Comment on "Emission of Band-Gap-Energy Positrons from Surfaces of LiF, NaF, and Other Ionic Crystals"

Recently Mills and Crane[1] reported that ionic crystals bombarded with low-energy (kiloelectronvolt) positrons (e^+) reemit a large fraction of these with an energy distribution measured to be approximately the width of the band gap. Positronium (Ps) was also emitted, and the probabilities of both e^+ and Ps emission had a similar dependence on the incident e^+ energy. It was concluded that the emitted e^+ and Ps have a common origin, namely, from Ps formed in the bulk, which then diffuses back to the surface, where it is directly emitted as Ps or as an energetic e^+ (after the electron is stripped from the Ps into an unoccupied electron surface state).

This interpretation necessitates the assumption of a high density of unoccupied electron states at alkali-halide surfaces. Since Ps is the source of both emissions it also requires that the Ps fraction formed in the bulk is large (i.e., 0.62 for NaF[1]). The high fraction can only be explained by the formation of Ps predominantly by a e^+ capturing an electron from the track of electron-hole pairs that it creates while slowing down (spur model[2]). In this case, however, the Ps fraction should increase with energy at low incident positron energy since more electron-hole pairs are created in this case. Such an increase has been observed in ice[3] but not in ionic crystals.[1] The formation of Ps by a mechanism whereby a positron of the right energy brings an electron from the valence band to the conduction band as a result of gaining the Ps binding energy has a lower expectation (0.28 for NaF according to the Ore model,[4] i.e., the width of the energy region where stable Ps can be formed relative to the band gap). Further, the model of Mills and Crane implicitly assumes that the fraction of positrons that did not form Ps has an insignificant probability of emission.

In contrast, we propose that the e^+ and Ps emission are due to positrons which reach the surface, still having part of their initial kinetic energy (i.e., nonthermal). The positrons are directly emitted and there is no requirement of the presence of empty surface electron states. Ps is formed by the nonthermal positron's picking up an electron, and the observed fraction of emitted Ps is in agreement with the Ore model applied at the surface.

Positrons that are injected into the crystal will rapidly lose energy, mainly by means of electron-hole pair creation, until they enter the band gap. Ps is can be formed whenever energetically favorable. Positrons that enter below the threshold for Ps formation can only lose energy by phonon scattering. The positron energy-loss rate, therefore, becomes orders of magnitude lower. The relatively long escape depth associated with reemission in these cases is not surprising considering the low loss rate and the high velocity of the nonthermal positrons. Recently reported diffusion lengths for nonequilibrium positrons in metals[5] and rare-gas solids[6] are also consistent with this explanation. It is more difficult to explain why the energy distribution does not change significantly with incident energy.[1] One possibility is the presence of a dominant energy-loss mechanism that totally removes a positron from the reemitted spectrum rather than change its energy within the distribution. This would change the intensity of reemitted positrons but not the shape.

Positron and Ps interaction with the electron-hole pairs created in the track during the positron energy-loss processes might be important. Positrons can interact with an electron in the conduction band and form Ps, as mentioned. Ps can possibly interact with one of the created holes resulting in electron-hole recombination where the excess energy can be transferred to the positron with the possibility of a repeated sequence. As a result energy stored in the track would be transformed to positrons and Ps. This might explain why the energy distribution of reemitted positrons is seemingly independent of incident energy.[1] The observed positron and Ps emission would still be due to positrons reaching the surface with high kinetic energy, provided that their mobility is significantly higher than the mobility of Ps. The presence of the positron (i.e., third body) enhances the electron-hole recombination cross section. This process is in many respects analogous to the proposed interaction between excitons and F centers in alkali halides resulting in the emission of an energetic electron.[7] Nonthermal Ps could possibly explain why the component in the angular correlation of the annihilation quanta which is associated with Ps is very broad.

We wish to thank P. Sferlazzo, A. Mills, and S. Linderoth for useful discussions.

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Received 13 June 1986
PACS numbers: 71.60.+z, 73.20.Cw, 78.70.Bj

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