Ruthenium, a detailed study of which will be performed in the project, is a little-studied metal. Suffice it to say that in the literature there are only two rather old publications on the EAM potential of ruthenium (M. Igarashi, M. Khantha, V. Vitek, "N-body interatomic potential for hexagonal close-packed metals", Phil. Mag. B, 63, 603-627 (1991), S. Chen, J. Xu, H. Zhang, "A new scheme of many-body potentials for hcp metals", Computational Materials Science, 29, 428–436 (2004)). They describe ruthenium in a small neighborhood of the equilibrium density and room temperatures. Meanwhile, for our purposes, a potential is needed that is suitable for significant stretching and noticeable compression and for strong heating, which corresponds to the conditions of laser irradiation with optical and X-ray lasers.

The value of the study is that ruthenium is an important material of X-ray optics, as well as the material of protective films, including in photolithographic machines, discussed above.

F) Laser melting of powders

3D printing technologies, also called additive technologies, are very popular in the media. Sometimes they talk about the omnipotence of this kind of production. In fact, today many fundamental problems are connected with these processes. The most significant of them, referring specifically to the laser, will be considered in our project. Without solving these problems, it is impossible to successfully advance in this direction.

G) Computational physics, large-scale high-performance numerical simulation

Algorithms, acceleration of computations, the use of multiprocessor codes, the expansion of space-time scales (in the case of molecular dynamics) - these are the actual challenges facing

computational physics. In our project, significant progress will be made to improve the software systems, to saturate them with real physics.

Such physics includes many components - from describing the absorption of laser energy to the processes of heat transfer, diffusion, modeling of complex, often three-dimensional movements of melts and a deformable solid with a package of elastic-plastic phenomena plus melting/crystallization phase transitions, intensive evaporation, cooling and condensation . Moreover, as a rule, the processes proceed quickly and often far from thermodynamic equilibrium.

This section of work has extremely clear practical value.

H) Characteristics of silicon irradiated by laser

In describing the thermal conductivity of the electron subsystem of silicon excited by an ultrashort laser, the values obtained from the reference books are still used and do not take into account the evolution of this quantity, except for its most dramatic change at the melting point. At the same time, previous

studies by the authors show ed the importance of adequately determining the dependence of the thermal conductivity on the electron and ion temperature and density. The very relevance of studying the surface treatment of silicon films with an ultrashort laser and solving related probl

ems is beyond doubt, since it can be considered as one of the most promising surface treatment methods with a resolution of several tens of nanometers.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals

As mentioned above, in Section 4.1, to solve the electron-phonon heat exchange rate problem, only two common methods are used (the modified Kaganov-Lifshitz-Tanatarov method and the Allen-Downer method), between which there is no unambiguous theoretical connection that would allow boundaries of their mutual compatibility. It should be noted that the data obtained in the second way are most common in third-party sources, in which the dependences of electron-phonon heat transfer on electron temperature are used to solve various problems on the conditions of electron-ion relaxation. At the same time, the assessment of the effect of electron heating on the phonon spectrum and on the results of the Allen-Downer method is an important task. To calculate the electron-ion relaxation, the modern approach of the electron force field (electron force field) will be used, which is applicable to describe such relaxation in different phases of the heated substance.

4.3. *The specific task (s) within the framework of the problem that the project is intended to solve, its scale and complexity*

We list the specific problems that will be solved.

A) Spatially distributed heating due to a combination of plasmon and laser EM fields.

The formation of the dome by the first shot will be simulated. For this, the previously developed approach will be used, see references [10] to section 1.4 of the application and the movie as a files «Au-220, 225, 226» on website http://laser.itp.ac.ru/RNF2019/index.html accompanying project. The near EM of a standing wave associated with a laser, a surface and a dome will be calculated by means of numerical methods of electrodynamics. The heating of the film in the standing wave due to the absorption of the EM field of the standing wave in the skin layer of the film will be calculated. Both film movement and thermal processes in a moving film will be modeled using molecular dynamics and SPH method. As a result, data will be obtained on the formation thresholds and on the characteristics of the spatial structure consisting of the dome and the standing wave imprint in the film and substrate. The results will be compared with the results of experiments from reference [11] to section 1.4 and the new experiments of the Vladivostok group.

It will be understood what happens as a result of lighting the above structure with the third shot. For this, additional electrodynamic modeling will be performed.

Today in the world literature there is neither a description nor a solution to such a problem. This is due to the difficulties of creating a physical model and a numerical scheme that matches the electrodynamic calculation with thermal-hydro-physical modeling. From the decision of the problem there are significant benefits associated with the creation of technologies for meta-surfaces and holograms.

The lack of solutions to this problem in the world literature, with its importance, indicates the non-triviality of the problem.

The formation of radial corrugation on the domes will be explained, see the example shown in fig. 1. Although the observations recorded these structures for a long time (6 years have passed since Wortmann et al., J. Laser Appl. V. 24, 042017 (2012)), no explanation has yet been provided.

B) Action of vortex beams

A theory will be created in the project, and an explanation will be found for the phenomenon shown in fig. 2 in file attached to the application , this problem will be solved and numerical calculations will be performed. The results will be compared with the results of experiments

that are conducted in the FIAN in the department of prof. A.A. Ionin. No quantitative calculations that would explain the origin of the structures in this figure, today is not available.

That, despite the publication of the results of the group of prof. T. Omattsu in prestigious editions, see [5] in section 1.4, there are still no quantitative results, indicates the intricacy, complexity of the problem and its value.

C) The formation of nanoparticles during ablation into a liquid.

A very difficult problem about the ablation of a metal into a liquid will be solved. Currently, there are only the very first attempts to solve this problem. These attempts cover only either the initial (see [6] in section 1.4) or the final (see [13] in 1.4) stages of the processes taking place.

In the project, an exhaustive end-to-end solution will be obtained that covers the initial stage, follows the development of phenomena at several intermediate stages and continuously moves to the vaporization stage in the hot contact layer of the liquid with the appearance of the vapor bubble, its expansion, stop of expansion and the begining of the return movement leading to compression of the bubble.

D) Laser fragmentation of liquid droplets and jets.

The problems of fragmentation of liquid microdroplets by laser action are very complex. Difficulties are associated with rich physics (from the interaction of radiation with a target mater and the creation of extreme conditions in temperature and pressure to capillary phenomena) and the sharply unsteady three-dimensional nature of flows. Moreover, the flow structure is hierarchical, covers several orders of magnitude in time and space: from fast to slow processes and on a spatial scale from the order of the size of a drop to the smallest fragments of fragmentation. We have a positive experience in solving the problem, see reference [7] in section 1.4.

The project will solve the problem of the action of a thin cylindrical beam of hard X-rays on a microdroplet of water or a liquid jet. The beam diameter is 1 μm, the size of the droplet and the diameter of the jet are several tens of μm. Task setting is shown in fig. 3.

Typical data of the experiments conducted by the Stanford accelerator Linac Coherent Light Source are shown in fig. 4. Coherent X-ray Imaging (CXI) instrument was used.

To solve the problem presented in Fig. 3 and 4, the program complex will be modified and new approaches will be added, both in physics and in the algorithms used. In physics, we are talking about the description of the interaction of the X-ray beam with a target matter and about the description of two-temperature phenomena. There is a great experience in the study of X-ray influences in a team, see the list of our works in reference [1] to section 1.5. The same applies to our research on two-temperature models, see reference [2] in section 1.5. Subroutines with X-

ray physics and two-temperature effects, as well as detailed information about the equation of state of water, will be inserted into the SPH algorithm.

In addition to problems with a hard impulse X-ray and a drop of water, research on a drop of tin will be continued. It is necessary to replace the equation of state of Mi-Grüneisen, used in [7] (see the literature for § 1.4), with a tabular equation of state.

E) Ablation of refractory metals.

A potential of interatomic interaction of ruthenium will be created. An equation of state for ruthenium will be developed taking into account two-temperature effects. DFT (density functional theory) calculations will be carried out to develop the potential and to create the equation of state. They will be performed using quantum-mechanical computation packages (VASP, Elk, etc.). In such calculations, the cold ruthenium curve is determined. It is necessary for building the interatomic interaction potential using the stress matching algorithm. In DFT calculations, two-temperature effects will be defined. For this, a series of calculations will be performed on the electron temperature, in which the electron subsystem is excited to a given temperature in the hcp ruthenium crystal. As a result, electronic contributions to pressure and internal energy are determined, and the electronic heat capacity is found. These values are non-trivial functions of density and temperature. They cannot be approximated by functions that correspond to the free Fermi gas.

Next, two-temperature hydrodynamic and molecular dynamics calculations will be performed. Work will be conducted in conjunction with the experiment. Ultrashort action of lasers with different wavelengths from optical to hard ultraviolet and hard x-rays at different angles of incidence will be considered. Our team has begun preliminary work in this area [3] - a reference in the list of references to section 1.5.

F) Laser melting of powders.

The project will solve the problem of melting metal microparticles with a laser pulse.

G) Computational physics, large-scale high-performance numerical simulation.

Work will be carried out to improve our numerical arsenal. This includes work on the development of codes and on the inclusion of the physics required for solving the problems listed above.

H) Characteristics of silicon irradiated by laser.

In the case of silicon, the main task is to accurately describe the process of nano-modification of its surface when irradiated with one or several laser pulses with a duration of 10-100 fs and with an energy input of 10-100 mJ / cm2, which determines the range near the ablation threshold. To solve this problem, it is planned to use the method of two-temperature hydrodynamics, where in addition to the data on the thermal conductivity of silicon in different phases, data on electron-phonon heat transfer and the thermodynamic potentials of the electron and ion subsystems are also required. To solve the last two problems, it is planned to use a combination of a number of methods: the modified Kaganov-Lifshits-Tanatarov method, the Allen-Downer method with an independently determined electron-phonon interaction constant, molecular-dynamic modeling in the electron force field approach, and the density functional theory. The main computational capacity here will be the problem of calculating the electron thermal conductivity according to the Kubo-Greenwood formula, since such a task, as was shown by the authors (Migdal, J. Phys .: Conf. Ser. 774, 012103, 2016), will require a quantum-mechanical analysis of the system at least a hundred atoms in the framework of the density functional method.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals.

When considering the Allen-Downer method in the two-temperature case, the main focus will be on those metals whose potential application in such areas as nanoplasmonics and nanophotonics (A. Kuchmizhak et al, Nanoscale, 8, 12352, 2016; DG Baranov et al, Optica, 4 (7), 814, 2017) is undoubted, and, on the other hand, there is evidence of the effect of electronic heating on their phonon properties (gold and copper). In addition, as follows from the previous paragraph, a similar study will be made for silicon, where earlier (V. Recoules et al. Phys. Rev. Lett, 96, 055503, 2006) the appearance of a “soft mode” in the phonon spectrum with increasing electronic temperature was found.

In the framework of the density functional method, the ground state energies will be calculated for systems with infinitesimal displacements of atoms into lattices corresponding to the main directions of its deformations. This will allow us to construct a matrix of force constants, with the help of which it will be possible to reconstruct the phonon spectrum, to calculate the dependence of the Eliashberg function on the frequency of the excited phonon. This will take into account the change in the electronic spectrum with temperature, recently discovered using ab initio calculations (V. Recoules et al, Phys. Rev. Lett, 96, 055503, 2006; Petrov, App. Phys. B. 2015). According to the obtained Eliashberg function corresponding to the state of matter with hot electrons, the electron-phonon interaction constant will be calculated by its definition. By its computational complexity, this problem is comparable to the calculations of electronic thermal conductivity by the Kubo-Greenwood method within the framework of quantum molecular dynamics, since it will require many different deformations of the original cell corresponding to

the crystal under consideration, containing several tens of atoms and immersed in periodic boundary conditions.

4.4. *The scientific novelty of research, the rationale for the attainability of solving the problem (s) and the possibility of obtaining the planned results*

A) Spatially distributed heating due to a combination of plasmon and laser EM fields

Today, there is neither a description in the world literature, nor a solution to the problem of a combination of plasmon fields and a laser electromagnetic (EM) field in intensive exposure modes. In such modes, the energy of the resulting EM wave, embedded in the skin layer, is sufficient for strong heating, which leads to the melting of the metal. This refers to the novelty.

The solution of the previous problem with the Kretchman scheme justifies our belief that we have a set of tools to solve the stated problem.

This also applies to the problem of the formation of radial goffering on the domes, see the example shown in Fig. 1.

B) Action of vortex beams.

Since there are no quantitative calculations in the literature of how chiral structures are formed during vortex exposure (see Fig. 2), we do not doubt the novelty of our research. The confidence that this study will be completed on time is based on our experience in solving previous problems with complex geometry.

C) The formation of nanoparticles during ablation into a liquid.

As stated in sections 1.5 and 4.1, 4.2 above, there are attempts to solve the problem of ablation into a liquid. But they do not give us the required complete picture from the initial stages to the completion of the process with the formation of a bubble, i.e. with evaporation of the near-surface layer of ablation fluid. The project will receive a complete picture. This is a new stage in the development of ideas about liquid ablation. Before the start of the project, we are armed with the necessary tools, we have relevant experience, there is no doubt that the tasks will be solved on time.

D) Laser fragmentation of liquid droplets and jets.

The project will continue to solve the problem of crushing a drop of molten tin. In contrast to the previous stage, fixed in the publication [7] in section 1.4, instead of the equation of state of Mie-Grüneisen used in [7], a tabular equation of state will be used. This is a significant novelty. In the two-temperature hydrodynamic program, we used both the Mie-Grüneisen equation and the tabular one, so there is confidence in the feasibility of this important improvement.

The project will solve a new difficult problem of the action of a thin cylindrical beam of hard X-rays on a microdroplet of water or a liquid jet.

The conclusion that the problem will be solved is based on our previous research on the fragmentation of a drop.

E) Ablation of refractory metals.

The problem of ablation of ruthenium with laser pulses of different wavelengths from optics to hard X-rays will be solved. There is no such solution in the literature, so the task is new. The solution of the problem is achievable in a timely manner, since we have the necessary experience and tools.

F) Laser melting of powders.

The problem of melting of powders will be solved. Optimal exposure regimes will be found. The task is new, unexplored in the literature. We have experience in working with porous media, with layered targets (see, for example, reference [2] in section 1.4). Therefore, the team is confident of success in this area.

G) Computational physics, large-scale high-performance numerical simulation.

Our team permanently leads the improvement of numerical tools, see, for example, reference [15] in the list to section 1.4. In this project, this improvement is due to the need to solve the above physical problems.

H) Characteristics of silicon irradiated by laser.

With regard to the problem of calculating the electronic thermal conductivity in the framework of first-principle methods and the Kubo-Greenwood formula, it should be noted that it is completely solved only in the case of such a simple metal as aluminum (D. Knyazev, Phys. Plasmas, 21 (073302), 2014). Currently, there are a number of works on the distribution of this approach to other metals, including transition and noble ones, that have many valence electrons

that require direct description in quantum mechanical calculations. In our case, we are talking about silicon, whose electronic structure is not so different in the number of valence electrons from aluminum. The only problem arising in the description of semiconductors in this case is the violation of the homogeneity of the electron gas due to the presence of directional bonds between the silicon ions. However, a number of authors (Duffy, Shokeen) showed that a good description of the electronic structure of silicon in the solid state can be achieved using hybrid functionals within the framework of the density functional theory.

Thus, the authors are confident in the applicability of the claimed approach with respect to silicon. Calculations of thermal conductivity by various approaches within the framework of the classical molecular dynamics method, such as the Green – Cuba approach, nonequilibrium molecular dynamics, were repeatedly performed for silicon, but only for some of its states, mainly for amorphous phases lying between 1300 and 1700 K. In this work the goal is to study the state of the liquid phase of silicon up to temperatures corresponding to the formation of supercritical fluid, the experimental study of which is still difficult.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals

The calculations of the electron-phonon heat transfer in the framework of the Allen-Downer approach, as already mentioned above, are carried out using the electron-phonon interaction constant defined in the equilibrium case and at ultralow temperatures. Thus, the novelty of the proposed such calculations should include carrying out the calculation in those conditions that are directly observed with ultrashort laser exposure: high electron temperatures exceeding the lattice / ion temperature. The possibility of such calculations comes from the proposal to use the density functional method, which allows the electron temperature to be set independently of the lattice state. To correctly determine the phonon spectrum, several dozens of atoms are required in the calculation cell, which is described in periodic boundary conditions, which is quite consistent with the performance of a great number of supercomputers operating in Russia.

4.5. *The current state of research on this issue, the main directions of research in world science and scientific competitors*

A) Spatially distributed heating due to a combination of plasmon and laser EM fields

Plasmonics is an important branch of modern physics, which has significant applications today and many promising applications for the future. It generates great interest among many groups (see the example in section 4.2 with the METANANO conference).

Another major direction is connected with laser technologies that use the laser heating, melting and thermomechanical effects. All listed tasks from A to G refer to this scientific direction. Generally speaking, plasmonics and laser thermomechanics develop independently, since the used theoretical methods differ fundamentally.

Our work on task A is aimed at creating a bridge between these two scientific fields.

Scientific competitors. The first works approaching this direction were performed in recent years. But they refer to the melting of nanoparticles in colloids, which is far from our task.

The closer to us work is performed by the group headed by Prof. Jean-Philippe Colombier from University Jean Monnet Saint-Etienne, Laboratoire Hubert Curien and Dr. R. Stoian - head of the Laser-matter interaction group at the same university. They consider thermal and hydrodynamic effects along with plasmon fields, but in dielectrics. These studies are mainly focused on the analysis of periodic structures like laser induced periodic surface structures (LIPSS) in the bulk and on the surface of dielectric materials.

B) Effect of vortex beams

This direction appeared relatively recently from the works [5] in the list of references to p. 1.4. It is currently divided into two sub-directions. In the first one, the beam diameter on the target is of the order of the wavelength. Here they are interested in the central feature of the structure in the form of a spiral elevation, see fig. 2. This sub-direction belongs to our task B.

On the second sub-direction, the diameter of the vortex beam on the target is large — many wavelengths fit on the diameter. They are interested in the usage of multiple pulses and the formation of spiral structures like LIPSS (laser induced periodic surface structures) on the surface. A conventional (non-vortex) large-diameter beam produces a system of periodic crests (like frozen sea wave). The direction along the ridges is perpendicular to the polarization vector of the laser electromagnetic wave. For a wide vortex beam, the direction of polarization changes inside the spot from point to point.

Accordingly, the ridges are fancifully turned. In such studies, the most advanced group is one headed by Prof. Salvatore Amoruso from Neapolitan University of Naples Federico II University. But this filed is far from our task B.

C) The formation of nanoparticles during ablation into a liquid.

The active scientific work is observed in this direction. It is considered promising with the possibilities of substantial commercialization. Basically, as it can be seen from recent reviews [12] to Section 1.4, the lasers physicists and chemists are involved to such work. They enumerate the parameters of laser exposure, targets (pure substances, alloys, laminates) and

ablation-receiving fluids (inorganic and organic, salt solutions). At the same time, fundamental issues remained unresolved yet due to the complexity of the processes.

The final stage of the process, when the bubble is clearly visible, has been studied in detail both in experiments and theoretically. The last work of this kind is [13] cited in the list of references to Section 1.4. This is the work of David Amans from Claude Bernard University Lyon 1. The theory relies on integrating the Rayleigh-Plesset equation. Bubble observations in [13] start from several microseconds, while the duration of the applied laser pulses varies in different experiments from subpicoseconds to nanoseconds. The "invisible era" in the experiments remains at times shorter than a microsecond.

About five years ago [1], the first works [1-5] appeared that shed light on the initial stages. The most significant contributions are made by the Povarnitsyn's group from JIHT RAS [1], and T.E. Itina [1] from Laboratoire Hubert Curien, Université de Lyon, Université Jean Monnet, and Prof. L.V. Zhigilei [2,4] from the University of Virginia. At present, studies have only been performed with ultrashort laser pulses (on the order of picoseconds or less). Evolution is tracked over the first few nanoseconds after exposure. In our work [3,5], the process is brought to a record of 0.2 microseconds, which, however, is still far from the bubble stage.

A significant achievement of the works [2-5] is the study of hydrodynamic stability at the contact zone between the metal and the receiving liquid. It is shown that under conditions of ultrashort pulses, the Rayleigh-Taylor instability develops due to the braking of a heavy metal by a liquid. This leads to the penetration into the liquid of rather large nanoparticles with dimensions of the order of a dozen nanometers.

As mentioned in the preceding paragraphs, the project will follow the complete evolution of the flow from the initial stage to the formation and dynamics of the micro-bubble. The effect of the pulse duration over the entire range of applied fluences will be studied. Such work requires detailed information about the fluid. This will be done with the example of water. Reference data on the thermal conductivity of water and the equation of state that covers the entire range of compressions and expansions of water from the Hugoniot adiabat to the two-phase region will be used. Note that in previous studies, the simplified descriptions of water were utilized.

D) Laser fragmentation of liquid droplets and jets

The great interest arose to laser-induced fragmentation of tin drops or a mixture of tin with iridium in connection with the program for creating photolithographic machines operating with extreme ultraviolet light (EUV) or a soft X-ray. The customers are ASML (Holland, https://www.asml.com/asml/), the University of Twente (Holland) and the Institute of Spectroscopy of the Russian Academy of Sciences in Troitsk. The site ASML says that the company began selling EUV systems recently. The machine is called NXE: 3400B system. EUV systems use 13.5 nm shortwave light. Accordingly, the diffraction limit decreases and the packing density of elements on the chip increases. However, it is necessary to work in vacuum,

and not in a liquid, as in the case of DUV (deep ultraviolet), and to use X-ray multilayer mirrors as optics; review of works on multilayer coatings is given in [6].

Another problem of phenomena, induced by the X-ray laser pulses to expose a droplet of water, arises in connection with the work [14] of Prof. Claudiu Stan, cited in Section 1.4. Their group will provide experimental data with which our numerical simulation will be compared. Prof. Claudiu Stan's group conducts experiments on free electron lasers (Linac Coherent Light Source, SACLA, FEL FLASH to DESY). This is a fundamental study of the initial stages of phase transitions associated with the generation of nuclei of a new phase. Moreover, X-ray lasers with an ultrashort pulse are involved into research. Such a pump pulse drives the substance motion in the target, while a subsequent diagnostic (probe) pulses probe the evolution of a substance at the micrometer-sized scale. The research includes diffraction measurements at a frequency in units of MHz of the X-ray laser pulse repetitions. Experimental capabilities are the most advanced in his group.

E) Ablation of refractory metals

The phenomenon of laser ablation has long been known. There are two regular international ablation conferences: HPLA (high power laser ablation, https://www.usasymposium.com/hpla) and COLA (conference on laser ablation, https://cola2017.sciencesconf.org/, https: / /cola2019.org/). However, this topic is also presented at other international conferences: for example, ICPEPA or FLAMN. Laser ablation of simple metals has been the subject of many papers. Today, the specificity associated with ultrashort pulses, when thermomechanical effects play an important role, is well recognized.

But there are complications. They belong to the so-called "non-standard" metals, X-ray lasers and irradiation at small sliding angles. Such irradiation is used in X-ray mirrors in the case of a hard X-ray. This is necessary to increase the reflection coefficient. Such a task will be solved in the project. Our "non-standard" material is ruthenium. The situations formed by a femtosecond pulse generated by lasers will be analyzed. The range of electromagnetic wavelengths is considered: optics - soft X-rays - hard X-rays.

There are groups that systematically apply hard X-rays for heating purposes (for example, [14], in Section 1.4) or diagnostics (same [14], and [7] here) or check the hard radiation coming from rapidly hot targets [8]. The soft x-rays are used for sensing in work [9] (in references to Sec. 4.1). Ref. [9] gives a review of the research done by late Anatoly Yakovlevich Faenov on the ablation of metals and dielectrics with soft X-rays.

The applied aspect of the problem under study is described in [10]. The application of the Monte-Carlo/XCASCADE (3D) code describing the kinetics of photo-ionization, in conjunction with the two-temperature model (but without the movement of material), is presented in [11]. The two-temperature model of ruthenium (without hydrodynamics) is analyzed in [12]. In our project the complete task will be solved, i.e. taking into account both purely thermal and

hydrodynamic effects. This will allow us to solve the issue of ablation thresholds and with comparison with experiments.

F) Laser melting of powders

The project will explore the most important part of the modern cutting-edge technology called as 3D printing. At present, this popular technology is expanding rapidly; several generations of automated machine tools have been created. The printing consists of several linked steps. First, a project of the future product is created in the computer-aided design (CAD) system. Then the product is dissected into thin sections 50–200 μm thick in the same 3D system. Secondly, a flat horizontal layer of micro-powder is formed in a horizontal bath. Finally, thirdly, the laser beam, adjustable by mirrors, melts the powder particles. The melting contour, along which the laser beam moves, is specified by a computer according to the sections specified in the CAD program.

The most complex and poorly studied link is associated with the physics of laser melting and recrystallization of micro-powder. A significant study is required in this field. This is mainly an experiment [13,14]. In numerical approaches, researchers use finite-difference methods or the finite element method [15]. Our project is based on a physical model and collectively developed programs with Lagrangian hydrodynamics, molecular dynamics with Monte Carlo method for electron thermal conductivity, and SPH code, which is specially adapted to describe 3D situations with complex geometry (powders, porous or layered media).

G) Computational physics, large-scale high-performance numerical simulation

Our team constantly leads the improvement of numerical tools, see, for example Ref. [15] in Sec. 1.4. In this project, because it is necessary to improve those tools for solving the above physical problems.

(Subsection G-1: Two-temperature hydrodynamics)

The hydrodynamic code in Lagrangian variables was created in our team 15 years ago. It is based on the well-known scheme suggested by Samarskii and Popov [48]. The scheme was drastically modified to match the laser effects with femtosecond pulse durations. With such an impact, it is necessary to take into account the strong excitation of the electronic subsystem. With our laser intensities (with an absorbed energy greater than 1 mJ/cm2), the electron-electron relaxation ends in a time shorter than the pulse duration.

Therefore, the electron subsystem can be described as a thermodynamically quasi-equilibrium system with an effective electron temperature Te. The concept of internal separation into the electronic and ion subsystems was created at one time in the pioneering work [49]. This work

helped to realize the fundamental difference between the effects of nanosecond (ns) and femto-picosecond (fs-ps) pulses. In ns pulses, the target substance evaporates or, at higher energies, a plasma corona is formed. Whereas at the fs-ps range, the thermomechanical effects in the condensed phase prevail. Thus, the physics of laser effects on materials changes qualitatively.

After creating a way to form ultrashort pulses with a compressor and stretcher (Gerard Moore and Donna Strickland, 1985), the era of the most active applications of these pulses in various applications (the Nobel Prize in Physics for 2018, the creation of tools from light) began. The researchers, who used ultrashort pulses, tried to first explain the effects of exposure using the then usual ideas applicable for ns pulses. Nothing worked. Only after using the ideas and approach of [49] (published 11 years before the work of Moore and Strickland, 1985) it became clear what was happened.

So, the physics of two-temperature states was added to the scheme [48]. The energy balance was split into two balances — the energy equations for the electron and ion subsystems, written separately. Then, the work began on establishing and building state equations in two-temperature conditions, calculating the thermal conductivity coefficient in two-temperature conditions, and determining the coefficient controlling the rate of energy exchange between the electron and ion subsystems in a condensed-phase material. Currently, our hydrocode is quite close in spirit to that developed in the JIHT RAS, in the Povarnitsyn's group [1].

Unfortunately, there is no universal recipe for this information. Each metal requires independent research. Moreover, the coefficients differ strongly from one group of metals (noble) to another (for example, iron, nickel, platinum), see [50] and references in this work. The ability to use the tabular equations of single-temperature states prepared by colleagues from JIHT RAS [51-55] has been added to our hydrocode. Creating equations of state is a very important work.

The two-temperature hydrocode needs to be improved for each specific application. The code modification for the calculation of subnanosecond actions was completed this year; see the second article in reference [6] to Sec. 1.4. The project will carry out the works on expanding calculations for nanosecond pulses and record-breaking times (up to μs). A complete equation of the state of water will be added to the hydrocode, which, as stated in this proposal, will cover a wide range of water states from double compression on the Hugoniot curve to rarefaction up to hundredths of the atmosphere of two-phase mixtures. In our previous work with water, the Grüneisen adiabat was used, see [6] to Sec. 1.4. A block for calculation of ruthenium will be also added in this project.

(Subsection G-2: Molecular dynamics)

In the last decade, the rapid growth of available computing resources made it possible the atomistic modeling of large systems having dimensions of several micrometers, which is approaching the scale of experiments with the influence of femtosecond lasers on films of

micrometer thickness. Thus, straightforward molecular dynamic (MD) simulation of a variety of laser-induced phenomena, including shock-wave phenomena, elastic-plastic transformations and phase transitions in materials under the action of high-speed deformations, has become possible [16-27]. At present, MD studies of such phenomena on a class of multiprocessor computers (available to us) can be performed on micrometer-sized samples within a few nanoseconds of the physical time of the process in a sample for a reasonable wall-clock time.

We use our own multiprocessor high-performance classical molecular dynamic simulation program with efficient parallelization. The scheme was first introduced in [45]. The method is named: material particle - dynamical domain decomposition (abbreviated MPD3) method. Note that, following similar principles, we developed an effective high-performance algorithm for SPH (Smoothed Particle Hydrodynamics, see the next subsection for reference) simulation, see the description in [15] in the list of references to Sec. 1.4. At present, the corresponding code is called CSPH-VD3 (Voronoi dynamical domain decomposition), since, like MPD3, it is based on three-dimensional decomposition of material samlpes into moving Voronoi subdomains, see detailed description below in the next subsection G-3.

Relatively recently, the MD program has been combined with a Monte-Carlo (MC) module for the calculation of electronic thermal conductivity. As it is known, in metals the electron thermal conductivity is much higher than the thermal conductivity associated with the thermal motion of ions. In our combined MC-MD code, each ion carries a quasi-electron with which it exchanges their momenta [46]. Random exchanges of electrons between neighboring ions at a given rate preserve the electro-neutrality of the material and allow the electron energy to diffuse through the grid of ions. Dips of density and discontinuities in material naturally reduce the coefficient of electronic thermal conductivity. Thus, the MC module allows you to correctly simulate the distribution of heat in metals and mesoscopic structures such as metal foams, and in particular the propagation of the melting and recrystallization fronts in such complex environments, that it is very difficult to achieve by the popular combination of MD with a mesh method for the problem of heat conduction [2, 4, 16].

(Subsection G-3: SPH)

Parallel modeling of non-stationary problems of continuum mechanics in extreme states characterized by significant pressure and velocity gradients, free surfaces and contact density discontinuities is faced with the problem of efficient use of computational resources due to the lack of a high-performance parallel processor with rapid changes in the spatial distribution of matter. Under these conditions, approaches using a static spatial decomposition of the computational domain (for example, LAMMPS: Large-scale Atomic/Molecular Massively Parallel Simulator) cannot provide an acceptable parallel calculation efficiency, since the distribution of the payload determined by the computational cost of calculating the motion of a substance is not tied to this movement.

We successfully develop an efficient load balancing algorithm and create a parallel program for large computational clusters that can evenly and maximally load available processors with useful work, and thereby ensure a high parallel efficiency of computation of hydrodynamic problems characterized by high-speed motion of matter and its fast redistribution [15] to Section 1.4.

Such tasks include modeling the proposed tasks of this project, in particular the laser effect on heterogeneous media and the calculation of the passage of the melting front along the mesostructure of the granular medium (powder), see the project text. Also in demand is effective parallel modeling of the problem of fragmentation of droplets and jets after irradiation with a light pulse (see project text), impact destruction of fragile materials [47], and high-speed collision of bodies.

Using the meshless SPH method [40], improved by solving the Riemann problem for interacting SPH particles [41], is preferable to use the mesh methods for modeling the processes listed above, which are very difficult to accurately resolve contact and free boundaries (for the Eulerian formalism) building mobile adaptable grids with Lagrangian medium description.

Solving the problem of uniform distribution of computational work between threads, processes or processor cores of a computer cluster is the key to building an effective parallel program. For the above problems of hydrodynamics, this task reduces to an optimal distribution of computational work between processors, i.e. to the decomposition of the simulated material samples between processes. In this case, even decomposition is a necessary, but not sufficient condition for optimality, since the exchange of information between processes is determined by the number of interacting particles that are in different processes. These particles are distributed in the volume of the border strip between the processes in the case of spatial decomposition of the medium and provide interaction between adjacent areas of the medium belonging to different processes.

A frequently used method of spatial decomposition is the method of division into parallelepiped subregions [42,43]. Under conditions of spatial inhomogeneity of the particle density, such a division can be performed recursively, by the method of orthogonal recursive bisection [44]. The idea of the method is simple: a rectangular area is recursively divided into two parts along the long side, so that each has an equal number of particles. Borders between rectangular subregions are planes parallel to the axes of coordinates. Balancing is carried out through the mobility of these planes separating the subregions. But with rebalancing, connectivity between processes can change significantly. Since the subdomains have a different number of neighbors, the reorganization of the decomposition requires multiple particle exchanges. This method of decomposition does not take into account the mixing of particles. All this, taken together, increases the calculation time due to significant exchanges of particles located in the frontier bands between the processes.

For a more efficient dynamic load balancing, we developed and use the method of dynamic decomposition of the material samples (not the space of the computational domain) into

moving Voronoi subdomains [15] to Sec. 1.4. Voronoi decomposition is uniquely defined by a set of generator points of the Voronoi diagram, where each point of the diagram corresponds to one computational process. The particles closest to the point-generator of the Voronoi subdomain are contained in the memory and updated with the corresponding process responsible for this subdomain. The mobility of the Voronoi diagram is carried out through the mobility of generator points, since their position is associated with the movement of the particles belonging to them. Loads of individual subdomains may vary in time, and the reason for which are the following factors. First, in the Voronoi subdomain, the number of particles can vary both for algorithmic reasons (fragmentation and merging of particles, adjusting the chart boundary due to a shift in the center of the diagram), and for physical reasons: according to changes in the density distribution and/or discontinuity of the environment surrounding point generator. Secondly, and this is very important, the physical processes inside each of the particles are local, which means that they can be calculated by their specific algorithms of different time consuming.

These factors lead to the fact that the sets of SPH particles in each Voronoi subdomain are processed at different times, which means that the processes are unevenly loaded. Therefore, the positions of the generator points are additionally shifted by the balancing displacement [45], redistributing the boundary particles from one region to another, which equalizes the computational load. Such an algorithm for load-balancing Voronoi decomposition is used together with the SPH-method for modeling problems of continuum dynamics for the first time.

The Voronoi auto-balancing decomposition algorithm allows one to naturally take into account the mass redistribution in the computational domain during the simulation. The algorithm is able to adapt to arbitrary flows with a minimal exchange of particles between cells, without requiring the preservation of connectivity between the Voronoi diagram generators. Data exchange between the subdomains of the diagram is localized pair-wise communication; at the same time, the surfaces through which the exchange takes place are usually smaller than in the methods with block (by parallelogram) decomposition of the region. Balancing decomposition is fully adaptive and to maximize the efficiency of the calculation does not require its rebuilding from scratch.

Decomposition according to Voronoi method with load balancing does not have the drawbacks characteristic of static decomposition or dynamic with bisection methods noted above. The experience of our calculations shows that the geometry of the sundomains tends to a cellular structure that has a minimum volume of border zones. Maximizing the load reduces the number of particles to be exchanged. The Voronoi subdomains also tend to an equal number of subdomains-neighbors, and the connectivity of the subdomains is not fixed and may change, following the mutual movement of the substance. Changing connectivity in this case is a local process that does not require massive communication between all processes. All communications between subdomains are carried out only within the circle of their nearest neighborhoods. Thus, despite the fact that the Voronoi decomposition is more difficult to program than the methods described above, it has indisputable advantages in solving problems of continuum mechanics in extreme states.

(Subsections G-4, 5: Development of potentials using cold stresses from DFT calculations)

The potentialities inherent in atomistic modeling are so great that they can lead to a deeper understanding of various physical phenomena caused by high-speed deformation, which can be caused by ultrafast release or energy transfer in metals under the action of a laser pulse, electrical discharge or shock wave front. All such effects on materials create extreme pressure gradients (~ 1 GPa/nm) and temperatures (~ 100 K/nm), which lead to complex highly non-equilibrium flows of matter with possible phase transitions and discontinuities in the form of bubbles and cracks. It is worth noting that, in contrast to MD, approaches based on continuum mechanics and the equation of state, which are widely used in modeling, are internally unable to describe the physics of all various high-speed nonequilibrium processes, such as cavitation, cracking and spalling, dislocations, and elastic-plastic transformations, as well as the kinetics of nonequilibrium phase transitions. Nowadays, the MD method is becoming a serious competitor to hydrodynamic methods in modeling phenomena, where large gradients of physical quantities arise, leading to rapid deformations and transformations of matter.

The reliability of the interatomic potential used in such extreme conditions is a critical requirement necessary for the predictive power of MD simulation. One of the most successful approaches for MD modeling of metals is the embedded atom model (EAM), which is a multi-body potential that is necessary for modeling a metallic bond [28-32]. The first generation of EAM potentials was based on simple analytical functions of charge density and energy, which have physical bases in the density functional theory [33].

The above works gave potentials that are optimized only for the general properties of metals, such as equilibrium density, cohesive energy, and elastic constants under normal conditions near zero pressure and room temperature.

Most of the intensively used modern EAM potentials were developed without regard to theoretical ideas about interatomic forces in a solid body in order to gain more freedom for fitting to experimental data and first-principle quantum mechanical calculations. Therefore, these second-generation potentials, having the form of tables or a set of splines, are more accurate in their ranges of definition than the previously proposed first-generation potentials. However, outside the range of parameters where fittinf was carried out, the potentials of the second generation are often not able to correctly describe the properties of a substance. For example, the widely used Mishin potentials for aluminum and nickel [34] are fairly well optimized for small strains and strains near room temperature, but lead to incorrect behavior of the metal with strong compressions of tens of GPa and higher. In particular, there is a decrease in the sound speed with compression and the appearance of rarefaction shock waves in aluminum and nickel, which fundamentally contradicts the experimental data. Similar restrictions on the field of application are typical for most EAM potentials of the second generation, including potentials for refractory metals, for example, for ruthenium [35,36].

Since the physical processes of interest to us occur as a result of extreme conditions caused by ultrafast localized energy release, then for credible MD simulation of these processes, potentials are needed that have been developed specifically for use in a wide range of pressures and temperatures.

There are two common methods for fitting interatomic EAM potentials based on first-principle databases: energy matching [37] and force matching [38]. When the energy is adjusted, the set of ab initio energies is calculated for various atomic configurations and crystal states. This set is commonly referred to as a fitting database. Then, parameters/coefficients of the EAM potential are searched/adjusted to reproduce the energy from the database as accurately as possible. A similar scheme is used for fitting by forces, for which ab initio forces between atoms are calculated. A combination of these two methods is often used also.

The main disadvantage of such fitting methods is that the atomic configurations entered into the database are not related to each other by any continuous physical process, such as isothermal compression or isochoric heating. Thus, the selected atomic configurations are physically poorly connected and strongly scattered in the multidimensional configuration space of atomic coordinates, and there is no guarantee that even a perfectly fitted interatomic potential will give accurate energies/forces in atomic configurations that are noticeably different from the fitted ones.

At the same time, the set of atomic configurations is usually limited to several thousand forces/energies, which is clearly not enough for sufficiently dense filling of the selected region of the configuration space. In such a case, it may well turn out, so even ideally fitted potential in MD simulation of a substance, say, with continuous compression, will quite often fall into the state regions of a substance where there is a shortage of adjustable atomic configurations. In these cases, the accuracy of the potential will fall sharply, and even non-physical/incorrect properties of the substance, such as a decrease in the rigidity of aluminum and nickel with compression, are not excluded, as indicated above in the case of Mishin potentials (with these compressions only a few adjustable points with small weights).

We have developed a new stress matching method [23]. This method aims to design EAM potentials specifically tuned for reliable reproduction of the behavior of materials in a wide range of pressures and temperatures. The basis for constructing a fitting database is the choice of atomic configurations of substances corresponding to the states that arise during continuous cold compression. Thus, the database is based on the ab initio equation of state of matter at absolute zero temperature, namely the cold pressure curve P (V) under uniform compression/tension and components of the stress tensor (pressure tensor) under uniaxial crystal deformations along the main crystallographic axes. Such a choice of configurations for a fitting database ensures that the potential will correctly describe the mechanical response of a solid to various strains with large compressions/strains. Moreover, the smoothness of the potential function and the cold pressure tensor curves constructed on it ensures good agreement not only with points from the fitting database, but also between them along the entire smooth cold curve P(V). Taking into account the fact that thermal energy and thermal

pressure are small compared with the potential energy of the interaction of atoms and cold pressure in the dense condensed phase, it can be expected that the potential will also give a reasonable thermodynamic behavior of the substance up to temperatures close to critical. It must be said here that ignoring the physical monotonicity condition for P(V) under uniform or uniaxial compression is characteristic of most of the works on the development of interatomic potentials.

Thus, the inclusion of the cold pressure tensor P(V) calculated by the DFT method in the fitting database is necessary for the development of interatomic interaction potentials, the use of which can provide the predictive power of MD modeling of highly compressed/stretched states of a condensed material.

The minimization of the stress deviation from the database is carried out by the combined search method, which includes the rolling polyhedron method (downhill simplex algorithm) [39] and the random walk method.

The found local minimum is disturbed by the vector of random displacement, from which the search for a new local minimum begins again. This process is repeated until the search finds deeper local minima in the allotted time. If the depth of the newly detected local minima does not increase for about an hour, the search stops. Then the procedure is repeated with new initial coefficients of an arbitrary non-pathological EAM potential. After several such attempts, the best potential among all is considered to be found and the search is completed. The sequential algorithm described above is actually implemented in our parallel search program, in which each processor independently searches for its best minimum, and the master processor compares them and keeps the best one. Using hundreds of CPUs, the program can scan multidimensional atom coordinate space in much more detail and find a better option than a sequential program in the allotted time. But even the use of parallel search does not guarantee finding a global minimum, the task of finding which is tremendously difficult. Fortunately, solving the global search problem is not our goal.

Examples of EAM potentials developed by the cold stress fitting method are presented on our page https://www.researchgate.net/project/Development-of-interatomic-EAM-potentials .

In this project we are going to develop a new potential for interatomic interaction of ruthenium using the described approach.

For the fitting base of cold stresses in ruthenium, the packages of quantum mechanical DFT (density functional theory) calculations of VASP, Abinit, Elk, etc. will be used.

H) Characteristics of laser irradiated silicon

Considering the calculation of electron heat conductivity in the framework of the first-principles methods with the Kubo-Greenwood formula, it should be noted that it is completely solved only in the case of such a simple metal as aluminum (D. V. Knyazev, Phys. Plasmas, 21 (073302),

2014). To this date, there are some works on the extension of this approach to other metals, including transition and noble, which have a lot of valence electrons that require a direct description in quantum mechanical calculations. In our case, we are talking about silicon, the electronic structure of which is not so much complicated in the sense of a number of valence electrons. The only problem that arises when describing semiconductors, in this case, is the strong deviation from the homogeneity of the electron gas due to the presence of directional bonds between silicon ions. However, a number of authors (R. Darkins et al, Phys. Rev. B. 98, 024304, 2018) have shown that a good description of the electron structure of silicon in the solid state can be achieved using hybrid functionals within the density functional theory.

Thus, the authors rely on the applicability of the discussed approach with respect to silicon. Calculations of heat conductivity by various approaches within the framework of the classical molecular dynamics method, such as the Green–Kubo approach, nonequilibrium molecular dynamics, were repeatedly performed for silicon, but only for some of its states, mainly for amorphous phases lying between 1300 and 1700 K. In this work the goal is to study the state of the liquid phase of silicon up to temperatures corresponding to the formation of a fluid, which experimental study is still difficult.

I) New approaches to calculations of the constant of electron-ion interaction in metals

Calculations of electron-phonon heat transfer in the Allen-Downer approach, as mentioned above, are carried out using the electron-phonon interaction constant defined in the equilibrium case and at ultra-low temperatures. Thus, the originality of the proposed calculations should be attributed to the conditions that are directly observed in the ultrashort laser irradiation: high electronic temperatures exceeding the temperature of the lattice / ions. The possibility of such calculations comes from the suggestion to use the density functional theory, which allows setting the electron temperature regardless of the lattice state. The correct determination of the phonon spectrum will require several tens of atoms in the computational cell described in periodic boundary conditions, which is quite consistent with the current performance of the existing supercomputers which has been constructed in Russia.

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4.6. *Proposed methods and approaches, a general work plan for the entire project implementation period and expected results* ***(not less than 2 pages in volume; including the expected specific results by year; an overall plan is given by year)***

A) Spatially distributed heating due to a combination of plasmon and laser EM fields.

A physical model will be created, analytical and numerical calculations of the electromagnetic fields produced by the laser and surface plasmon-polariton (SPP) modes will be carried out. The corresponding inhomogeneous dissipation along the surface in the skin layer will be calculated. The SPP modes are excited by the same laser pulse on a previously created inhomogeneity of the surface of the metal film. Thermal phenomena (heat spreading due to thermal conductivity), melting, hydrodynamic motion taking into account capillary forces (which are quite significant, as estimates show) and recrystallization into surface structures will be simulated. The final frozen surface structures will be compared with those that were observed in the experiments in [11], see the references to section 1.4 of the abstract of the project.

Work will be performed for 2019 and 2020.

In 2019, the formation of radial corrugation on the domes will be explained, see fig. 1 in the attached file 4.13 file 1.

B) Action of vortex beams

To solve the problem, the whole arsenal of techniques will be used, except for SPH modeling. Lagrangian hydrodynamics, molecular dynamics with a Monte-Carlo electronic thermal conductivity technics, and a modified semi-analytical model of thin film dynamics taking into account the surface tension and pressure of the evaporated substance will be required (for this model, see [10] in section 1.4, JETP, 2015).

The work is complex, it will be carried out in stages for 2019-2021.

C) The formation of nanoparticles during ablation into a liquid.

A lot of work will be done in this direction.

Firstly, it is necessary to incorporate detailed up-to-date data related to water into the computational programs; in the following steps, features related to other liquids will be considered. Water data will cover a wide range of liquid states (numerous solid water phases are excluded) of water from compressions along the shock adiabat to pressures of 20 GPa (higher levels cannot be created due to low acoustic impedance of water) to negative pressures

upto a critical water pressure of 220 bar and below to large expansions and pressure drops to hundredths of a bar (due to over-expansion of the bubble). A detailed description will be created of what is happening inside the two-phase water region.

Secondly, mutually complementary calculations by the next programs will be performed: (a) a two-temperature hydrodynamic program, (b) a molecular dynamics program taking into account the electronic thermal conductivity of the metal and the molecular thermal conductivity of water and (c) an SPH program. It is necessary to draw up a clear general picture of what is happening on the basis of the obtained calculated data. The picture of the thermal and dynamic interaction of the evaporated metal layer, in which condensation takes place, with the surrounding liquid, which in turn changes from a supercritical state with low compressibility to a subcritical state with high compressibility and begins to form a bubble. Subtle details that follow from molecular dynamics will be taken into account - this is the kinetics of evaporation and condensation, variation of surface tension under the conditions of the problem, and diffusion processes. With the help of molecular dynamics and SPH modeling, the role of the Rayleigh – Taylor instability under different conditions (variation of the energy deposited on the target and the pulse duration) will be understood.

Thirdly, it is necessary to clarify the question of the transition from one-dimensional flat expansion to three-dimensional spherical expansion - the formation, development and inhibition of a bubble.

Sections “firstly” and “secondly” will be completed in the first two years of the project. For the execution of the last section ("thirdly") apparently, it will take the 2021st year.

D) Laser fragmentation of liquid droplets and jets

Research will be continued on a drop of tin. It is necessary to replace the equation of state of Mie-Grüneisen used in [7] (see the literature for section 1.4) with the tabular equation of state - 2019 and 2020.

In collaboration with the group of prof. C.A. Stan (Rutgers univ.), working on XFEL (x-ray free electron laser) LCLS (LINAC coherent laser source) and other XFEL (FLASH DESY, SACLA RIKEN/HARIMA, Hyogo prefecture, Japan), a physical model will be created and numerical simulation of a problem of the interaction of a thin cylindrical hard X-ray beam with a microdrop or microjet of water will be carried out. Modification of our programs is required. All programs will be used.

Two-temperature Lagrangian hydrodynamics will be required to describe the initial stages of the development of a process around a cylindrical jet. Molecular dynamics modeling and SPH code will be applied to describe the middle and late stages. At the middle stage, the shock wave comes from a thin heating cylinder in the middle part of a drop or jet. At the final stages, the picture becomes very complex - oblique shock waves reach the free surface and are reflected

from it. This leads to the appearance of complex three-dimensional rarefaction waves, the simplest analogue of which is the Prandtl-Meyer wave.

The work will require 2019-2021 years. As a result of the research, a complete picture of the most complex process will be obtained, the scheme of which and the first experimental observations are shown in Figures 3 and 4, respectively.

E) Ablation of refractory metals.

A rolling polyhedron in multidimensional space (this is a simplex method) in combination with Monte Carlo, which produces fairly coarse noise, allows us to bypass the multidimensional parameter space that defines the potential of multiparticle interaction and find hundreds or thousands of local minima. From these minima is selected the most profound. So potential is built. The combination with Monte-Carlo is necessary, otherwise the simplex will roll into the nearest, but, as a rule, shallow minimum. This technique will be applied in 2019 to build the potential of interatomic interaction of ruthenium. The technique works together with quantum-mechanical means (VASP, Abinit, Elk, etc. software packages) for constructing cold curves taking into account the anisotropy of the crystal (usually along the main axes of the crystal cell) and taking into account the c/a parameter of the hcp (hexagonal close-packed) lattice, which includes ruthenium crystal.

Further, the interatomic potential will be applied to calculate the strength of the crystal and the ruthenium melt in our temperature and strain rate range using molecular dynamics methods. The strength data, together with the data on thermal conductivity and the coefficient of electron-ion interaction and the equation of state, will be used in two-temperature hydrodynamic modeling of ruthenium ablation under the action of laser pulses (all ultrashort) with different photon energies of ~ 1 eV, 90 eV, 7-12 keV.

In addition, the interatomic potential of ruthenium will be used in molecular-dynamic modeling of ablation with full consideration of non-one-dimensional geometry — foaming of the ruthenium melt after nucleation of the nuclei of the vapor phase in the melt.

The results of hydrodynamic and molecular dynamics calculations will be obtained in 2019. This will make it possible to understand what happens during laser irradiation of ruthenium.

F) Laser melting of powders

A hydrodynamical code in Lagrangian variables, molecular dynamics with scaling, and an SPH code will be applied.

A one-dimensional hydrodynamical code is needed to describe the initial and middle stages of absorption of laser radiation and the propagation of absorbed heat in the thickness of the powder microparticle. The duration of heating is determined by the diameter of the laser spot

on the surface (usually of the order of fractions of mm - mm) and the speed of scanning the beam along the surface (usually 10-100 cm / s). The absorption coefficient is calculated using the Fresnel formulas, taking into account the angle of incidence. Also, using hydrodynamic modeling, an estimate of the dynamic role of the saturated vapor pressure of the heated metal microparticle will be obtained.

An important role will be played by molecular dynamics simulation taking into account (the Monte-Carlo technics is involved) high electronic thermal conductivity in the bulk of the metal and using a scaling technics. The importance of this role is that the properties of interparticle contacts, "points" of contact, will be studied. In fact, these are not points, but small contact areas. Their area changes at partial compactification upon compression, upon heating, and upon melting. The size of the plots is extremely important for calculating the transfer of heat from one microparticle to another.

With the help of molecular dynamics simulation, the process of melting the microparticle, which starts from the illuminated surface area, will be studied. It is important to correctly describe the development of the melting process on the particle, taking into account the mesoscopic environment of neighboring particles.

The SPH code will be applied to calculate the thermal and dynamic effects in the mesoscopic ensemble of microparticles.

The work is great in scope and complex. For three years, a pattern of laser action on powders will be created. And the most important general pattern will be received in 2019.

G) Computational physics, large-scale high-performance numerical simulation.

(1) In the course of all forthcoming studies, the hydrodynamic code will be modernized for the corresponding specific task. Therefore, work on the code will be carried out throughout the whole time of the project.

(2) Molecular dynamics is an important tool in solving problems A – F listed above. Each time it will be adjusted to the problem. Using the physical model, the scaling parameters will be configured when required. Molecular dynamics will apply for the duration of the project.

(3) In the years 2019-2020 the part relating to the tabular equation of state will be added in SPH code (Smoothed Particle Hydrodynamics) and will be tested. It is clear that this will greatly increase the coverage of physical tasks with SPH code. This code is currently used with the equation of state in the form of Mie-Grüneisen. SPH is a very effective code when solving geometrically complex problems using a multimillion number of particles.

The code allows one to deal with the most complicated problems, for example, particle crushing (see [7] to section1.4 and the move attached to this publication) or the effect on powders. The disadvantage of an SPH code is the lack of a melting description. Usually,

melting in the SPH code is mimicked by calculating the temperature field, while the melt is the part of the material in which the temperature has exceeded the melting point. With a tabular equation of state, this disadvantage will be eliminated - the melting point will depend on pressure, a transition zone with a mixture of solid and liquid phases will appear and the latent heat of melting will be automatically taken into account. Such is the situation when simulatiion is made by a Lagrangian hydrocode.

By 2021, work will be completed on a program that will allow surface tension to be included in SPH. This will certainly raise the capabilities of the program to a new level.

(4, 5) The simplex plus Monte Carlo code was used by us earlier. In 2019, this code together with the DFT computation programs will be used to create, firstly, the interatomic interaction potential in ruthenium and, secondly, to construct a two-temperature state of ruthenium.

(6) Codes from ready-made COMSOL Multiphysics © and LS-DYNA packages will be adapted for solving problems A, B. Results will be obtained in 2019.

(7) In all the tasks listed above, a combined approach will be used. As mentioned, this approach is to use two or more codes to solve one problem. This is done either for verification and clarification. Either the task is complicated, it is divided into sections in time (initial and subsequent stages) and/or space (near-surface zone and volume), in which one code is used in one area and in another area - another code. At the same time, the results of the work of one code are incorporated into another code (hybrids).

H) Characteristics of silicon irradiated by laser.

For the study of silicon, the whole set of modern methods for calculating thermal conductivity in the framework of quantum and classical molecular dynamics will be used: the Kubo-Greenwood formula (Green-Kubo in the classical case) as an element of the theory that relates the kinetic coefficients of the system under consideration with the correlators of speeds and fluxes. In the case of quantum molecular dynamics, the basis of the electronic wave functions will be considered using the projected augmented wave method (PAW); to describe the lower electron states, than the valence, the pseudopotentials libraries that are included in the VASP computation package will be used.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals

Consideration of electron-phonon heat transfer will be carried out using quantum calculations using the density functional method using the approaches mentioned above using the computational package VASP, as well as ABINIT and Elk. In the latter case, the electron spectrum and the force constant tensor will be calculated in the full electron basis for cases where the transition from valence electrons to lower ones in energy is blurred due to the

presence of semi-valent states, as happens in some transition metals. An effective force field approach will also be used, which allows, within the framework of classical molecular dynamics, to describe the interaction of semiclassical electrons and ions, without resorting to e-jelly models, such as, in particular, the embedded atom method.

Let's sum up what was said.

A) Spatially distributed heating due to a combination of plasmon and laser EM fields.

Work on the combination of plasmonics and thermo-hydrodynamics will be performed for 2019 and 2020. In 2019, the formation of radial corrugation on the domes will be explained, see fig. one.

B) Action of vortex beams.

The work is complex, it will be carried out in stages for 2019-2021. Important results will be obtained as early as 2019.

C) The formation of nanoparticles during ablation into a liquid.

The main results will be obtained in the first two years of the project. To obtain a description of the spherization of the expansion flow, all three years of work on the project will be needed.

D) Laser fragmentation of liquid droplets and jets.

Translation of SPH to the tabular equation of state - 2019 and 2020 A full description of the problem with the action of the hard LCLS X-ray beam on the micro-droplet / jet will take all three years of work on the project.

E) Ablation of refractory metals.

It is planned to complete and present practical recommendations on X-ray mirrors for 2019. For the same period, to prepare articles.

F) Laser melting of powders.

The work is great in scope and complex. For three years, a pattern of laser effects on powders will be created. And the most important general pattern will be received in 2019.

G) Computational physics, large-scale high-performance numerical simulation.

All the years of work on the project will be accompanied by the modernization of computational algorithms.

H, I) These problems will be solved in 2019 and 2020.

4.7. *The scientific background of the project available to the research team*

(the results obtained earlier, the developed programs and methods are indicated)

The research team established for the project has extensive experience in the interaction of laser radiation with matter. Already in the widely cited work [1], the foundation was laid for the physics of the interaction of ultrashort laser pulses with matter in a condensed state. The most important features of such an interaction are widely covered in large-scale reviews [2, 3]. The research group covers a wide spectrum of laser radiation from infrared and optical [4-8] to ultraviolet and hard X-rays [9-11], as well as various targets of condensed matter - metals [12], dielectrics [13], solids, fluids [14] and various pulse durations, see, for example, recent work [6], the 2nd reference in the list of references to § 1.4.

With the help of our works [7] (literature to section 4.1), the observations of Newton's rings with a variable number of rings in time [6] were originally explained (see Section 4.1).

Our research team has developed theoretical models for the interaction of ultrashort laser pulses with metals, the ablation of both volume targets [15] and thin metal films [16] under the action of such pulses: see references in § 1.4 under the number [1]. These articles are supplemented with additional illustrations in the form of films Au-220, Au-225, Au-226 on the site http://laser.itp.ac.ru/RNF2019/index.html . These films show how the films evolve nontrivially after a sharply focused, ultrashort effect (melting - rebound from the substrate - braking due to surface tension - the onset of recrystallization - jet formation - continued solidification).

Work is underway to analyze the effect of longer subnanosecond [17] and nanosecond laser pulses on complex targets (films, laminates, powders). The effect on liquid microdroplets is being studied, see the SV.mp4 film at http://laser.itp.ac.ru/RNF2019/index.html . This is a film about the fragmentation of a tin microdroplet at a source of shortwave radiation for the photolithographic machines of the future. The film relates (illustrates) to article [7], see the list of references to paragraph 1.4.

In studies on the ablation of volume targets under the action of ultrashort laser pulses, molecular-dynamic modeling of the expansion of aluminum heated with a laser pulse with an interatomic interaction potential was performed, taking into account many-particle effects. An ablation pattern was obtained with the formation of a spall liquid part of the target filled with two-phase foam from liquid and vapor [18–20].

In the works carried out by the research team, the interaction of femtosecond laser pulses with thin (from 60–100 nm to several microns) flat metal films (gold used) on a dielectric substrate (fused quartz) was considered, see [1.10] - literature p. 1.4. The ablation of such targets as a result of the action of laser pulses with a duration of 30–300 fs has been studied. The thermal and mechanical properties of these targets are qualitatively different from the behavior of bulk targets and from free-hanging films, here the substrate works as a heat insulating wall, slowing down the cooling of the metal due to thermal conductivity in comparison with the situation of a bulk target. At the same time, the hydromechanical interaction of the film with quartz changes the situation in comparison with the case of a free-hanging film.

A combined approach combining two-temperature hydrodynamics and molecular dynamics simulation was applied. For the first time, descriptions of the possible modes of the dynamics of the metal film / quartz system are presented. The implementation of certain regimes depends on the magnitude of the surface density of the absorbed energy (absorbed fluence), see [1,10] - literature for p. 1.4. Found two thresholds for absorbed fluence and three modes of movement compared with one of the free-hanging film. There is an oscillatory mode in which the film oscillates, remaining on the substrate at the values of the absorbed fluence not exceeding a smaller threshold. When the fluence is in the interval between two threshold values, the metal film is detached from the substrate, because the negative pressure overcomes the adhesive force of the film-substrate contact. For fluence values exceeding the larger of the thresholds, there is a gap inside the film and ablation of the target in the form of spalling of the condensed target fragment before the metal is separated from the dielectric substrate [21, 22].

The formation of surface nanostructures as a result of ablation [23–25] under the action of ultrashort laser radiation on metallic films was studied. The dynamics of a thin gold film on a glass substrate caused by rapid heating using a subpicosecond laser pulse was studied. The pressure waves generated by such heating can lead to the peeling of the film and its departure from the substrate. Due to the inhomogeneity of the heating of the film surface in the radial direction of the laser spot, the velocity distribution in the film substance flying away from the substrate has a maximum in the center of the spot, and the separating film has a dome-shaped shape that swells with time (inflationary stage). The volume of the cavity between the film and the substrate increases during inflation, lasting from several to several tens of nanoseconds. Typical flight speeds are in the range of 30–200 m / s. Capillary forces acting along the flying film slow down the inflation of the dome and lead to the concentration of the substance of the dome along its axis. This leads to the formation of an axial jet and drops at its end, the recrystallization of which leads to the appearance of characteristic nanostructures on the surface.

A large complex of works was carried out to study the occurrence and propagation of ultrashort elastic and plastic shock waves in laser targets under the action of ultrashort radiation pulses. The existence of ultrashort elastic waves was found at pressures far exceeding the elastic limit [26,27], which relates to waves traveling along samples 100 mm – 1 mm thick.

A new propagation mode of shock waves was discovered, characterized by a two-zone elastic-plastic structure consisting of an elastic front and a plastic front following it, moving at the same average speed, and having a fixed effective thickness, reaching micron-scale [28]. In this case, the substance in the elastic zone is in a metastable state at a pressure that can significantly exceed the usually accepted values for dynamic yield strength [28,29].

The work [26] and the work of our colleagues, experimenters from the JIHT RAS (Ashitkov et al.), Were ahead of American papers on the same effect: Whitley et al. for 4 months and a year, an article in PRL of Jonathan and Mike and co-authors:

V.H. Whitley et al., The elastic-plastic response of aluminum films to ultrafast laser-generated shocks, JOURNAL OF APPLIED PHYSICS 109, 013505 (2011)

Jonathan Crowhurst, Michael R. Armstrong et al., Invariance of the Dissipative Action at Ultrahigh Strain Rates Above the Strong Shock Threshold, PRL 107, 144302 (2011)

S.I. Ashitkov, M.B. Agranat, G.I. Kanel', P.S. Komarov, and V.E. Fortov, Behavior of Aluminum near an Ultimate Theoretical Strength in Experiments with Femtosecond Laser Pulses, JETP Letters, 2010, Vol. 92, No. 8, pp. 516-520.

Studies of polymorphic transformations in metals under the action of shock waves [30, 31] have been performed. Polymorphic transformations of the alpha phase (body-centered cubic structure) into the epsilon phase (hexagonal close-packed structure) in iron under conditions of ultrashort loads are considered. Molecular dynamics modeling shows that in crystalline iron films oriented in the [110] and [111] directions, alpha epsilon polymorphic transformation in the experimental conditions under consideration can occur only in the first 100-200 nm film thickness, where the pressure in the shock wave exceeds 30 GPa. And in monocrystalline iron with the [100] orientation, the polymorphic transition is easily accomplished under the action of elastic shock waves with a pressure exceeding 23 GPa. The transition is not associated with the dynamics of dislocations and is reversible in the discharge part of the shock wave, where it begins with pressures of 23 GPa. For other crystal orientations, the reverse epsilon-alpha transition begins at pressures of the order of 13 GPa in the discharge tail. Molecular dynamics calculations were performed using the interatomic potential of iron in the immersed atom method, which takes into account the multiparticle effects of interatomic interaction in metals, in which parameters were selected in quantum mechanical calculations of the density functional theory taking into account the specificity of uniaxial deformation.

In addition to theoretical models, the team developed effective computational methods and created high-performance programs for numerical calculations and computer simulation of the problems of interaction of laser radiation with matter. A one-dimensional Lagrangian (as well as for radial motion with spherical and cylindrical symmetry) hydrodynamic code was developed for a substance subjected to a laser pulse, taking into account a nonequilibrium two-temperature state, energy exchange between electrons and ions, a wide-range two-temperature equation of state, a change in the phase state of a substance, and electronic heat conduction. This hydrodynamic code is also used to calculate the initial conditions for the subsequent molecular dynamics simulation [4,8,10,11,13-15,17,21,22,24,25,27].

The team has created highly efficient programs for molecular-dynamic calculations, based on parallel calculations and allowing to bring the number of particles involved in the simulation to several hundred million. The use of the capillary and thermal dimensionless parameters developed in a team for scaling allows us to significantly expand the spatial and temporal limits for molecular dynamics modeling [4,5,7,8,10-31].

The team has a lot of experience on the basis of calculations using the density functional theory of interatomic interaction potentials for both metals and non-metallic substances. In the "immersed atom" model, many-particle interaction potentials in metals such as aluminum, gold, tin were obtained, which adequately describe the interatomic interaction in these metals in a wide density range [5,14-16,28,32]. The density functional theory and based on it the program of calculating the electronic spectrum, electronic thermodynamic functions, quantum molecular dynamics for the movement of atoms with their interaction on the density functional theory were widely used in the project team.

In the VASP, Abinit, Elk software packages, electronic energy zones of both simple metals (aluminum, tin) and transitional (gold, copper, tantalum, nickel) were obtained, their electronic thermodynamic functions were calculated [33,34]. Using the quantum molecular dynamics, the coefficient of electronic thermal conductivity of copper in the liquid state was calculated over a wide range of density and electron temperature [35]

Collectively developed methods for calculating the kinetic coefficients of a substance in a two-temperature state, such as the coefficient of electron thermal conductivity and the coefficient of electron-ion heat transfer, and the computational programs created for finding them are important in numerical hydrodynamic and molecular-dynamic modeling of ablation under the action of laser radiation. The coefficient of electronic thermal conductivity of metals, both simple and transitional, was obtained in the approximation of the kinetic equation [36-40].

The coefficient of electron-ion heat transfer of both metals [38–40] and ionic dielectric crystals, such as LiF [11], was calculated.

Among the important computational programs are the hydrodynamic SPH code (Smoothed Particles Hydrodynamics), which allows two- and three-dimensional hydrodynamic calculations [41], as well as a set of programs for carrying out numerical electrodynamic calculations [42].

The group has considerable experience in calculating the electronic thermal conductivity of metals in a two-temperature state (Yu.V. Petrov, N.A. Inogamov, K.P. Migdal, JETP Letters, 97, 27, 2013; K.P. Migdal et al, App. Phys. A, 122 (4), 408, 2016; Yu.V. Petrov et al, JETP Letters, 104, 431, 2016), where they used both an analytical approach based on solving the Boltzmann kinetic equation in the relaxation approximation for hot electrons with the two-parabolic dispersion law proposed by the authors, and Kubo-Greenwood formula combined with a quantum molecular dynamic description of a copper melt. The results of the two approaches proved to be in qualitative agreement. Comparing different first-principle calculations with analytical data allowed us to express the idea of the limited accuracy of describing the electron-electron interaction of hot electrons using the density functional method (K.P. Migdal et al, App. Phys. A, 122 (4), 408, 2016, K.P. Migdal et al, J. Phys.: Conf. Ser. 774, 012103, 2016). Comparison of less computationally intensive analytical approach, conducted for both aluminum and third-party work (D.V. Knyazev, P.R. Levashov, Phys. Plasmas, 21, 073302, 2014, G. Norman et al, Contrib. Plasma Phys. 53 (4-5), 300, 2013), and for copper it shows a satisfactory agreement of the results in the temperature range above 10 000 - 20 000 K.

The study of electron-phonon heat transfer in metals has been one of the most urgent tasks of the group over the past six years (Yu.V. Petrov, N.A. Inogamov, K.P. Migdal, JETP Letters, 97, 27, 2013; K.P. Migdal, Yu.V. Petrov, N.A. Inogamov, Proc. SPIE, 9065, 90653, 2013; N.A. Inogamov et al., Cont. Plasma Phys. 53 (10), 796, 2013, K.P. Migdal et al, J. Phys.: Conf. Ser. 653, 012086, 2015; K.P. Migdal et al., App. Phys. A, 122 (4), 408, 2016). Data has been accumulated to describe a number of metals, including simple, transitional, and noble, in the electron temperature range up to 50,000 K. The effect of hydrostatic compression/tension, achieved by the action of electronic pressure forces in the final two-temperature stage, is also considered. Comparison with other models, among which the mentioned Allen-Downer model, shows in

general a good agreement of the data obtained by the authors for those metals where there are jointly results of research obtained by several methods.

Theoretical studies and numerical modeling are carried out in close collaboration with known experimental groups.

Such cooperation is conducted with the JIHT RAS (Department of Laser Plasma under the supervision of Dr. M. Agranat):

A study was made of the dynamics of aluminum melt produced by femtosecond laser pulses.

(N.A. Inogamov, V.V. Zhakhovsky, S.I. Ashitkov, M.B. Agranat, P.S. Komarov, V.A. Khokhlov, V.V. Shepelev, *Pump-Probe Method for Measurement of Thickness of Molten Layer Produced by Ultrashort Laser Pulse* AIP Conf. Proc. 1278, 590 (2010)) ;

M.B. Agranat, S.I. Anisimov, S.I. Ashitkov, V.V. Zhakhovskii, N.A. Inogamov, P.S. Komarov, A.V. Ovchinnikov, V.E. Fortov, V.A. Khokhlov, V.V. Shepelev, *Strength properties of an aluminum melt at extremely high tension rates under the action of femtosecond laser pulses*, JETP Lett. 91 (9), 471-477 (2010)),

The formation of nano-cavities inside an aluminum target was studied when the intensity of laser radiation was less than the ablation threshold.

(S.I. Ashitkov, N.A. Inogamov, V.V. Zhakhovskii, Yu.N. Emirov, M.B. Agranat, I.I. Oleinik, S.I. Anisimov, V.E. Fortov, *Formation of nanocavities in the surface layer of an aluminum target irradiated by a femtosecond laser pulse*, JETP Lett., 95(4), 176-181 (2012)),

properties of twotemperature states of metals are investigated

(N.A. Inogamov, S.I. Ashitkov, V.V. Zhakhovsky, V.V. Shepelev, V.A. Khokhlov, P.S. Komarov, M.B. Agranat, S.I. Anisimov, V.E. Fortov, *Acoustic probing of two-temperature relaxation initiated by action of ultrashort laser pulse*, Appl. Phys. A 101(1), 1-5 (2010);

N.A. Inogamov, Yu.V. Petrov, V.V. Zhakhovsky, V.A. Khokhlov, B.J. Demaske, S.I. Ashitkov, K.V. Khishchenko, K.P. Migdal, M.B. Agranat, S.I. Anisimov, V.E. Fortov, I.I. Oleynik, *Two-temperature thermodynamic and kinetic properties of transition metals irradiated by femtosecond lasers*, AIP Conf. Proc. 1464, 593-608 (2012)),

The propagation of elastic and plastic waves in metals under the action of femtosecond laser pulses was studied

(V.V. Zhakhovsky, B.J. Demaske, N.A. Inogamov, V.A. Khokhlov, S.I. Ashitkov, M.B. Agranat, I.I. Oleynik, *Super-elastic response of metals to laser-induced shock waves,* AIP Conf. Proc. 1464, 102-112 (2012);

N. Inogamov, V. Khokhlov, Yu. Petrov, S. Anisimov, V.V. Zhakhovsky, B.J. Demaske, I.I. Oleynik, S.I. Ashitkov, K.V. Khishchenko, M. Agranat, V. Fortov, C.T. White, *Ultrashort elastic and plastic shock waves in aluminum*, AIP Conf. Proc. 1426, 909-912 (2012)),

The formation of surface nanostructures in metals under the action of femtosecond laser radiation pulses was studied

(N.A. Inogamov, V.V. Zhakhovsky, Yu.V. Petrov, V.A. Khokhlov, S.I. Ashitkov, K.P. Migdal, D.K. Ilnitsky, Y.N. Emirov, K.V. Khishchenko, P.S. Komarov, V.V. Shepelev, M.B. Agranat, S.I. Anisimov, I.I. Oleynik, V.E. Fortov, *Ultrashort laser - matter interaction at moderate intensities: two-temperature relaxation, foaming of stretched melt, and freezing of evolving nanostructures.* SPIE Proceedings 9065, 906502,1-14, (2013);

N.A. Inogamov , V.V. Zhakhovsky, Yu.V. Petrov, V.A. Khokhlov, S.I. Ashitkov, K.V. Khishchenko, K.P. Migdal, D.K. Ilnitsky, Yu.N. Emirov, P.S. Komarov, V.V. Shepelev, C.W. Miller, I.I. Oleynik, M.B. Agranat, A.V. Andriyash, S.I. Anisimov, and V.E. Fortov *Electron-Ion Relaxation, Phase Transitions, and Surface Nano-Structuring Produced by Ultrashort Laser Pulses in Metals* Contributions to Plasma Physics, v. 53, p. 796-810 (2013);

Inogamov, N. A.; Zhakhovsky, V. V.; Khokhlov, V. A.; Ashitkov, S. I.; Emirov, Y. N.; Khichshenko, K. V.; Faenov, A. Y.; Pikuz, T. A.; Ishino, M.; Kando, M.; Hasegawa, N.; Nishikino, M.; Komarov, P. S.; Demaske, B. J.; Agranat, M. B.; Anisimov, S. I.; Kawachi, T. & Oleynik, I. I. *Ultrafast lasers and solids in highly excited states: results of hydrodynamics and molecular dynamics simulations* Journal of Physics: Conference Series, 2014, 510(1), 012041;

Inogamov, N. A.; Zhakhovsky, V. V.; Ashitkov, S. I.; Emirov, Y. N.; Faenov, A. Y.; Pikuz, T. A.; Ishino, M.; Kando, M.; Hasegawa, N.; Nishikino, M.; Kawachi, T.; Agranat, M. B.; Andriash, A. V.; Kuratov, S. E. & Oleynik, I. I. *Surface nano-structuring produced by spallation of metal irradiated by an ultrashort laser pulse* Journal of Physics: Conference Series, 2014, 500, 112070;

Ashitkov, S. I., Komarov, P. S., Ovchinnikov, A. V., Struleva, E. V., Zhakhovskii, V. V., Inogamov, N. A. & Agranat, M. B. *Ablation and nanostructuring of metals by femtosecond laser pulses* Quantum Electronics, 2014, 44(6), 535;

S.I. Ashitkov, S.A. Romashevskii, P.S. Komarov, A.A. Burmistrov, V.V. Zhakhovskii, N.A. Inogamov, M.B. Agranat *Formation of nanostructures under femtosecond laser ablation of metals.* Quantum Electronics, 2015, v. 45, pp. 547-550;

Inogamov, N. A., Zhakhovsky, V. V., Ashitkov, S. I., Emirov, Yu. N., Faenov, A. Ya., Petrov, Yu. V., Khokhlov, V. A., Ishino, M., Demaske, B. J., Tanaka, M., Hasegawa, N., Nishikino, M., Tamotsu, S., Pikuz, T. A., Skobelev, I. Ya., Ohba, T., Kaihori, T., Ochi, Y., Imazono, T., Fukuda, Y., Kando, M., Kato, Y., Kawachi, T., Anisimov, S. I., Agranat, M. B., Oleynik, I. I. & Fortov, V. E. *Surface Nanodeformations Caused by Ultrashort Laser Pulse,* Engineering Failure Analysis, 2015, 47, 328-337),

ablation of gold by femtosecond laser pulses is considered

(Ashitkov, S. I.; Komarov, P. S.; Zhakhovsky, V. V.; Petrov, Y. V.; Khokhlov, V. A.; Yurkevich, A. A.; Ilnitsky, D. K.; Inogamov, N. A., Agranat, M. B. *Ablation of gold irradiated by femtosecond laser pulse: experiment and modeling* J. Phys.: Conf. Ser., 2016, V. 774, No. 1, 012097[1-60]),

polymorphic transformations in iron under the influence of femtosecond laser pulses were studied

(S.I. Ashitkov, V.V. Zhakhovsky, N.A. Inogamov, P.S. Komarov, M.B.Agranat and G.I.Kanel. *The behavior of iron under ultrafast shock loading driven by a femtosecond laser.* AIP Conf. proc., 2017, 1793, 100035).

In collaboration with experimenters from IAPU, Far East Branch, Russian Academy of Sciences and FEFU, Vladivostok, as well as from FIAN (department under the hands of Prof. A. Ionin) the problems of laser printing of plasmonic nano cavities in silver and gold were considered

(Kuchmizhak, A.; Vitrik, O.; Kulchin, Y.; Storozhenko, D.; Mayor, A.; Mirochnik, A.; Makarov, S.; Milichko, V.; Kudryashov, S.; Zhakhovsky, V. Inogamov, N. *Laser printing of resonant plasmonic nanovoids* Nanoscale, 2016, 8, 12352-12361),

In collaboration with experimenters from IAPU, Far East Branch, Russian Academy of Sciences and FEFU, were considered

(Wang, X. W.; Kuchmizhak, A. A.; Li, X.; Juodkazis, S.; Vitrik, O. B.; Kulchin, Y. N.; Zhakhovsky, V. V.; Danilov, P. A.; Ionin, A. A.; Kudryashov, S. I.; Rudenko, A. A. & Inogamov, N. A. *Laser-induced Translative Hydrodynamic Mass Snapshots: non-invasive characterization and predictive modeling via mapping at nanoscale* Physical Review Applied, 2017, 8, 044016 - 1-17)

The joint work is carried out with experimenters from the Institute of Spectroscopy, Russian Academy of Sciences, Troitsk;

In collaboration with experimenters from the University of Twente, Institute of Nanotechnology, Netherlands, the ablation dynamics of the refractory ruthenium metal under the action of ultrashort laser pulses of the optical or X-ray range was considered.
(V. A. Khokhlov, I. Milov, I. A. Makhotkin, V. V. Zhakhovsky, D. K. Ilnitsky, K. P. Migdal, V. V. Shepelev, Y. V. Petrov and N. A. Inogamov. Dynamics of ruthenium mirror under action of soft x-ray or optical ultrashort laser pulse, J. Phys. Conf. Ser., accepted (2018)).

Much work has been done to study the interaction of short laser pulses of the optical range and soft X-rays with metals and dielectrics, the ablation of these substances, the formation of surface nano-structures together with experimenters from Kansai Photon Science Institute (KPSI), Quantum Beam Science Research Directorate, QST, X-ray Laser Group, group leader prof. M. Nishikino, Japan. This large work is reflected in a significant number of joint articles [1], references to which are given in the literature to section 1.5.

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4.8. *The list of equipment, materials, information and other resources available to the research team for the project (including the need for their use to implement the project)*

The project participants are provided with personal computers, the PARMA parallel computing complex of the Noginsk Scientific Center of the Russian Academy of Sciences (Chernogolovka) is used, the MD simulation is carried out on several multiprocessor machines, including the K-100 cluster at IPM im. Mv Keldysh (960 calculus), supercomputer "Lomonosov" (Moscow State University). VVZhahovsky has access to the Dutch Cartesius supercomputer (48,000 callers) https://userinfo.surfsara.nl/systems/cartesius.

The original, developed by the project participants two-temperature hydrodynamics program, the scheme of MD calculations with the original paralleling technique, the SPH scheme and others are used.

COMSOL, LS-DYNA, LAMMPS, Abinit and VASP computational packages (classical and quantum molecular dynamics), symbolic computation packages, etc. are used.

This whole device will be used in the execution of the project. Modeling by the methods of MD-MK and SPH is based on the application of the supercomputers listed above.

When calculating the electron-phonon interaction constant based on the calculation of the Eliashberg function, codes based on the density functional method ABINIT and Elk will be applied.

The equipment group is provided enough.

4.9. *Work plan for the first year of the project (including the planned trip (expedition) for the project)*

A) Spatially distributed heating due to a combination of plasmon and laser EM fields

Work on a combination of calculations of the electromagnetic field of surface plasmon-polaritons and thermo-hydrodynamics. Work on the calculation of radial corrugation on the domes, see fig. 1.

B) Action of the vortex beams

Calculation of the action of the vortex beam of light.

C) The formation of nanoparticles during ablation into a liquid

Work on the inclusion of the full equation of state of water in the hydrodynamic calculation of the ablation of gold into water. Molecular dynamics simulation of metal and water interpenetration due to diffusion. Condensation into gold clusters during expansion and cooling of gold vapor in a diffusion layer with water and inside pure gold vapor. The first calculations of metal ablation into liquid using the SPH code.

D) Laser fragmentation of liquid droplets and jets

Transfer of SPH code to tabular equation of state. Beginning of work on the problem of the interaction of a hard X-ray LCLS beam with a microdroplet or microjet of water.

E) Ablation of refractory metals

Complete a computational part of the work on the X-ray mirrors with ruthenium. Prepare and submit relevant articles.

F) Laser melting powders

The hydrodynamic calculations of the laser heating of the microparticles will be performed. The melting threshold of the first layer of microparticles will be determined. A picture of melting of two layers of the microparticles will be created. Molecular dynamics calculations will be initiated. An SPH code will be prepared for calculating the heating of microparticle powders.

G) Computational physics, large-scale high-performance numerical simulation

The necessary improvements will be embedded in the codes for performing calculations in 2019.

H) Characteristics of silicon irradiated by laser.

Most of the work planned for two years will be completed.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals.
Calculations of the interaction between the electron and ion subsystems of the metal will be performed using a new approach.

4.10. *Planned for the first year of the content of the work of each main executor of the project*

1. Anisimov Sergei Ivanovich, head of the project. General project management. Monthly/quarterly internal reporting of each team member. Making decisions. Physical models of processes. Analysis of the results. Adjustment of work if necessary.

2. Inogamov Nail Alimovich.

Development of a model for task A (a hybrid of plasmonics and thermo-hydrodynamics). Contact with performers.

Calculations for problem B (vortex structures). Theory of the process. Selection of parameters for scaling task B in the framework of molecular dynamic modeling. Writing an article.

Task B (ablation into a liquid): analysis of the thermodynamic data of water, comparison with the thermodynamics of gold. The initial stages, thermal conductivity and diffusion, are far stages of the process when gold vapor expands by two orders of magnitude. Preparation of materials for publication.

Task D (fragmentation of droplets / jets). Together with team members, setting parameters for calculating the initial dynamics (absorption of hard X-ray photons, relaxation of the electronic subsystem, expansion of a cylindrical shock wave), transfer of data of the initial dynamics to the input of molecular dynamics and SPH code.

Task D (ablation of ruthenium). Physical model Analysis of the results of hydrodynamic and molecular dynamic calculations.

Task E (powders). Physical picture. A list of the main points, those that require calculations to understand what is happening.

3. Petrov Yury Vasilyevich.

The complete equation of state of liquid and vaporous water. The calculation of the shock adiabat, the calculation of the two-phase region, the calculation of the adiabat connecting the Hugoniot adiabat and passing into the two-phase region. The equation of state of ruthenium, the equation of state of molybdenum in two-temperature and single-temperature conditions. Calculation of the coefficient of thermal conductivity and the coefficient of electron-ion interaction for ruthenium and molybdenum in two-temperature and single-temperature conditions.

4. Khokhlov Victor Alexandrovich.

Hydrodynamic calculations for problems A, B, C, D, D, E. Adaptation of the complete equation of state of water in the liquid and vapor states to the hydrodynamic calculation scheme. Adaptation of the code scheme for solving problems of ruthenium and molybdenum.

5. Zhakhovsky Vasily Viktorovich.

An important team member. Creates physical models. Adapts codes to the real situation that you want to describe. Develops interatomic interaction potential for ruthenium. Perform work on molecular-dynamic and hydrodynamic SPH modeling of problems A, B, C, D, D., E. Develop new and modify existing codes in the framework of task J.

Team members up to 39 years old:

6. Migdal Kirill Petrovich.

He will use his experience in using quantum mechanical modeling packages to find the required thermodynamic and transport data for ruthenium and molybdenum in the calculations. Perform work on the properties of silicon by laser irradiation. Refine the calculations of the coefficient of electron-ion interaction. All these works are important for the success of the project.

7. Grigoriev Sergey Yurevich.

Very necessary for the project specialist. Perform work on the application of the SPH code (Smoothed Particle Hydrodynamics) and molecular dynamics for solving problems in paras. C, D, E. Perform work on the development of the algorithmic base of the team (p. J).

8. Dyachkov Sergey Alexandrovich.

Required for the project specialist. Perform work on the application of the SPH code (Smoothed Particle Hydrodynamics) and molecular dynamics for solving problems in paras. C, D, E. Perform work on the development of the algorithmic base of the team (p. J).

9. Egorova Maria Sergeevna.

Required for the project specialist. Perform work on the application of the SPH code (Smoothed Particle Hydrodynamics) and molecular dynamics for solving problems in paras. C, D, E. Perform work on the development of the algorithmic base of the team (p. J).

10. Murzov Semen Alexandrovich.

Required for the project specialist. Perform work on the application of the SPH code (Smoothed Particle Hydrodynamics) and molecular dynamics for solving problems in paras. C, G, E. Perform work on the development of the algorithmic base of the team (p. J).

4.11. *Specific scientific results expected at the end of the first year (the presentation should provide an opportunity to examine the results and assess the degree of implementation of the work plan stated in the draft)*

A) Spatially distributed heating due to a combination of plasmon and laser EM fields.

Calculations of plasmon fields initiated by an external incident laser wave will be performed. The total effective field in the skin layer of the metal will be found. The corresponding dissipation will be calculated.

We emphasize that the calculations of 2019 are qualitatively different from the simpler calculations described in the articles [4], see the list of references to section 1.4 of the project. In [4], the geometry was relatively simple, the waves were two-dimensional, i.e. were in the plane of the wave vectors of the laser waves, one propagating in the Kretchmann wedge, and the other falling on the film from a vacuum. In our case, the waves are three-dimensional, since they are excited on the tubercle-dome of the film and run in different directions from the dome.

A set of thermo-hydrodynamic calculations will be performed that describe the target response to dissipation into heat in the skin layer. This dissipation is not uniform over the film. Description of the response means that we will recreate the picture of melting, movement and freezing into final structures, which will be compared with the results of experiments of colleagues from Vladivostok and FIAN.

The movements of the domes shown in fig. 1 will be calculated. We will not use the axial symmetry approximation. An unknown and intriguing reason for the strong radial corrugation on the domes will be established.

B) Action of vortex beams.

Much work will be done to prepare for the calculations and performing calculations of the action of the vortex beam, see fig. 2. We will apply all the means at our disposal and describe the mechanism for the formation of chiral points. Note that today in the literature there are two opposing points of view. Japanese authors and some others argue that the cause of chirality is the angular momentum brought by the vortex photon beam, see the first two papers in the list of references to section 1.4 under the number [5]. At the same time, colleagues from FIAN and the university in Samara believe that it is caused by the heterogeneity of the illumination in the spot on the surface of the target. Thus, the situation is very interesting and complex.

C) The formation of nanoparticles during ablation into a liquid.

The work on the inclusion of the complete equation of state of water in the hydrodynamic calculation of the ablation of gold into water will be completed. Molecular dynamics (MD) modeling of the processes of metal and water interpenetration due to diffusion will be performed. Condensation into clusters of gold will be simulated when the gold vapor expands

and cools in the diffusion layer with water and inside pure gold vapor. Calculations of metal ablation into liquid using the SPH code will be performed. It is necessary to compare the MD and SPH results. Hydrodynamic modeling will be performed using a code in Lagrange variables. It will be understood when and how nanoparticles are formed.

D) Laser fragmentation of liquid droplets and jets.

The SPH code will be transferred from analytic to a tabular equation of state. Work will be started on the problem of the interaction of a hard X-ray beam LCLS with a microdroplet or microjet of water. It is necessary to create a reserve for further work and publish the first data obtained on the dynamics of a drop or jet after a strong concentrated X-ray exposure along a thin thread.

E) Ablation of refractory metals.

Calculations on x-ray mirrors using ruthenium will be completed. Articles on this work will be written and put into print.

F) Laser melting of powders.

The hydrodynamic calculations of the laser heating of the microparticles will be performed. The melting threshold of the first layer of microparticles will be determined. A melting pattern will be created for the two or three first layers of microparticles. Molecular dynamics calculations will be initiated. An SPH code will be prepared for the heating of mesoscopic ensembles of microparticles. The results will be prepared for publication.

G) Computational physics, large-scale high-performance numerical simulation.

The necessary improvements will be embedded in the codes for performing calculations in 2019.

H) Characteristics of silicon irradiated by laser.

Most of the work planned for two years will be completed.

I) New approaches to the calculation of the coefficient of electron-ion interaction in metals.

Calculations of the interaction between the electron and ion subsystems of the metal will be performed using a new approach.