Referee's Report on "Boron-doping of cubic SiC for intermediate band solar cells: A scanning transmission electron microscopy study" by P.A. Carvalho, A. Thøgersen, Q. Ma, D.N. Write, S. Diplas, A. Galeckas, A. Azarov, V. Jokubavicius, M. Syväyärvi, B.G. Svensson, and O.M. Løvvik, submitted to SciPost Physics

This manuscript presents a scanning transmission electron microscopy study of the annealing behavior of epitaxial 3C SiC heavily implanted with Boron (1 – 3 at..%). The concentration profile of the Boron was measured by SIMS. The principle finding is that implantation and annealing does not lead to isolated substitutional Boron at the high concentration levels required for application as an absorber in single-junction solar cells based on an intermediate band.

Since I have no previous experience with SciPost Physics, and in fact was not aware of its existence, I had a look at several recent issues as part of the process of deciding whether to accept the invitation to review this manuscript. It appears to me that most of the papers in this journal are on fashionable and/or esoteric subjects, and many are theoretical in nature. I did not notice any papers that would be regarded as materials science or characterization, so I'm surprised both that the authors chose to submit to this journal and that the editors are seriously considering it for publication. It does not appear to fit, and it's not clear whether others working in silicon carbide and/or solar cells will find it. However, I assume that the editors are willing to publish this manuscript, so I proceed to discuss it.

The work is sound and worthy of publication after the authors take into account the following comments and suggestions, listed in order of appearance.

Page 2: Experimental

The authors omit some information, which should be provided. They do not state the thickness, doping type and concentration of either the epilayer or substrate (Perhaps these are provided in [11]). They do not state the penetration depth of the Boron ions, although the TEM images and SIMS profiles suggest that all of the effects are within about a micron of the surface, so that an epilayer thickness of a few microns would be sufficient. How close is the ion fluence to that required to render the implanted layer amorphous? Because the implantations were performed at 773K, amorphization is not an issue. Figure 1 shows evidence for good periodicity before annealing.

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It may be helpful to provide details about the sample preparation for the electron microsopy.

Results and Discussion

Line 1: "STEM images obtained" → "Cross sectional STEM images obtained"

Line 5: "rather than from the introduction of the weakly-scattering B atoms" Presumably Carbon atoms are also displaced, but the same comment applies to C as to B.

Line 8: "B preferentially substitutes for Si" However, note that boron-nitrogen donor-acceptor pair spectra in 3C SiC indicate that there is a boron acceptor with an ionization energy of about 0.735 eV (A value of about 749 meV might be more reasonable). Since the DAP spectrum is "Type I" and nitrogen donors substitute for carbon, this boron also presumably substitutes for carbon. The story of boron in SiC is quite complicated. Relevant references for my comment are:

1) H. Kuwabara, S. Yamada and S. Tsunekawa, J. Lumin. 12-13, 531 (1976) and 2) J.W. Sun, I.G. Ivanov, S. Juillaguet and J. Camassel, Phys. Rev. B83, 195201 (2011).

Lines 8-10: "At high collection angles (98 – 200 mrad), no contrast between the implanted layers and the underlying material was discerned …" The lower part of Fig. 1(b) is a bit brighter, although there is no distinct boundary between bright and dark regions.

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Figure 1: Part (d) is fuzzy. The axes and tick marks (or grid lines) are barely discernable and must be made more bold.

Text: Line 1: "Magnified images of the region in Figure 1…" Would it be helpful to specify the position/depth? Does it matter, or is the implanted region uniform with respect to this measurement?

Line 14: What is meant by "apparent strain localization perpendicular to (111)"? Are you saying that there are localized regions of high strain which are needle-like with the axis perpendicular to a (111) face?

Page 6

Line 1: "a large density of stacking faults was observed on (111) planes parallel to the surface" For a reader who is not an expert in electron microscopy, it would be helpful to point out examples of such features on an image and/or describe their appearance.

Line 4: "(see Figure 2)" → "(see Figure 2 (a))"?

Figure 3 (c) is fuzzy, and the axes/grid lines are too light.

Note that there is lots of empty space surrounding most of the figures. The larger the figures, the more effective they will be. Efforts should be made, where possible, to enlarge the figures/images to use all of the available space.

Below Fig. 3, Line 8: A different B concentration was used for the sample annealed at 1873 K compared to the one annealed at 1773 K. Why? More generally, the reason for choosing three (at least) distinct boron concentrations should be stated.

Page 8, Figure 5: The images are very small, while there is much empty space available. Can something be done? Note that three distinct values of B concentration are represented in the images. Why? The caption might explain the purpose of the white arrows in the final image in part (a).

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Figure 9: In this case, some of the panels are so small that they are unreadable, although there is plenty of available space to make them bigger. Please use all of the available space to enlarge the images and panels, especially c, d, e, f.

Below Fig.6, Lines 4-5: Various types of brackets are used, associated with directions, lattice planes, etc. Are they all correct?

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Figure 9 Caption, Line 5: Should "(b) and (f)" be "(b) and (e)"?

Line 10: The “greater than or equal to” sign is rather subtle. I believe that it is associated with the largest boron concentration observed in the SIMS profile after annealing, highlighted by an arrow (which I failed to notice on first reading but do now). I suggest being a bit more explicit in the text.

Page 12: Figure 10

For part (a), make the axes/ticks/grid lines bolder.

In the caption for part (b), specify whether the cross-section image was obtained after annealing at 1873K.

References: Please check all of the references carefully, as there are quite a few minor errors.

[3]: “(IPV). Effect” → “(IPV) effect” would make more sense.

[5]: “*in SiC in Properties”* → “*in SiC* in *Properties*” (The second “in” should not be italicized.

[6]: I believe that the correct volume number is 93, not 3.

[9]: I believe that the correct journal is Phys. Rev. Lett., not Appl. Phys. Lett.

[17]: Should the ‘4” in “B4C” be a subscript?

[18]: Should the “x” in “BxC” be a subscript?

[18] and [20]: Unlike the other references, the year of publication is given before the page/article number. Please use a consistent set of conventions.

[29]: The “R” in “Radiation” should not be upper case, for consistency.

[31] and [33]: “App.” → “Appl.” is conventional.