First principles modeling of three-phase interface system of ZrB_2-ZrC-$ZrSi_2$

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I. 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 depends on different compositions. For example, ZrB_2 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 ZrB_2, 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 ($ZrSi_2$ in equilibrium). ZrSi and $ZrSi_2$ show low electrical resistivity and high thermal conductivity compared to ZrB_2 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 ZrB_2, ZrC and $ZrSi_2$ 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 (ZrB_2, ZrC and $ZrSi_2$) and binary (ZrB_2-ZrC, ZrB_2-$ZrSi_2$, $ZrSi_2$-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.

II. Images

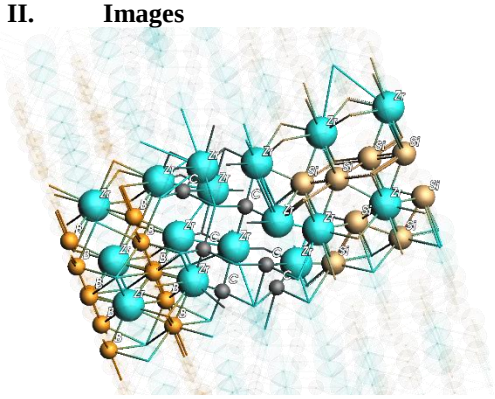


Fig.1 Ternary ZrB_2-ZrC-$ZrSi_2$ layer studied with density functional theory.

III. Referance:

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3. Xue, C., Zhou, H., Hu, J. et al. Fabrication and microstructure of ZrB2–ZrC–SiC coatings on C/C composites by reactive melt infiltration using ZrSi2 alloy. J Adv Ceram 7, 64–71 (2018). https://doi.org/10.1007/s40145-017-0257-x.

IV. Biography:

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