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Reply to "Comment on 'Multiple encounters of thermal positrons with surfaces' "

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In replying to Jensen and Walker's Comment, we point out the inconsistency that exists in theoretical modeling and experimental data analysis for positron remission measurements. For the modeling aspect, Jensen and Walker have correctly emphasized that the diffusion-equation theory includes the multiple-encounter effects for positrons at surfaces.

We agree with Jensen and Walker[1] in that the multiple encounters are included in the classical solution of the diffusion equation. Unfortunately, the results of the experiments that have been discussed in Ref. 2 have not necessarily been interpreted using such a classical solution. While is is unclear about which approach Ref. 3 has adopted, Ref. 4 certainly has not followed all the assumptions in the classical solution. This point is also agreed upon by authors of Ref. 1 [see discussions after Eq. (7) in Ref. 1]. In Ref. 2, we have suggested that the modeling in Refs. 3 and 4 may have neglected multiple-encounter effects. We have not directly discussed the diffusion equation in those references especially in relation to its "classical solution." Thus, we are not indicating that the classical solution of the diffusion equation does not include the multiple-encounter effects. However, having not discussed explicitly the existence of such a classical solution may have caused the inference by authors of Ref. 1.

To be more specific about the experimental treatments in Refs. 3 and 4, although they have employed the "diffusion equation," they have not related ν to the evaluated reflection (or transmission) coefficient (see Ref. 1 for definition of symbols). The detail of the data analysis is not given in Ref. 3, but it is mentioned that the model of Britton *et al.*[4] is referenced. Thus we will discuss the data analysis consequences of Britton *et al.*[4] below.

In Ref. 4, ν is related to positron and positronium emission and surface trapping rate ν_{e+}, ν_{Ps}, ν_s by the following equation:

$$\nu=\nu_{e+}+\nu_{\text{Ps}}+\nu_s \ . \tag{1}$$

ν_{e+} and ν_{Ps} are both proportional to a surface transition probability T, which is evaluated from a step potential model [Eq. (4) of Ref. 4]. These two terms vanish as the temperature approaches zero. However, the surface trapping rate ν_s in Ref. 4 is assumed to be temperature independent,[5] and is in fact larger than the other two surface escape channels. Thus from Eq. (1), ν will be nonzero at all temperatures. According to the equations given by Ref. 1, if the authors have evaluated the reflection coefficient from $1-P_{\text{enc}}$, they should have obtained a zero ν in order to obtain total reflection. This is certainly against the conclusion drawn in Ref. 4. Therefore, the experimental results are not, as one would deduce from the classical solution of the diffusion equation, related to the single encounter parameter ν. In general, we feel that the diffusion theory and experimental data analysis are not yet fully consistent with each other. It is not totally clear what the experimentally extracted parameters mean.

Reference 1 has also discussed the experimental results on positron-annihilation-induced Auger electrons (PAES) from a Ge(100) surface.[6] We have estimated that the near-surface contribution to PAES is on the order of 10^{-2} when compared with surface state positrons, and we note here that other contributions such as those discussed by the original authors[6] can all be significant. The authors in Ref. 1 have reached the conclusion that the near-surface contribution is two to three orders of magnitude smaller than the surface-trapped positrons which do not deviate much from our estimate. It is agreed also by the authors of Ref. 1 that a more detailed, and possibly first-principle calculation can quantify the contribution of near-surface positron contributions. Therefore, it is yet too early to claim that the PAES observation of 5% cannot be, to an observable extent, related to the near-surface positron annihilations. Quantitative attempts, such as those based on the diffusion approximation implied by the authors of Ref. 1, are subject to questions since the validity of the diffusing approximation no longer holds at 10 Å from the surface.

In conclusion, we look forward both to improved compatibility between theory and experiment when extracting, e.g., reflection coefficients, and to future theoretical progresses in quantitative evaluation of, e.g., near-surface positron annihilation contributions toward PAES.

[1] K. O. Jensen and A. B. Walker, preceding paper Phys. Rev. B **48**, 2215 (1993).

[2] Y. Kong and K. G. Lynn, Phys. Rev. B **44**, 13 109 (1991).

[3] G. R. Brandes, K. F. Canter, and A. P. Mills, Jr., Phys. Rev. B **43**, 10 103 (1991); G. R. Brandes, *ibid.* **43**, 10 111 (1991).

[4] D. T. Britton, P. A. Huttunen, J. A. Makinen, E. Soininen, and A. Vehanen, Phys. Rev. Lett. **62**, 2413 (1989).

[5] We note that the absolute surface trapped positrons may possess temperature dependence, whereas the branching ratio can be temperature independent [see Y. Kong and K. G. Lynn, Phys. Rev. B **44**, 10 843 (1991)]. Thus, one should be careful when making assumptions about ν_s in Ref. 4.

[6] E. Soininen, A. Schwab, and K. G. Lynn, Phys. Rev. B **43**, 10 051 (1991).

