**Comment on "Identification of Lattice Vacancies on the Two Sublattices of SiC"**

In a recent Letter [1] Rempel *et al.* proposed that a positron lifetime of 210 ps was associated with positron annihilation (PA) in the Si + Si divacancy in high-energy (2.5 MeV) electron-irradiated SiC, supported by coincidence Doppler broadening (CDB) data [1,2]. In this Comment we propose that it is the Si + C, not Si + Si, divacancy which gives rise to this lifetime.

There have been a number of experimental PA studies of defects in SiC over the past 10 years or so, but none unambiguously supports the conclusions of [1]. For example, by combining PA with deep level transient spectroscopy Kawasuso *et al.* concluded that Si vacancy-related defects act as the major positron trapping centers after electron irradiation [3]; their data were not, however, conclusive with regard to the formation of Si + C divacancies. Although Arpiainen *et al.* [4] tend to accept the view of the Stuttgart group [5] that the 210 ps lifetime is due to PA in Si vacancies, they explicitly state that they are unable to distinguish between the single Si vacancy and the Si + C divacancy. Theoretical PA studies of vacancylike defects in SiC are given in [6–9] and a comparison of different computational approaches is presented in [10].

Our main point is that the 210 ps lifetime agrees well with the calculated values for the Si + C divacancy [6–9] but not with the values for the Si + Si divacancy. The latter behaves rather as two isolated Si vacancies [7], thus giving a lifetime very close to that for the single Si vacancy. In our opinion the Si environment is not detected in CDB because PA in the Si part of the divacancy is about 3 times more probable than in the C part [11]. Therefore, a signal coming from Si atoms in the vicinity of the C part has to be weak — see Fig. 2 of [9] and the discussion in [10].

A recent paper dealing with atomic displacements in SiC [12] suggests that the threshold displacement energies for Si and C atoms are about 40 and 20 eV, respectively. This means that at higher electron energies more C than Si vacancies are produced, and the creation of nearest-neighbor Si + C divacancies is, therefore, very probable. Electron spin resonance [13] gives another strong indication that the Si + C divacancy is formed after high-energy electron irradiation.

Various charge states of the Si + C divacancy in SiC were examined in a recent *ab initio* study [14]. Defect charging is important when determining the relaxed geometry of defects, and its influence on PA characteristics should be considered in detail in future positron studies of SiC.

A second point is that after irradiation by 0.5 MeV electrons both Si and C vacancies are produced, but in [1] it is proposed that positrons annihilate predominantly in Si vacancies. In our opinion an estimated lifetime of 176 ps represents a mixture of signals from C and Si vacancies (153 and 192 ps [7]) and perhaps also from Si + C divacancies (214 ps [7]). In addition, calculated CDB ratio curves [9] indicate an almost negligible difference — both in slope and position — between the signals from the Si vacancy and the Si + C divacancy. Considering this, and the difference (found in [1]) between the positions of CDB ratio curves for 0.5 and 2.5 MeV electron-irradiated samples, we again conclude that positrons should annihilate in both Si and C vacancies.

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[1] A. A. Rempel *et al.*, Phys. Rev. Lett. **89**, 185501 (2002).
[2] A. A. Rempel *et al.*, Mater. Sci. Forum **389–393**, 485 (2002).
[3] A. Kawasuso *et al.*, J. Appl. Phys. **90**, 3377 (2001).
[4] S. Arpiainen *et al.*, Phys. Rev. B **66**, 075206 (2002).
[5] M. A. Müller *et al.*, Mater. Sci. Forum **363–365**, 70 (2001).
[6] G. Brauer *et al.*, Phys. Rev. B **54**, 3084 (1996).
[7] G. Brauer *et al.*, Phys. Rev. B **54**, 2512 (1996).
[8] B. Barbiellini *et al.*, Mater. Res. Soc. Symp. Proc. **640**, H5.25.1 (2001).
[9] T. E. M. Staab *et al.*, Mater. Sci. Forum **353–356**, 533 (2001).
[10] J. Kuriplach, Appl. Surf. Sci. **194**, 61 (2002).
[11] J. Kuriplach (to be published).
[12] L. Malerba *et al.*, Phys. Rev. B **65**, 045202 (2002).
[13] N. T. Son *et al.*, Semicond. Sci. Technol. **14**, 1141 (1999).
[14] L. Torpo *et al.*, Phys. Rev. B **65**, 085202 (2002).

  