Brief information about the project

Title	AP25793533 «Synthesis of nanostructured silicon and tungsten
	carbides: study of structure and new approaches to production
	methods»
Relevance	The project is highly relevant for Kazakhstan as it focuses on the development of advanced technologies for the synthesis of nanostructured silicon and tungsten carbides. This will help reduce dependence on imported high-tech materials, strengthen the country's scientific and technological potential in the fields of nanotechnology and materials science, train qualified specialists, develop scientific infrastructure, and provide environmentally safe and economically efficient solutions for industry, energy, and the defense sector.
Goal	Development and optimization of methods for the synthesis of nanostructured silicon and tungsten carbides using plasma-enhanced chemical vapor deposition and electron beam irradiation, as well as computer modeling to establish relationships between synthesis parameters, structural properties, and characteristics of the obtained materials.
Tasks	Task 1. Experimentally identify the effect of plasma-enhanced chemical vapor deposition process parameters (synthesis temperature, operating pressure, plasma power, etc.) on the formation of SiC and WC nanostructures. This will ensure the creation of controlled conditions for obtaining high-quality nanomaterials.
	Task 2. Conduct a comprehensive study of the structure and morphology of SiC and WC nanostructures in order to establish correlation dependencies between the characteristics of the obtained materials and the synthesis parameters. This will establish a relationship between the process parameters and the properties of the final product, which is critical for quality control of materials.
	Task 3. Establish the effect of crystal-chemical parameters of metal nanoclusters on the structure formation and growth of SiC and WC nanostructures. Provide a theoretical interpretation of the mechanism of nucleation and growth of SiC and WC nanostructures obtained by plasma-enhanced chemical vapor deposition. Conduct computer simulation using molecular dynamics and density functional theory to establish a correlation between SiC and WC nanostructures and synthesis parameters. This will establish a connection between the process parameters and the properties of the final product, which is critical for material quality control.
	Task 4. Experimentally study the dependence of the characteristics of SiC and WC nanostructures obtained by electron beam synthesis on varying such process parameters as electron energy, electron current density, irradiation duration, and others. This is necessary to optimize the electron beam synthesis process and obtain nanostructures with the required properties.
	Task 5. Determine the structure and morphology of SiC and WC nanostructures and establish the effect of electron beam synthesis parameters on the structure formation and growth of SiC and WC nanostructures. This will establish correlations between the process parameters and the quality characteristics

of nanomaterials, ensuring their precise control. Task 6. Provide a theoretical interpretation of the mechanism of nucleation and growth of SiC and WC nanostructures obtained by electron beam irradiation. Conduct computer modeling using molecular dynamics and density functional theory methods to establish a correlation between SiC and WC nanostructures and synthesis parameters. Modeling will provide a deep understanding of the synthesis mechanisms, which will allow theoretical justification and improvement of experimental approaches. **Expected and Achieved Results** Expected result 1: the effect of plasma-enhanced chemical vapor deposition process parameters (synthesis temperature, operating pressure, plasma power, etc.) on the formation of SiC and WC nanostructures will be experimentally determined. Expected result 2: a comprehensive study of the structure and morphology of SiC and WC nanostructures will be conducted and the dependencies between the characteristics of the obtained materials and the synthesis parameters will be established. Expected result 3: the effect of crystal-chemical parameters of metal nanoclusters on the structure formation and growth of SiC and WC nanostructures will be established and a theoretical interpretation of the mechanism of nucleation and growth of SiC and WC nanostructures will be given. Computer modeling will be carried out using molecular dynamics and density functional theory methods; correlations between SiC and WC nanostructures and synthesis parameters will be established. Expected result 4: the dependence of the characteristics of SiC and WC nanostructures obtained by electron beam synthesis on the variation of such process parameters as electron energy, electron current density, irradiation duration, etc. will be experimentally determined. Expected result 5: the structure and morphology of SiC and WC nanostructures will be determined and the effect of electron

beam synthesis parameters on the structure formation and growth of SiC and WC nanostructures will be established.

Expected result 6: a theoretical interpretation of the mechanism of nucleation and growth of SiC and WC nanostructures obtained by electron beam irradiation will be given. Computer modeling will be carried out using molecular dynamics and density functional theory methods and correlations will be established between the SiC and WC nanostructure and synthesis parameters.

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