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Transport Characteristics of Amorphous Borocarbides: A Variable Range Hopping Treatment NASEER DARI, DONALD PRIOUR, JR, University of Missouri, Kansas City — We calculate the temperature dependent conductivity of amorphous borocarbide materials within a variable range hopping framework. We study the impact of disorder on borocarbide transport characteristics by beginning with a regular rombahedral lattice of periodically placed icosahedral arrangements of boron and carbon atomic species. A self consistent numerical procedure is used to calculate the charge occupancy factors. Three dimensional lattices containing several hundred icosahedral clusters are considered; disorder is introduced in the form of random translational displacements of the icosahedral cages. In addition, we use stochastic rotations about three independent randomly selected axes to implement orientational disorder for each of the icosahedral clusters. We find the sensitivity to random lateral displacements of the boron-carbon icosahedra to be on the order of 5%, whereas the effects of even appreciable orientational disorder appears to be negligible within the assumptions of our model. In sum, we find temperature and the density of icosahedral clusters to have the strongest effect on the conductivity, while the transport characteristics are largely robust with respect to the introduction of disorder.

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