Abstract

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First principles modeling of three-phase interface system of ZrB2-ZrC-ZrSi2

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Abstract

Advanced zirconium compounds show superior properties such as high refractory characteristics, abrasion resistance, corrosion resistance, fracture toughness and hardness. These products are useful candidates specifically for high temperature applications. The production is a challenge because of high temperature and/or pressure requirements to give enough densification for applications while most of them depend on different compositions. For example, ZrB2 known for its high refractory properties like good thermal shock resistance, chemical stability to liquid metals, high oxidation resistance and high melting point but requires sintering aid to lower porosity. ZrC has high abrasion resistance and similar thermal properties like ZrB2, but its low resistance to oxidation prevents some features. SiC is the most used C source during composite synthesis of ZrC structures and Si will form Zr-Si structures (ZrSi2 in equilibrium). ZrSi and ZrSi2 show low electrical resistivity and high thermal conductivity compared to ZrB2 and ZrC. It performs well to inhibit oxidation of underlying structures. Therefore, it is rational to use boride, carbide and silicide structures of zirconium together for high performance applications. On the other hand, both production and characterization methods for these type of materials need extreme conditions which is a bottleneck for experimental studies. To explore stable structures as candidates, we modeled crystalline layers of ZrB2, ZrC and ZrSi2 to explore interfacial properties of binary, ternary-layered nanocomposites and ternary periodic composites with density functional theory. We studied the energy, bonding lengths and electron densities to describe stable interfaces and compared ternary models with mono (ZrB2, ZrC and ZrSi2) and binary (ZrB2-ZrC, ZrB2- ZrSi2, ZrSi2-ZrC) model results. Then we simulated unstable periodic conditions like high pressure, high and low temperature and corrosive atmosphere to get insight about model behaviors and performance metrics.

Biography

Serzat Safaltin received his BSc degree in metallurgy and materials science engineering from Istanbul Technical University (ITU), Istanbul, Turkey, in 2015. He received his MSc degree in extractive metallurgical technologies engineering from ITU, in 2017. He is currently a PhD student and a research assistant in the metallurgical and materials engineering department at ITU. His research interests include modeling & simulation, 2D materials and metallic alloy nanoparticle production, cleanroom fabrication, and characterization methods