Confirmation of Positron Mobility Edge in Gaseous Helium by Monte Carlo Simulation

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Positron lifetime spectra in helium gas, subjected to a uniform dc electric field, are calculated by a Monte Carlo simulation procedure which is based on an earlier scheme developed by Farazdel and Epstein. These calculations clearly show that introduction of a positron mobility edge E_c^+ alone produces a striking improvement in the agreement between theory and experiment. By visual inspection it is estimated that $E_c^+ = 10^{+5}_{-2}$ meV at an electric field of 52 V/cm.

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Recently a positron mobility edge E_c^+ in helium gas has been reported by Tawel and Canter,[1] using a pulsed electric field technique. Aside from the inherent interest of the physics involved, this observation is of particular importance since it has been suggested by these investigators that E_c^+ is a possible candidate for the long sought mobility edge E_c separating Anderson localized and extended states, proposed by Mott and expounded by Mott and Davis.[2]

The existence of a mobility edge for positrons in helium gas was first suggested by Canter *et al.*[3] Subsequently Azbel and Platzman proposed[4] the existence of two distinct energy thresholds, namely E_c^+ (i.e., the mobility edge) and the well-known cluster formation threshold[5] E_R, in their model for cluster nucleation. Ruttenberg, Tawel, and Canter[6] later proposed that the Azbel-Platzman model might be responsible for a small disagreement in their experimental positron lifetime spectrum (PLS) from that of the Farazdel-Epstein (FE)[7,8] Monte Carlo simulation procedure.

Here preliminary results on the effect of introduction of such a mobility edge in the FE Monte Carlo simulation procedure are reported. As it turns out, the addition of E_c^+ alone, while other simulation parameters are kept fixed at their zero-field values, brings a dramatic improvement in the agreement with the experimental PLS at the electric field of 52 V/cm. By visual inspection[9] the optimum value of E_c^+ is chosen which gives a PLS that matches the experimental one. The value of E_c^+ chosen this way agrees with the reported experimental value[1] within estimated errors. The FE Monte Carlo simulation scheme for the determination of PLS is based on an entirely different method from the experiment. Hence the present work constitutes an additional confirmation of the existence of a positron mobility edge in gaseous helium. In addition, the Monte Carlo scheme reported here opens the possibility of future estimates of E_c^+ at high densities.

In a typical positron lifetime experiment, an ensemble (essentially one at a time) of positrons with an energy of 0.5 MeV is emitted along with 1.28-MeV photons into a sample chamber containing the host gas helium by a radioactive source such as ^{22}Na or ^{64}Cu. These high-energy positrons undergo many collisions with the helium atoms before their eventual annihilation. At first the positrons rapidly lose energy, primarily by excitations and ionizations, until they reach first 24.5 eV, the ionization energy, then 19.8 eV, the lowest excitation energy of ground-state helium, and finally 17.7 eV, the difference between the ionization energies of helium and positronium. A significant fraction of positrons is scattered below 17.7 eV. In the absence of applied electric fields, entrance into this low-energy region is essentially irreversible, and these so-called "slow positrons" can undergo only elastic collisions (about 30000 at temperature of 5 K and density of 3.5×10^{21} cm^{-3} with no external field) and annihilation. The rate of annihilation, $A(t) = -dN(t)/dt$, of slow positrons as a function of time t measured from the moment of emission of the positron constitutes a PLS. Here $N(t)$ is the number of positrons yet to be annihilated at time t.

The chief features of a low-temperature–high-density PLS in helium gas are the following: (i) There is an initial slowly varying linear shoulder for free annihilation of positrons; this linear region is broad because of the existence of a minimum (so-called Ramsauer minimum) in the momentum-transfer cross section of positron with helium. (ii) After the initial linear region, a peak appears resulting from the rapid nucleation of a cluster of helium atoms around a positron, i.e., self-trapped states of the positron. (iii) After the peak, $A(t)$ levels off and resumes the linear dependence but now at a high slope corresponding to the self-trapped state.

The theoretical method used in the present report to calculate the PLS in helium is based on a streamlined version of the semiclassical Monte Carlo procedure developed by Farazdel and Epstein.[7,8] The FE simulation makes very simple assumptions consistent with the experiment and uses only two simulation parameters. The first is the energy threshold E_R for the cluster formation around the positron, and the second parameter is Z_R,[10] the corresponding enhanced decay-rate parameter (i.e., slope of the tail of PLS on a semilog scale). This method has been able to simulate successfully[6] the "anomalous" peak in PLS due to the positron cluster as well as the variations (position and shape) of the peak with external electric field and ambient temperature of helium.[8] References 7 and 8 explain the details of the FE simulation scheme. Briefly, in this method the motion of positron through the host gas helium is treated classically but the cross sections (momentum transfer σ_e and annihilation σ_a) used, as functions of positron energy, are high-quality quantum-mechanical calculations[11] in agreement with experiment.

A salient feature of the FE method is that instead of tracking one positron at a time from its "birth" to its "death" (i.e., annihilation), a swarm of independent positrons with identical energies (randomly sampled from some assumed energy distribution) is followed. This is necessary if the method is to have a practical efficiency since for slow positrons the ratio σ_a/σ_e is small (about 10^{-4}). At each collision, a fraction $\sigma_a/(\sigma_a+\sigma_e)$ of the positron swarm is annihilated, while the rest is scattered elastically and moves on to the next collision. During the slowing down all positrons in the swarm have the same energy. The dispersion of the energy distribution comes from the sampling of several swarms and not from the positrons in only one swarm. In a typical PLS, about 250 swarms are needed to achieve an accuracy comparable to that of the best available experiments. In the present work an additional energy threshold, namely the positron mobility edge E_c^+, is added to the FE simulation. Below E_c^+ the electric field is "turned off" until the positron reaches E_R below which it forms the cluster. The mobility edge is assumed to have no effect on the form of the collision cross sections involved. The input to the simulation program consists of the number of positron swarms, ambient temperature and density of the host gas helium, electric field strength, and the three simulation parameters E_R, Z_R, and now E_c^+. The output includes a histogram of $A(t)$ (i.e., PLS), and the average and width of the positron energy distribution, versus time.

In Fig. 1 calculated PLS's in helium vapor at 5.5 K and 129 amagats (1 amagat $=2.6868\times10^{19}$ cm^{-3}) subjected to a uniform electric field of 52 V/cm (dashed curves) and no external field (solid curve) are shown on a semilogarithmic scale. The only parameter that is different among these PLS's is E_c^+, while everything else is kept the same. Specifically, the simulation parameters $E_R=0.005$ eV and $Z_R=18.2$ are chosen[8] to give good agreement with the experimental zero-field PLS.[6] To have PLS in the limit of $E_c^+=+\infty$, the calculated zero-field PLS is also included in Fig. 1 (the solid curve). All theoretical PLS's in this report are convoluted with the instrumental resolution function[12] which can be approximated by a standard Gaussian function of width 0.9 nsec. The effects of convoluting on the shape of PLS were minimal and it essentially helped smooth out the PLS. As can be seen in Fig. 1, the increase in E_c^+ alone

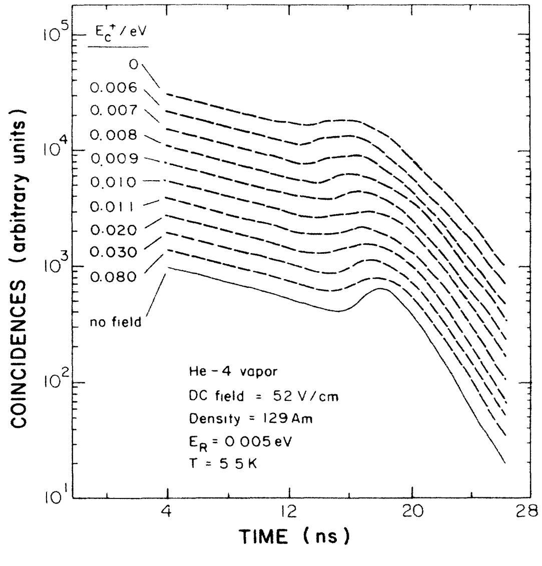

FIG. 1. Calculated lifetime spectra for slow positrons in helium gas in the presence of an external electric field (dashed curves) corresponding to different values for mobility edge E_c^+. All other parameters, namely $E_R=0.005$ eV, $Z_R=18.2$, and the type of positron initial energy distribution, are held fixed at their zero-field values (Ref. 8). The solid curve is the calculated zero-field (corresponding to $E_c^+=+\infty$) PLS of Ref. 8. All spectra are convoluted with the experimental resolution function.

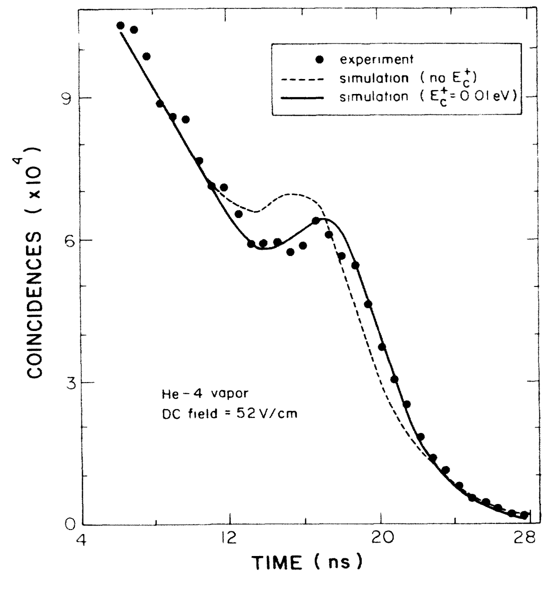

FIG. 2. Theoretical lifetime spectra with and without a positron mobility edge along with the experimental PLS at 5.5 K and 140 amagats. The theoretical spectra were calculated at 5.5 K, 140 amagats, $E_R=0.005$ eV, and $Z_R=18.2$. The two theoretical PLS's are convoluted with the experimental resolution function.

(i) delays the onset of the peak, (ii) sharpens the peak, and (iii) increases the apparent slope of the tail.[13] All these three trends are consistent with the theoretical observation[8] that the longer the positron is "exposed" to the external electric field (equivalent to lowering of E_c^+), the broader the positron energy distribution becomes.

In order to choose the value of E_c^+ which gives a PLS in best agreement with the experiment, the experimental PLS[6] was visually compared[9] with the theoretical ones. For this comparison all the PLS's were plotted on a linear scale in which the differences between PLS's are more pronounced. All theoretical PLS's were also normalized to have the same area under the curve as the experimental PLS of Ref. 6. The best value for E_c^+ from this visual inspection method is 10 meV with an estimated lower limit of 8 meV and upper limit of 15 meV. Further work is in progress to decrease this error limit and make our estimate of best E_c^+ more quantitative. The value of $E_c^+ = 10^{+5}_{-2}$ meV obtained here is consistent with the pulsed-field value of $E_c^+ = 15 \pm 3$ meV reported in Ref. 1. However, for more precise comparison, the electric field, gas density, and temperature dependences of E_c^+ have to be investigated further. In Fig. 2, the best theoretical PLS corresponding to $E_c^+ = 10$ meV is shown along with the experimental PLS of Ref. 6. Note the striking improvement that the addition of E_c^+ brings.

In summary it is established that the addition of a positron mobility edge alone, while other conditions and simulation parameters are at their zero-field values, brings a dramatic agreement between experiment and theory. In view of the fact that the simulation scheme here for calculation of PLS uses so few (actually three) simulation parameters and the degree to which the theoretical PLS matches the experiment, the present results constitute strong support for the recently observed positron mobility edge of Ref. 1. Additionally, the Monte Carlo scheme reported here can be used to determine E_c^+ at high densities at which the experimental (pulsed field) method usually has timing limitations.

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[9] Presently extensive simulations at more values of E_c^+ are being carried out to make the estimate of the best E_c^+ and its associated error more quantitative.

[10] The quantity Z_R can be thought of as the effective number of electrons "seen" by the positron in the cluster.

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[13] Of course in the limit of time $= +\infty$, all calculated positron lifetime spectra will have the same slope corresponding to the cluster with a given Z_R.