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New Si-B-C-N materials: Combining electrical conductivity with extremely high thermal stabilityJiri Houska¹, Simon Kos¹, Petr Zeman¹, Jiri Capek¹, Pavel Calta¹, Petr Steidl¹, Jaroslav Vlcek¹¹University of West Bohemia, Plzen, Czech Republic

jhouska@kfy.zcu.cz

Amorphous Si-B-C-N materials are becoming increasingly attractive due to their prospective high-temperature and harsh-environment applications. Depending on elemental composition, they feature one or more of extremely high thermal stability and oxidation resistance, electrical conductivity, optical transparency, high hardness or low stress. We report on ab-initio molecular dynamics (MD) calculations of structure, electronic structure and properties of Si-B-C-N materials in a wide range of compositions. In our liquid-quench simulations, the Kohn-Sham equations for the valence electrons are expanded in a basis of plane wave functions, while core electrons were represented using pseudopotentials. We investigate how the N content, the B content and the Si/C ratio affect characteristics of Si-B-C-N materials. On one hand, high Si/C ratio and high N content improve thermal stability and oxidation resistance. Thermal stability can be expressed in terms of formation of N₂ molecules and bond lifetimes. On the other hand, low Si/C ratio and low N content improve electrical conductivity. Electrical conductivity can be expressed in terms of electronic structure and localization of electronic states. We focus on detailed explanation of the role of individual atomic species, and consequently on identifying of Si-B-C-N compositions which exhibit non-zero electrical conductivity at maximum thermal stability. A special attention is paid to the comparison with experimental results obtained using reactive magnetron sputtering. Collectively, the results provide insight into the complex relationships between composition, electronic structure and properties of Si-B-C-N materials, and they consequently allow one to tailor the process parameters for producing electrically conductive Si-B-C-N materials for different technological applications such as high-temperature sensor devices.

KeywordsSi-B-C-N
electrical conductivity
thermal stability
oxidation resistance
molecular dynamics