

Quantum methods in the development of new materials

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The analysis of quantum methods for supercomputer simulations “ab initio”, quantum Monte-Carlo (QMC), Density Functional Theory (DFT) and semiempirical approaches like Tomas-Fermi at finite temperatures (TFFT) for gas, plasma and solid phases equilibrium thermodynamics and transport properties are presented. Thermodynamic potentials, entropy, specific enthalpy and their derivatives, specific heat capacity, velocity of sound, shock wave entropy behavior, diffusion, thermal and electrical conductivity, dielectric functions of the new materials for Atomic Energy Industry are analysed. The results are presented in the developed Data Base of Atomic Materials. Equation of state for aluminium melting, temperature dependence of Al thermal conductivity, the thermal pressure of the electrons for tungsten and Al dielectric function are obtained on the basis of experiment and simulation and compared with other works. Al shock adiabats, Al temperature – density and Al sound velocity are analysed by using QMD and MPTEOS simulations. Porous W pressure – mass velocity is investigated using experiments and simulations by QMD.

Key words: Material Data Base, DFT, QMC, Monte Carlo, Tomas-Fermi, EOS.

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1. Introduction

The progress in the real acceleration in the number of available materials is associated with an increase in the information component in their development. Exponential growth in computing power and data storage density, combined with advances in computer science (e-science), have produced an information revolution. Big Data management techniques have now found use in information retrieval technologies, Life Sciences, Economics, Social Media, etc. Recently, an innovative idea has been formulated to integrate materials development techniques with data management technologies, the so-called Materials Informatics (MI) or Materials Genome (MG). Its implementation will bring a change in the basic paradigm in Materials Science (MS), replacing the traditional method of trial and error with a highly productive scientifically-based approach. A number of countries have already launched programs with strong government support in this direction, such as “The Center for the Design of Materials for Functional Electronics” in the United States. In 2016, three Centers of Excellence for the study of

Big Data sets management in Materials Science begin their activities in Europe: MAX, NOMAD and ECAM. It is very important for Russia to take a leading role in this area. To this aim, we propose Interdisciplinary Project "Genome of nuclear energy materials" with the Rosatom (Russian Atomic Energy Commission) collaboration.

The task is set as follows. To create materials for the new types of reactors, to ensure the safety of existing nuclear power plants, there are problems with the creation of materials with properties that would meet the requirements of standards, long-term operation and reliability. After determining the required properties of the materials on the basis of existing interactive (constantly updated and corrected) databases can be analyzed candidates for new materials. Then the first-principle (ab-initio) calculations are made and the molecular structure of the new material is determined. After that, the technologies for obtaining these materials are determined and, as a rule, a new material is created on the basis of additive technologies. The resulting material must pass a full cycle of testing and certification. The proposed approach, which includes the use of interactive databases, primitive

quantum calculations, technology development and experimental research, is not trivial, but it is the only way that can lead to success in the field of nuclear engineering.

To achieve this goal, an interdisciplinary team of leading researchers with complementary expertise in material modelling, machine learning, database development, visualization, and experimental synthesis and analysis of the properties of new materials is being created. The developed approach will have sufficient potential to significantly reduce, by an order of magnitude or more, the cost, risks and time of discovery of new materials and bringing them to the commercial market.

2 Ab initio calculations and design of solid and liquid materials

2.1 Aims and goals of ab initio calculations

The strategic goal of the project is to provide the possibility of scientifically-based development of new materials based on the management of large data sets, proposed by the revolutionary progress of the theory of modeling, computing power, Informatics, statistics and visualization. We will produce, store and classify large amounts of material data based on our own computer simulations and experiments, as well as from a wide range of literature sources and databases available to us. Research of Big Data sets using effective machine learning (ML) algorithms will allow to discover new materials and phenomena with promising technological applications, to recognize new relations “parameter to properties” and “parameter to parameter”. It will allow to receive qualitatively new ideas, inaccessible for usual methods of research. Indeed, the effectiveness of the transition from data to knowledge depends on the adequacy and correctness of abstraction methods. Examples of successful abstractions are the Periodic table of elements or so-called Ashby diagrams, which graphically select relationships between two or more properties of materials or their classes. Such diagrams are widely used by material scientists and engineers. However, the use of approaches developed for Big Data sets in materials science until recently was limited to excessive labor-intensive experimental data acquisition. With the use of computer modeling, the efficiency of obtaining data on the properties of materials increases significantly. At the same time, the problem of transition from data to knowledge using traditional empirical methods becomes difficult to

solve. Using the new revolutionary approaches developed in the framework of our project, we will be able to identify the scientific context of key concepts in materials science, and use it to model and predict the properties and behavior of materials under various conditions and in a variety of applications.

2.2 Review of previous research developed by authors and their research groups

Previous research developed by the group developed Nuclear Gas Core Reactor is presented in [1-3]. The next scientific results for materials were obtained.

* A new generation of materials modeling methods has been developed with qualitatively new possibilities of taking into account real external conditions, namely temperature effects of crystal lattice oscillations, magnetic excitations, as well as multielectronic effects [4-5].

* The applicability of the developed methods to describe the behavior of materials in extreme conditions is demonstrated. A detailed experimental and theoretical study of the behavior of one of the incompressible Os metals at a pressure greater than 770 GPa was carried out, revealing a new type of electronic transition caused by the intersection of internal levels (CLC) [6].

* The importance of multielectronic effects in the case of Fe properties research is shown [4]. It is shown that their consideration leads to a theoretical prediction of the presence of electronic topological transitions in iron under pressure. Experimental measurements of sound velocity as a function of pressure confirm the presence of a transition [8].

* A study of the dependence on the pressure of the magnetic hyperfine field in Nickel oxide NiO [9], which confirmed the antiferromagnetic state of NiO up to 280 GPa. This is the highest pressure where magnetism has been observed so far in any material.

* The influence of stresses and multicomponent alloying on the phase stability of Fe-Cr alloys, which are the base materials for nuclear reactors, is studied [10].

* Within the framework of fundamental interdisciplinary studies, the evidence for stabilization of the Fe-10 at structure of the BCC is presented. % Ni alloys at pressures above 225 GPa and temperatures above 3400 K, and it is theoretically demonstrated that the alloy can be stable in the Earth's core [11].

* In our recent work, the structural properties of graphite and diamond as a function of applied

pressure were calculated using the Density Functional Theory (DFT) and various methods to incorporate the Van der Waals interaction.

* Theoretical and experimental study of structural and magnetic properties of FeCO_3 siderite at high pressure and temperature has been performed [12]. The reason for the increase in the Neel temperature and the stability of the AFM state of FeCO_3 when the pressure increases relative to the DLM structure is analyzed. It is shown that when heated to the temperature of the Earth's core and pressures above 50 GPa, siderite FeCO_3 practically disintegrates into various oxides.

* Peculiarities of pressure influence on properties of carbides and nitrides were studied. Calculations of monocrystalline and polycrystalline elastic properties in the range from 0 to 1200 K, taking into account temperature contributions, were carried out for a technologically important paramagnetic CRN alloy by a new TDEP method with force constant symmetrization [13]. It was shown that there is a significant increase in the isotropy of the elastic properties of CrN with temperature. The influence of anharmonic effects on phase stability was analyzed and physical properties of AlN nitride characterized by unusually high thermal conductivity were determined [14].

* Members of the scientific group have extensive experience in the field of thermodynamic modeling by Calphad methods both for individual substances and in dual and multicomponent systems, as well as in the field of experimental determination of phase rotations and thermodynamic properties, which is reflected in the relevant publications [16-20].

* We reviewed opportunities to improve job modeling in the new pure element database [21].

* As a result of joint work with RWTH Aachen, a detailed experimental analysis of the key system for the development of Fe-Mn-Al-C high manganese compounds was carried out [23-24].

* A new thermodynamic database for Precimn high manganese steels describing the Fe-Mn-Al - Cr-Nb-Si-Ni-Ti-V-C-N system and its subsystems was constructed [26].

* On the basis of thermodynamic calculations the reasons are revealed and recommendations on optimization of compositions of steels for the purpose of elimination of formation of nonmetallic inclusions at welding of HDV of branch pipes are issued

* On the basis of thermodynamic calculations and experimental studies, the causes and mechanisms of formation of harmful inclusions of non-ferrous impurities of non-ferrous metals on the surface of steels made of secondary raw materials were found.

* Work is underway to create a new generation pure and pure element substances database (Calphad 3-0) within the SGTE consortium to replace the existing Pure Elements Database 1991[22, 25].

* The technique of quantitative analysis of integral Auger spectra is developed, which provides an assessment of the content of all elements that can be detected on the surface of brittle intergranular fracture. With the help of the developed technique, spectra from the database of Auger studies of hull reactor steels (CR) obtained at the SIC "Kurchatov Institute" were analyzed.

* The mutual influence of the elements that make up the GZ, correlations between their content (P-C, P-Ni, C-Cr), kinetics of accumulation of P in the GZ are established. Preliminary estimates show that the concentration of P in GZ initially increases, and then, after about 16 and 22 years, respectively, changes slightly. This result is also confirmed by thermodynamic Calphad calculations. For binary systems Me-P and Me-Me3P, where Me = Fe, Cr, Ni, concentrations of phosphide and phosphorus in GZ were calculated at 315 C. Concentrations of iron phosphides (0.012 in mole fractions), chromium (0.014) and Nickel (0.012), and phosphorus (0.041) were obtained. The latter value is well compared with the experimental value of 0.037 obtained after exposure of 195,000 hours (more than 22 years) at T=315 S.

2.3. *Example of ab-initio modeling and experimental investigation of the properties of ultra-high temperature solid solutions $Ta_xZr_{1-x}C$*

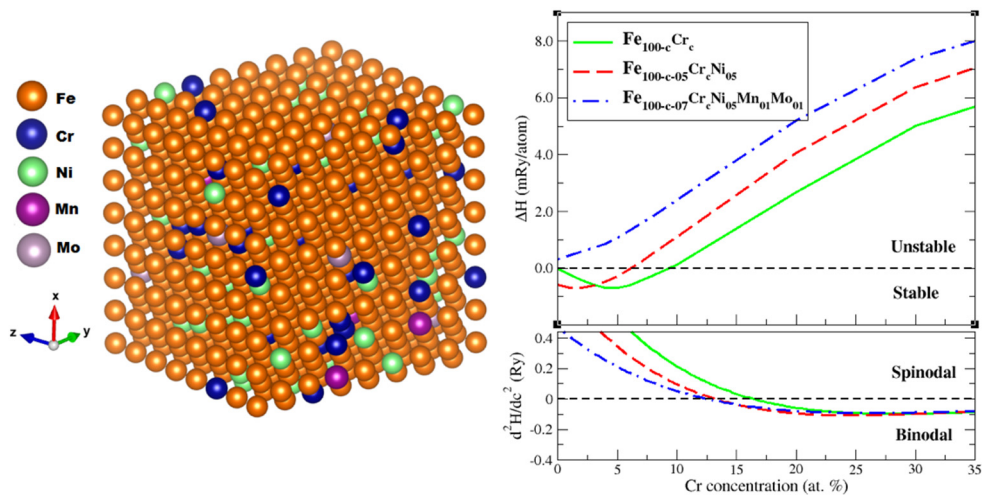


Figure 1 – Effect of multicomponent alloying with Ni, Mn and Mo on phase stability of bcc Fe-Cr alloys

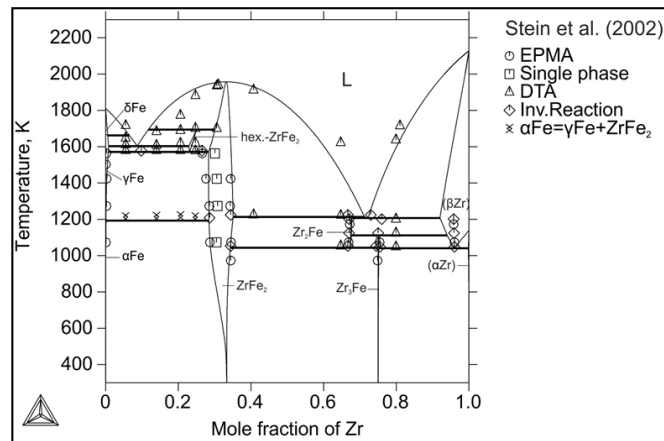


Figure 2 – Re-assessment of Zr-Fe phase diagram [49]

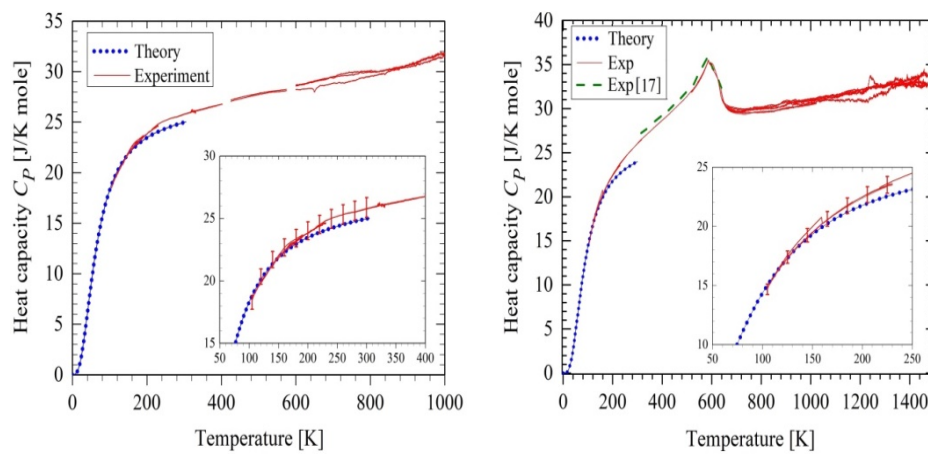


Figure 3 – Heat capacity Zr₃Fe a) and ZrFe₂ b) - theory and experiments (collaboration with Freiberg University of Mining and Technology, Germany)

3 Ab initio calculations and design of liquid and plasma materials including extreme states

3.1. Quantum Molecular Dynamics metals in extreme states

Quantum Molecular Dynamics (VASP)

- Adiabatic Approximation
- Electrons are quantum particles, defined by electron density in DFT at fixed ion positions
- Ions are classical particles in the fields of other ions and electrons described by Newton's laws.
- Number of particles – up to 1000, time simulation 1 ns,
- NVT - Ensemble

The quantum molecular dynamics method allows direct calculation of some thermodynamic functions, including pressure, energy, and heat capacity; additional calculations are necessary to calculate entropy. In addition, the quantum molecular dynamics method approximates the energy spectrum of the system, which makes it possible to apply the Kubo-Greenwood formula to calculate the dynamic Onsager coefficients and calculate the transport and optical electronic properties, including the static coefficients of electrical conductivity and thermal conductivity. Some results of VASP simulations are presented in Figures 4-8.

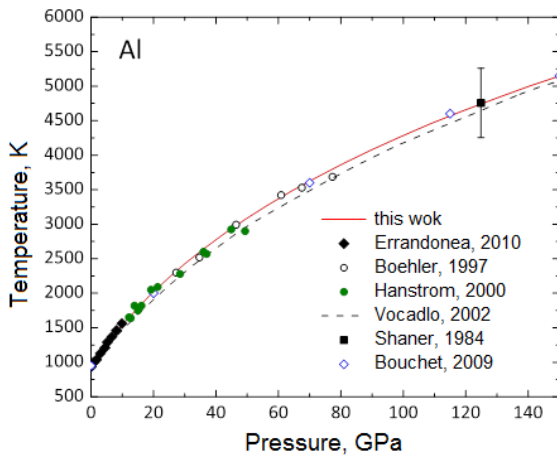


Figure 4 – Aluminum melting experiments and simulations

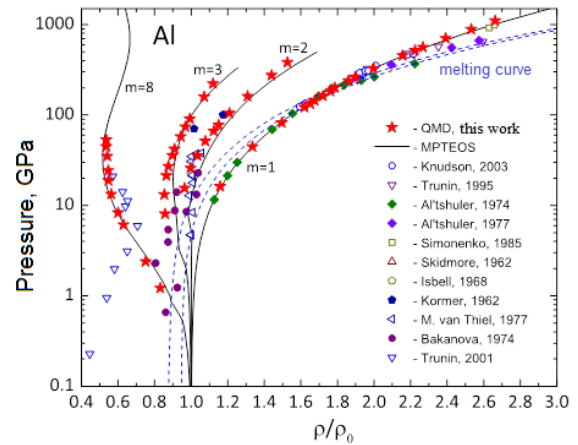


Figure 5 – Al shock adiabats simulations by QMD and MPTEOS

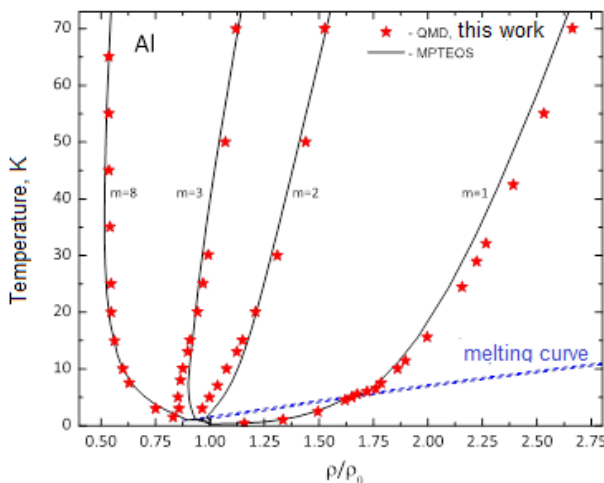


Figure 6 – Al temperature – density simulations by QMD and MPTEOS

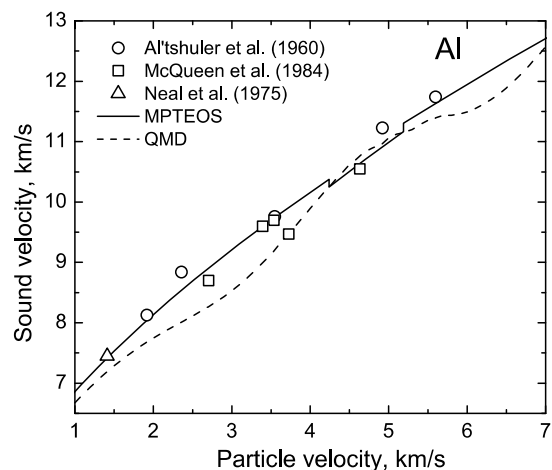


Figure 7 – Al sound velocity, experiments and simulations by QMD and MPTEOS

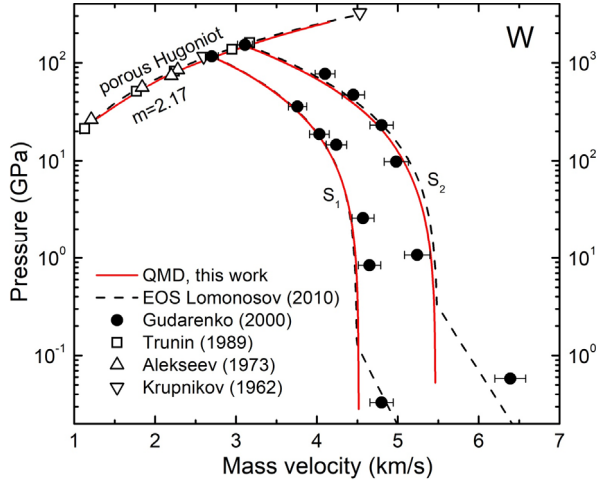


Figure 8 – Porous W pressure – mass velocity, experiments and simulations by QMD

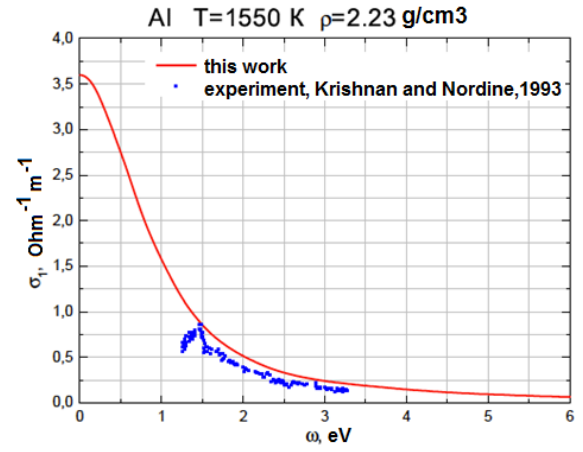


Figure 9 – Al dielectric function simulation and experiment

3.2. Thermodynamic functions in Thomas-Fermi model at finite temperatures

Thomas-Fermi model has been developed for matter thermodynamic properties by Feynman, Metropolis and Teller [50]. In our Data Base approach for high temperature material properties the Thomas-Fermi model in the next formulation. Let $V(r)$ - atomic potential for particle in cell. The Poisson equation has the form of [50]:

$$\Delta V = -4\pi Z\delta(r) + \frac{2}{\pi}(2\theta)^{3/2} I_{1/2} \left(\frac{V(r) + \mu}{\theta} \right)$$

$$F(V, T) = \frac{2\sqrt{2}v_a T^{5/2}}{\pi^2} \left[I_{3/2} \left(\frac{\mu}{T} \right) - 8 \int_0^1 u^5 I_{3/2}(\phi) du + 3 \int_0^1 u^5 \phi I_{1/2}(\phi) du \right]$$

Thermodynamic functions could be presented by second derivatives of free energy. For derivatives of pressure and entropy are:

$$P'_V = -F''_{VV} = \frac{(2\theta)^{3/2}}{2\pi^2} I_{1/2} \left(\frac{\mu}{T} \right) (\mu'_V)_{N,T}$$

$$P'_T = -F''_{VT} = \frac{(2\theta)^{3/2}}{2\pi^2} \left[I_{1/2} \left(\frac{\mu}{T} \right) (\mu'_T)_{N,V} + \frac{5}{3} I_{3/2} \left(\frac{\mu}{T} \right) - \frac{\mu}{T} I_{1/2} \left(\frac{\mu}{T} \right) \right]$$

$$S'_T = -F''_{TT} = \frac{3\sqrt{2}v_a}{\pi^2 T^{3/2}} \int_0^1 \left[5T^2 u^5 I_{3/2}(\phi) + 3u^3 (\phi'_T T^2 - 2\phi T) I_{1/2}(\phi) - u\phi (\phi'_T T - \phi) I_{-1/2}(\phi) \right] du$$

The boundary condition for potential are used for the cell center and at the boundary:

$$rV(r)|_{r=0} = Z \quad V(r_0) = 0 \quad \frac{dV(r)}{dr} \Big|_{r=r_0} = 0$$

At finite temperature electron densities could be expressed by integrals

$$I_k(x) = \int_0^\infty \frac{y^k dy}{1 + \exp(y-x)}$$

Free energy in the canonical ensemble has the form

Internal energy could be found from the 1st law of thermodynamics:

$$E_T = E(V, T) - E(V, 0) = \int_0^T T_1 S'_T(V, T_1) dT_1$$

Results of simulations are resented in figure 10 for thermal pressure of electrons and temperature dependence of thermal conductivity for aluminum.

4. Data Bases for Atomic Energy materials

All data from ab-initio and semiempirical simulations are used in the Data Base of Atomic Materials on the basis of approach described in [4-48].

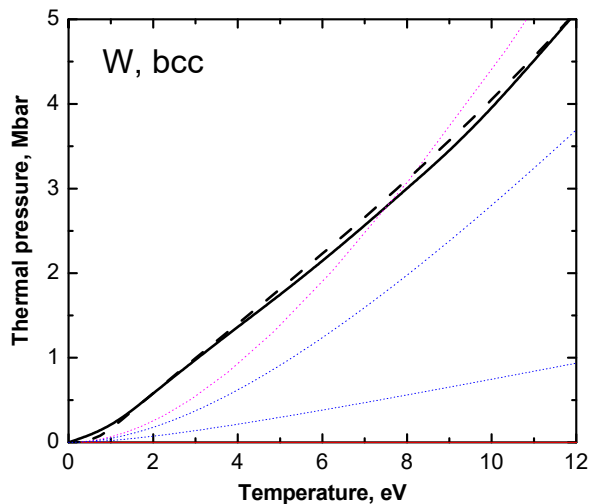


Figure 10 – The thermal pressure of the electrons for Tungsten, ion temperature $T_i = 0$, $V = V_0$.

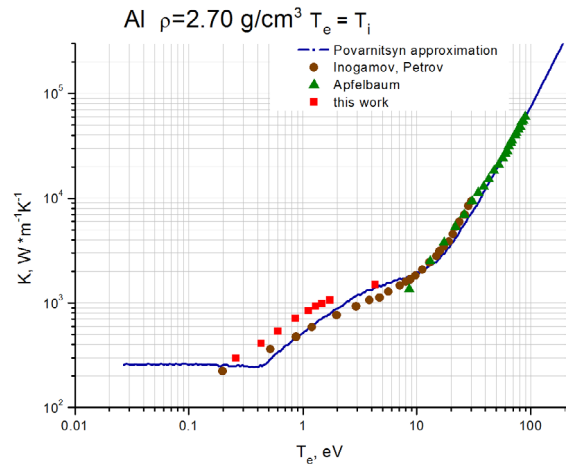


Figure 11 – Temperature dependence of thermal conductivity Al.

5. Conclusions

Modern quantum ab-initio approaches and powerful supercomputers have made it possible to directly calculate the thermophysical properties of substances. In many cases, even today, the calculations can replace the experiment. Calculations are possible for substances of complex composition and structure, this requires significant computing power. The results are presented in the developed Data Base for Atomic Energy Materials.

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