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Mechanical and electronic properties of al(111)/6h-sic interfaces: A dft study

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A density functional theory (DFT) calculation is carried out in this work to investigate the effect of vacancies on the behavior of Al(1 1 1)/6H SiC composites. DFT simulations with appropriate interface models can be an acceptable alternative approach to experimental. We developed two modes for Al/SiC superlattices, C-terminated and Si-terminated interface configurations. The results illustrate that C and Si vacancies are challenging to generate, while Al vacancies near the interface are easy to generate. C and Si vacancies reduce interfacial adhesion energy significantly, while Al vacancies close the interface have little effect on the adhesion energy. Young's modulus (E) is higher for C-terminated configurations than for Si-terminated configurations. Supercells are stretched vertically along the Z-direction to obtain tensile strength. The tensile properties show that failure usually occurs not at the interface but near the Al side. The existence of C and Si vacancies noticeably increases the tensile properties of the composite, particularly C and Si vacancies at the interface. According to the results, SiC and Al interfaces with C-terminated have better bonding properties. Furthermore, we systematically studied the surface energies (γ) and mode one fracture toughness (KIC). Finally, densities of states (DOS) were calculated to understand these systems' electronic properties better.

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Biography

Mostafa Fathalian, obtain a master's degree from Semnan University in 2017. He has a good background in manufacturing composites and nanocomposites. He collaborated with Prof. Ghorbanzadeh at Mazandaran University as a researcher. He published 5 papers in the journals of Fib &Pol, Vacuum, App Surf Sci, Phys E & Mater Chem & Phys. He also has a patent in the field of nanocomposite.

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