Model of fragile destruction of metal constructions at reduced temperatures

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Abstract. The paper presents the results of studies of metals with different types of crystalline structure in a wide range of low temperatures. Based on the data obtained, a model of brittle fracture of metals at low temperatures is proposed. The relationship between the lattice parameter of metals and the temperature of a viscous-brittle transition is established. A quantum-mechanical simulation of the effect of temperature on the lattice parameter has been carried out. It is shown that a decrease in the lattice parameter is observed with decreasing temperature.

1. Introduction
Low-carbon steel with a bcc lattice with high viscosity, are widely used in the manufacture of parts of critical units of vehicles and metal structures operating at low temperatures, in particular gas and pipelines [1-4]. Such steels contain carbon in α-iron up to 0.02%, phosphorus up to 0.003%, and a number of other impurities. Carbon impurity is considered useful, causing solid-solution hardening of α-iron. The use of low-carbon steels at low temperatures is due not only to their high cold resistance, but also to their economic efficiency. Metals operating at low temperatures should have a set of properties, such as the required level of ductility, strength, impact strength. This in turn requires tensile and impact bending tests.

2. Test materials and equipment used
Metals with different types of crystalline structures were selected for the study: steel 20, steel 45, austenitic steel 12Kh18N10T, and titanium alloy VT8 at low temperatures.

Tensile tests and impact bending were performed in the temperature range from + 20°C to -100°C. To cool the samples during the tensile test, a special cryocamera with a liquid nitrogen supply based on the Tinius Olsen H100KU breaking device was used. For carrying out tensile tests, samples were made with dimensions and requirements according to GOST 11150.

Impact bending tests were carried out on a pendulum scraper MK-300 with a potential energy reserve of 450 J using the developed cryochamber for cooling impact bend samples, where a mixture of alcohol and liquid nitrogen was used as a cooling medium. Preparation for testing, testing and processing of results produced according to GOST 9454.

To record the temperature during the preparation of samples for tests on impact bending, as well as during the tensile tests, an electronic thermometer was used - CENTER 300 type K (± 200...1370°C (± (0.3% + 1°C)).

Also according to the test results, the lattice parameter was determined - a. The determination of
the lattice parameter of the studied metals was carried out on the basis of X-ray diffraction analysis on a DRON-2 diffractometer using CoKa radiation.

3. Applicable software

Due to the complexity of studying the destruction of metals at low temperatures, requiring special climate chambers, other expensive equipment, as well as the well-known difficulties of studying the dislocation structure formed at low temperatures, quantum mechanical modeling of the main parameters at low temperatures is of particular relevance. Similar studies are also needed to study the mechanisms of destruction of low-carbon steels at low temperatures and to find effective ways to increase their brittle strength in harsh climatic conditions during long-term operation.

To perform quantum mechanical modeling, the electron density functional method was used, which was programmed in the CP2K and Quantum Espresso software.

Among modern high-performance systems, hybrid systems including graphic accelerators (GPU - graphic processing unit) are increasingly being used recently. Therefore, in the software packages used, GPUs were included to speed up the calculations and are used by us to simulate the equilibrium state of materials at different temperatures and pressures.

The program code CP2K and Quantum Espresso shows very good parallel efficiency and has a stable convergence. In particular, the code may work on many nodes that may or may not have a GPU. Shown with the use of a GPU can achieve significant acceleration: up to 15-20 times for some operations and up to 8-10 times for a full set of operations of a typical calculation within the framework of ab-initio molecular dynamics.

4. Experimental studies

During tests on impact bending, the dependences of impact strength (KCV) on temperature for the studied materials were obtained. These dependencies are shown in Figure 1.

![Figure 1](image)

**Figure 1.** Dependence of impact toughness (KCV) on temperature for the studied materials

According to the results of the study of fractures of the samples, the temperatures of the viscous-brittle transition were determined for the materials under study. Thus, 12Kh18N10T steel has a viscous-brittle transition temperature in the region of -112°C, D16 aluminum alloy does not have a viscous-brittle transition temperature, for a titanium VT8 alloy, the viscous-brittle transition temperature is about -88°C. Steel 20 and steel 45 have a viscous-brittle transition temperature, which is -43°C and -28°C, respectively.

According to the results of tensile tests, the values of the mechanical characteristics of the materials under study (conditional yield strength $\sigma_{0,2}$, relative elongation $\delta$, temporary resistance $\sigma_u$, and the dependence of the ratio $\sigma_u/\sigma_{0,2}$ on the test temperature) are determined.
The results of tensile tests are shown in Figure 2.

Figure 2. Values of mechanical characteristics of the studied materials

In the study of the cold resistance of these materials, the dependence of the viscous-brittle transition temperature on the lattice parameter was established (Fig. 3), which was determined on the basis of x-ray structural analysis.

Figure 3. Dependence of the temperature of the viscous-brittle transition on the lattice parameter

5. Analysis of the results of experimental studies

Analysis of data on the nature of changes in the mechanical characteristics of materials with decreasing temperature shows that with decreasing temperature, temporary resistance, the conditional yield strength of steels increases, and the relative elongation decreases. The highest relative elongation in a wide temperature range is shown by stainless steel, titanium alloy VT8 and low carbon steel 20. When tested for toughness, these materials provide a lower viscous-brittle transition temperature as compared to steel 45.

In the works [1-4] it is shown that in the process of long-term operation of steel structures (bridges) and pipes of main pipelines, they are subjected to deformation aging. Brittle fracture is the main factor limiting their use in metal structures at low temperatures upon reaching a certain operating time (25-30 years). In this regard, the problem of cold resistance of metals in conditions with low temperatures is
particularly relevant.

As it is known, the fundamental point of classical theories is the statement that cold brittleness is caused by a sharp increase in the flow stress with a decrease in temperature (Fig. 2).

Special studies [1] made it possible to establish that carbon leaves the saturated solid solution of the crystal lattice at the grain boundaries, forming carbon-iron compounds there, weakening their strength. The authors of [2, 3] adhere to a similar model of brittle fracture of low-carbon steels at low temperatures, where it was shown that at low temperatures during aging the coarse mesh mesostructure is formed in ferrite grains and at the grain ferrite boundaries. In [4], it was established that after long-term operation of main pipes, the lattice parameter of α-iron decreases from 2.8675 to 2.8664 nm, which indicates carbon outflow from the solid solution.

The change in the lattice parameter of iron at temperatures of 0K and 240K is investigated. By means of quantum mechanical modeling, an optimized orthonormal iron cell with carbon impurity at 0K and 240K is obtained. The distance after optimization between the selected Fe and C atoms is 1.925Å and 1.950Å. The distance after optimization between the separated neighboring Fe – Fe atoms is 2.843Å and 2.851 Å at 0K and 240K, respectively. The lattice parameter of pure iron without impurities is a=2.866 Å. Consequently, as the temperature decreases, the lattice parameter decreases, as studies using quantum mechanical modeling have shown.

From figure 3 it is clear that there is a dependency, the higher the lattice parameter of the metal, the higher its temperature of the viscous-brittle transition.

In [5], it was found that metals with a bcc lattice, prone to cold brittleness, have, as a rule, a lower lattice parameter than plastic ones. This explains their lower resistance to brittle fracture of refractory metals with a BCC lattice.

In the considered papers [1, 4], the driving force that affects the carbon withdrawal from the ferrite lattice is the saturation of the solid solution in α-iron. The question arises as to what caused the decrease in the distance between the atoms of iron and carbon, the withdrawal of carbon from the crystal lattice of α-iron, and the parameter of the crystal lattice of iron at low temperatures. Consider this phenomenon based on the quantum approach of the strength of solids.

The temperature of a solid is created by the motion of atoms [6]. It would seem that at low temperatures and even more so at absolute zero, i.e. at -273.15°C all atoms must be at rest. However, due to quantum effects, this is impossible, in particular, due to zero-point oscillations, which even a vacuum has, as well as a tunnel effect that provides carbon atoms as a result of fluctuations to overcome energy barriers at low temperatures.

Thus, the possibility of carbon withdrawal at low temperatures by its diffusion from the crystal lattice to the grain boundaries should be associated with a quantum thermo-lactation phenomenon. It also leads to a decrease in the lattice parameter and a decrease in brittle strength due to a decrease in the mobility of dislocations, its edge components.

The hardening of grain boundaries at low temperatures, in our opinion, is mainly due to the blocking of dislocations by impurities. The formation of new dislocations does not occur. Hardening of grain boundaries due to the grid of iron carbides, which are formed when carbon moves to grain boundaries due to energy fluctuations and a tunnel effect at low temperatures, is also unlikely. Apparently, if they are formed, then they should have nanostructured dimensions, i.e. less than 100 nm. This circumstance explains the fact of hardening of the grain boundaries of iron due to the diffusion of carbon on them from the solid solution of the lattice. The formation of a grid of iron carbides (mesostructure) at the boundaries of α-ferrite grains, which sharply reduce the tensile strength of carbon steels, is probably possible only with a high carbon content in steels and at certain temperatures in accordance with the iron-carbon diagram.

6. Conclusions
1. With a decrease in temperature for a wide range of materials, an increase in the temporary resistance, the conditional yield strength and the decrease in toughness, and also the relative
elongation are observed. Particularly intense change in the characteristics considered is observed for metals with a bcc lattice (steel 20 and steel 45).

2. Quantum-mechanical calculations allowed to clarify the mechanism of brittle fracture of steel structures. It is established that as the temperature decreases, the lattice parameter decreases. It is shown that when recognizing a viscous component in fractures of steel 45 using an INS, the recognition error does not exceed 8%.

3. The lattice parameter is a good indicator of the tendency of metals to brittle fracture. Studies have shown using X-ray analysis and tests for impact bending, the higher the lattice parameter of the metal, the lower the temperature of the viscous-brittle transition.

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