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A microscopic study of the electrical conductivity of hard and thermally stable SiBCN materials

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We present the results of a DFT-based microscopic study of features that determine the electrical conductivity of the novel hard and thermally stable SiBCN materials. The control parameters used are the silicon-to-carbon atom ratio, and the fraction of nitrogen atoms in the total atom count. We have studied the influence of these parameters on the following features: (1) the width of the gap between the valence and the conduction bands, (2) the localization of the electronic states quantified by the spread of the Wannier functions, by the inverse participation ratio, and by the number of atoms and clusters on which a given weight of a particular state resides, (3) the role of individual atom and bond types in the electronic states around the Fermi level, (4) the average bond length of states around the Fermi level, and (5) the spatial homogeneity of the samples. We have also studied correlations among these features. We have found that (1) in samples with high nitrogen content, the electrical conductivity is mainly associated with carbon atoms and carbon-carbon bonds, and hence decreases with an increasing silicon-to-carbon ratio, and that (2) as the nitrogen content decreases, conductivity increases and boron starts acting as an efficient dopant and forming boron-rich zones. All the samples simulated had been prepared experimentally as coatings by reactive magnetron sputtering. Hence, we could compare the results of our numerical calculations with the measurements of the electrical and optical conductivity, and we have found the trends to be in agreement. The consistent theoretical and experimental results provide a detailed insight into the complex relationships between the material composition and the electronic properties, and allow one to tailor SiBCN compositions that can combine high thermal stability with electrical conductivity.

[1] J. Houska and S. Kos, J. Appl. Phys. 108, 083711 (2010)
[2] V. Petrman, J. Houska, S. Kos, P. Calta and J. Vlcek, Acta Materialia 59, 2341 (2011)

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