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Letter to the Editor

Comment on "Spectral identification of thin film coated and solid form semiconductor neutron detectors" by McGregor and Shultis

S. Hallbeck[a,b], A.N. Caruso[a,c,*], S. Adenwalla[a,c], J. Brand[a,b], Dongjin Byun[d], H.X. Jiang[e], J.Y. Lin[e], Ya.B. Losovyj[a,f], C. Lundstedt[c], D.N. McIlroy[g], W.K. Pitts[h], B.W. Robertson[a,b], P.A. Dowben[a,c]

[a]*116 Brace Laboratory, Center for Materials Research and Analysis, University of Nebraska, P.O. Box 880111, Lincoln, NE 68588-0111, USA*
[b]*College of Engineering and Technology, N104 Walter Scott Engineering Center, 17th & Vine Streets, University of Nebraska-Lincoln, Lincoln, Nebraska 68588-0656, USA*
[c]*Behlen Laboratory of Physics, Department of Physics and Astronomy, University of Nebraska, P.O. Box 880111, Lincoln, NE 68588-0111, USA*
[d]*Department of Materials Science and Engineering, Korea University, Seoul, Korea*
[e]*Department of Physics, Kansas State University, Manhattan, Kansas 66606-2601, USA*
[f]*Center for Advanced Microstructures and Devices of Louisiana State University, 6980 Jefferson Highway, Baton Rouge, LA 70806, USA*
[g]*Department of Physics, Engineering and Physics Bldg., University of Idaho, Moscow, ID 83844-0903, Russia*
[h]*Pacific Northwest National Laboratory, Radiological and Chemical Sciences, P.O. Box 999 MSIN P8-01, Richland, WA 99352, USA*

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Abstract

We comment on some of the inferences and conclusions outlined by McGregor and Shultis [1].

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While we welcome the attention paid to boron-rich semiconductor devices, several clarifications are indicated to a recent paper [1] modeling neutron capture in boron-rich semiconductor solid-state detectors.

*Corresponding author. 262 Behlen Laboratory of Physics, University of Nebraska-Lincoln, Lincoln, NE 68588-0111, USA.
E-mail address: acaruso1@bigred.unl.edu (A.N. Caruso).

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First, some readers may infer that boron carbide and boron phosphide layers act only as neutron conversion layers to the active device and in fact are not active semiconductor layers. Although p–n junction formation can occur through the delta doping of silicon from the decomposition of borane cluster molecules [2,3], boron carbides and boron phosphides are nonetheless excellent semiconductors, even when deposited on silicon from suitable highly pure molecular source compounds [4–7]. The boron carbide [5–7] and boron phosphide [8,9] materials with good semiconductor properties can be doped n-type, while both n- and p-type 'self-doped' materials can be formed from an appropriate choice of the source compound isomer [10]. Behavior inconsistent with boron-doped silicon diodes can be observed, as $n–n^+$ heterojunction diodes have been fabricated with silicon [5–7]. Schottky barrier contacts are generally not a serious complication in boron carbide silicon heterojunction structures [11,12]. Indeed, all boron carbide n–p junction diodes have been fabricated both in a homojunction geometry [6] and in heteropolytype geometries [5,10]. We have successfully detected neutrons with "all boron–carbide" diode devices [10], to which models that assume a neutron "conversion layer geometry" (i.e. that the boron-rich layers are not part of the active semiconductor device but serve only to capture neutrons) are inapplicable. Heterojunction geometry devices do detect alpha particles from the boron carbide side of the junctions, indicating that the boron carbide, in such devices, are an active semiconductor part of the diode.

Second, boron-rich compound semiconductors are generally thought to be refractory [4,13], highly resistive ($\rho = 10^9$–$10^{12}\,\Omega\,\mathrm{cm}$, undoped [4]), with an indirect gap of about 0.7 eV [4,14] and diode characteristics that have been observed to elevated temperatures well above 200 °C [6,15], with depletion widths of the order of 0.5 μm or more [16]. The reason for exploiting main group molecular chemical vapor deposition, for making the boron carbide thin film materials, has more to do with the need to keep "doping" impurities out of the semiconductor material and make a highly resistive semiconductor over a large area (with few intrinsic carriers), than with an absence of high temperature materials stability, as has been suggested [1]. The electronic structure of the semiconductor material based on the packing of icosahedra is quite complex [17–20] and far from completely mapped in detail, with the added complication that are clear indications of several polytypes for the C_2B_{10} material, based on electronic structure studies [4,7,10]. Nonetheless, most researchers agree that the building block of these materials is the icosahedron [4,13,17–22], not tetrahedral coordinated B_4C as suggested in Ref. [1]. Application of another boron-based semiconductor electronic structure (say that of B_4C) is quite likely inappropriate for describing the icosahedral based semiconductors. The stability of the icosahedral cage and the tendency for the closo-1,2-dicarbadodecaborane to adsorb with the carbon atoms bonding toward the interface [23] may explain why double diode junctions are not routinely formed and observed in boron carbide/silicon heterostructures [4,11,12], except when a double heterostructure is explicitly formed [5,6].

Finally, as correctly noted by McGregor and Shultis [1], simulations of the actual boron-based neutron detector device characteristics (as reported in Ref. [24–30]) need to account for a number of complexities. These include the correct isotopic abundance of ^{10}B in the material, backscattering and forward scattering through interfaces and attenuation through the contacts (the latter a result of the perpendicular to plane detection geometry). The results obtained by the TRIM simulation in Ref. [1] are for devices enriched in ^{10}B, unlike the devices used in our heterojunction diodes reported in Refs. [24,25]. This will have a small but noticeable effect on the properties; specifically, the flux of neutrons reaching the farthest layer of the boron carbide will be reduced in the ^{10}B enriched devices.

We have carried out simulations, similar to those in Ref. [1], using a well-developed simulations package from CERN called GEANT 4.5.2 (GEometry ANd Tracking) [31], that allows us to perform a complete Monte Carlo simulation following an incident thermal neutron through the entire detector, all the way through to the

process of charge collection. The caveats are similar to those mentioned by McGregor and Shultis [1]: we assume complete charge collection and uniformity. While a surface barrier boron coated (conversion layer) detector and a thin semiconducting boron carbide layer heterojunction detector should be almost identical in response [25], our pulse height spectra simulation results are different from Ref. [1]. For boron carbide films on silicon that are thin, compared to the reaction product path lengths, our simulations of conversion layer and true solid-state devices show no noticeable differences in the positions of corresponding features, as is generally [24–29], but not always observed [30] in the experiment. A physical explanation for absence of capture product sum peak intensities for such thin boron carbide layers is that the available range of angles for total signal collection from both reaction products, compared to the total solid angle, is only significant once the boron carbide layer is at least about 1 μm thick.

A more significant difference from Ref. [1] is that the peaks corresponding to single capture products in our simulations have tails at *lower* energies for conversion layer devices, but at *higher* energies for true (non-Schottky) homojunction and heterojunction diodes, even for film thickness below 1 μm. This is a direct consequence of the fact that, in a heterojunction diode formed by semiconducting boron carbide and Si, electrical signals can be collected from along the reaction product paths within both boron carbide and silicon, whereas in a conversion layer, Schottky semiconductor device signals can only be collected from along the reaction product paths in the semiconductor, not the conversion layer. The simulations in Ref. [1] do not show this effect. It may be that such simulations must be applied with great care to the "all boron carbide" devices that are now being fabricated [6,10], for which neutron detection has been demonstrated [10].

We are grateful to McGregor and Shultis for calling attention to our efforts as well as for articulating, very clearly, part of the roadmap for future research in this area of boron-rich semiconductor detectors.

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