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Machine Learning Directed Search for W/SiC Plasma Facing Components

General Atomics is pursuing novel functionally graded tungsten/silicon carbide (W/SiC) composites as the material for an integrated blanket design that utilizes W at the plasma-facing side and SiC as the structure. The combination of W and SiC are naturally synergistic due to their similar coefficient of thermal expansion and high temperature operating window. Functional grading of the two materials leads to smoothly varying compositional gradients that may lead to the formation of novel phases. Here, we develop a machine learning algorithm to search for previously unidentified W-Si-C phases. An initial population of W-Si-C phases are created for a given composition with cell lengths, angles, and atomic positions randomly selected within a given range. A genetic algorithm is implemented that combines two parent structures utilizing various operators to create progenitor populations through successive generations. Each phase is minimized allowing for the free variation of atomic positions, cell lengths and angles. A population of the best W-Si-C phases is iteratively maintained such that successive generations are created from structures with progressively lower heats of formation. Winners of the algorithm are subsequently relaxed with density functional theory to confirm the stability of the phases produced by the ML algorithm. The present study has identified multiple previously unknown stable W-Si-C phases. These phases were then subject to density functional perturbation theory calculations to determine the elastic tensor to assess mechanical and thermal properties. The results show that these phases possess excellent mechanical and thermal properties, indicating the potential for new alloys capable of satisfying the strict requirements of a first wall. Efforts are on-going to synthesize these phases with a pulsed DC sputtering technique developed in-house. The results suggest that power exhaust/extraction from the fusion core may benefit from the use of functionally graded W/SiC materials, leveraging safety advantages and high-temperature compatibility for optimal thermal efficiency and flexibility.

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Primary author: BERGSTROM, Zachary (General Atomics)

Co-author: ABRAMS, Tyler (General Atomics)

Presenter: BERGSTROM, Zachary (General Atomics)