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LETTER TO THE EDITOR

Positive-hole mobility in liquid xenon as a function of temperature

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Abstract. The drift mobility of positive holes was measured in liquid xenon in the temperature range from 161 K to 280 K. The results are discussed on the basis of the model of small-polaron hopping.

Recently, measurements of the drift mobility of positive holes in liquid xenon were reported by us (Hilt and Schmidt 1994). At the melting point ($T = 161$ K), a mobility of $3.5 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ was measured. In the temperature interval from 161 K to 200 K the mobility was found to be thermally activated with an activation energy of 32 meV. The magnitude of the mobility and its temperature dependence suggested an interpretation of the data via the hopping model of charge carrier transport (LeComber *et al* 1968). In this model, the charge carrier carries out thermally activated jumps from one trapping site to another. The mobility is given as

$$\mu = (e_0 b^2 / k_B T) \omega. \quad (1)$$

Here b denotes the average jump distance and ω is the jumping frequency. In a semiclassical model (Emin 1973) the jumping frequency can be expressed as

$$\omega = P(\omega_0 / 2\pi) \exp(-E_a / k_B T). \quad (2)$$

E_a is the activation energy and P denotes the tunnelling probability for the case where adjacent sites have the same energy level. ω_0 is the phonon frequency. The hole data measured could be rationalized under the assumption of a fixed jump distance b . Since the density of liquid xenon decreases with increasing temperature it seems unlikely that b will remain unaffected. For this reason, we extended the measurements of the hole mobility up to a temperature of 280 K.

The time-of-flight measurement technique and the purification of the samples has been described already in detail (Hilt and Schmidt 1994). The results obtained on the temperature dependence of the drift mobility of positive holes along the saturation line (orthobaric conditions) are shown in figure 1. The fidelity of the present data is supported by a value at 230 K reported by Obodovski (1994). The surprising result is the decrease of the mobility at higher temperatures. We assume that the main reason for this lies in the variation of $b(T)$. The next-neighbour distance decreases with increasing temperature, and we take $b(T)$ as

$$b^3(T) = \sqrt{2} M / \rho(T) \quad (3)$$

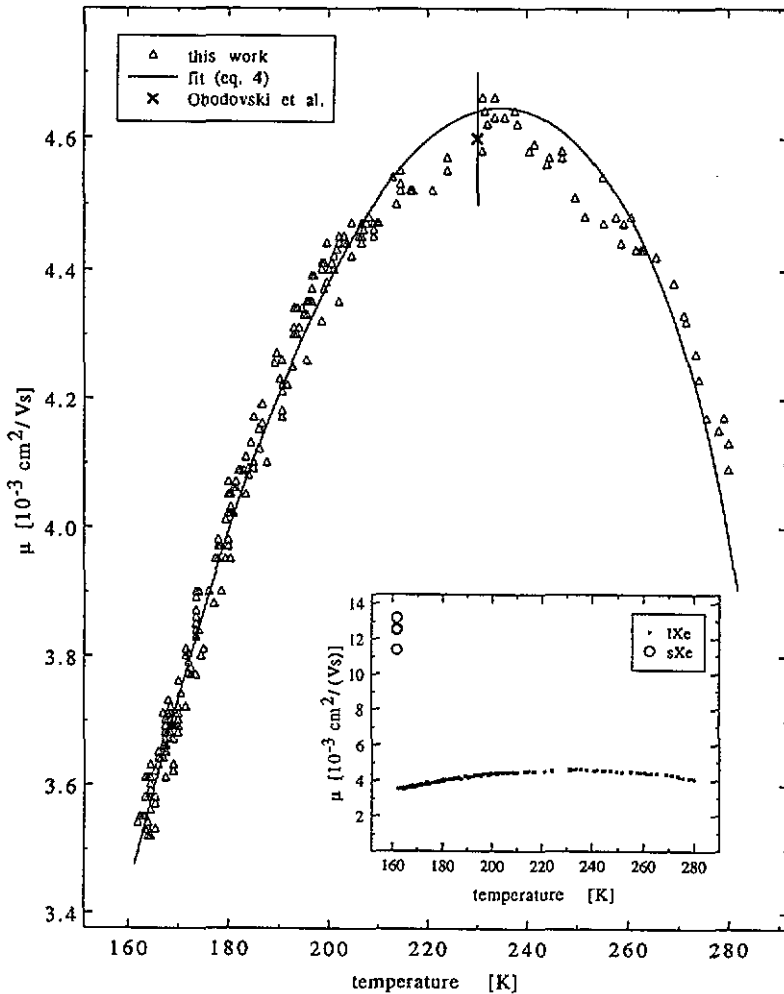


Figure 1. The drift mobility of positive holes in liquid xenon as a function of temperature; inset—drift mobility in liquid xenon and in solid xenon at the triple point; note the scale of the abscissa.

with M the mass of a xenon atom and $\rho(T)$ the density as a function of temperature. $b(T)$ is shown in figure 2. Increase in b leads to an increase in μ . At the same time, b signifies the separation of a filled and an adjacent empty trap. Increase in $b(T)$ reduces the overlap of the wave function with the empty level.

In the further discussion, we assume that the trapped state of the hole can be described as a small polaron (Holstein 1959). Although this picture was developed initially for electrons in perfect crystals it was later extended to electrons and holes in disordered materials (Emin 1973). The mobility of the small polaron is given by

$$\mu(T) = \frac{e_0 b^2(T)}{k_B T} \frac{2\pi}{h} \sqrt{\frac{\pi}{4E_a k_B T}} J_0^2 \exp(-2\alpha b(T)) \exp\left[-\frac{E_a}{k_B T}\right]. \quad (4)$$

h is Planck's constant. The transfer integral J , which describes the overlap, decreases with distance, r , as (Böttger and Bryskin 1985)

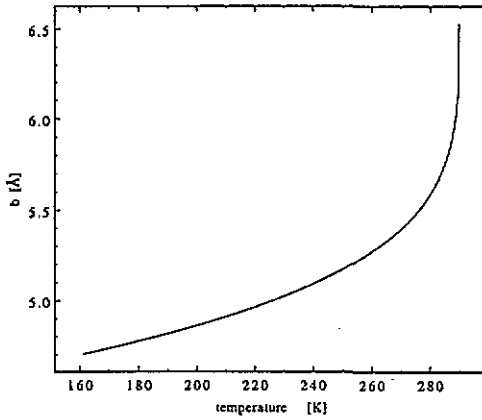


Figure 2. The mean atomic distance $b(T)$ for liquid xenon according to (3).

$$J(r) = J_0 \exp(-\alpha r). \quad (5)$$

α^{-1} is the decay length. With $b(T)$ given by (3), α , J_0 , and E_a were varied until agreement between the measured data and (4) was obtained. The solid line in figure 1 represents the best fit with $E_a = 44.5$ meV, $J_0 = 15.8$ meV, and $\alpha^{-1} = 2.39$ Å. $J(b(T))$ decreases with temperature from $J = 2.23$ meV at 161.4 K to $J = 1.54$ meV at $T = 280$ K.

Included in figure 1 are hole mobility data for solid xenon at the triple point which were also measured by us. The ratio of the mobilities at the triple point was found to be

$$\mu(\text{s-Xe})/\mu(\text{l-Xe}) \approx 3.5. \quad (6)$$

This is determined mainly by the variation of the binding energy, E_b , of the polaron. The binding energy of the small polaron depends on the lattice deformation energy, E_D . It can be expressed as (Mott and Davis 1979)

$$E_b = \frac{1}{2} B^2 / \kappa V. \quad (7)$$

Here, B is proportional to the polarization energy, E_p . The bulk modulus, κ , is proportional to E_D . V expresses the volume involved in the deformation. At the phase transition from the solid to the liquid state, B or E_p decreases with the dielectric constant ϵ_r :

$$E_p \sim 1 - 1/\epsilon_r. \quad (8)$$

The dielectric constant of solid xenon is $\epsilon_r(\text{s-Xe}) = 2.0$, while in liquid xenon at the triple point $\epsilon_r(\text{l-Xe}) = 1.8$ is reported (Bokov and Naberukhin 1981). The reduced coupling between the atoms in the liquid is reflected by a smaller value of κ . The bulk modulus is given by the velocity of sound, v_s ,

$$\kappa = v_s^2 \rho. \quad (9)$$

At the triple point the following values are reported: in solid Xe, $v_s(\text{s-Xe}) = 1020$ m s⁻¹ (Bezuglyi *et al* 1971); in liquid Xe, $v_s(\text{l-Xe}) = 655$ m s⁻¹ (Aziz *et al* 1967). The density changes by about 15% at the melting line (Pollack 1964). It follows that the binding energy

of the polaron is bigger in the liquid than in the solid. For the ratio of the polaron binding energies we obtain

$$\frac{E_b(s\text{-Xe})}{E_b(l\text{-Xe})} = \left(\frac{1 - 1/\epsilon_r(s\text{-Xe})}{1 - 1/\epsilon_r(l\text{-Xe})} \right)^2 \left(\frac{v_s(l\text{-Xe})}{v_s(s\text{-Xe})} \right)^2 \frac{\rho(l\text{-Xe})}{\rho(s\text{-Xe})}. \quad (10)$$

With $E_b(l\text{-Xe}) = 89.0$ meV, equation (10) yields $E_b(s\text{-Xe}) = 55.6$ meV. Since $E_b = 2E_a$, the mobility according to (4) decreases with increasing E_a at T_{tr} . The mean atomic distance b also increases during the melting process. At the triple point, the separation distances are $b(s\text{-Xe}) = 4.49$ Å and $b(l\text{-Xe}) = 4.71$ Å. The ratio of the hole mobility in solid and liquid xenon is then given by

$$\frac{\mu(s\text{-Xe})}{\mu(l\text{-Xe})} = \left(\frac{b(s\text{-Xe})}{b(l\text{-Xe})} \right)^2 \exp[2\alpha(b(l\text{-Xe}) - b(s\text{-Xe}))] \sqrt{\frac{E_a(l\text{-Xe})}{E_a(s\text{-Xe})}} \times \exp\left(\frac{E_a(l\text{-Xe}) - E_a(s\text{-Xe})}{k_B T}\right). \quad (11)$$

Equation (11) yields

$$\mu(s\text{-Xe})/\mu(l\text{-Xe}) = 4.3. \quad (12)$$

This ratio of the mobilities is in good agreement with the measured value (equation (6)).

In liquid xenon, the dielectric constant ϵ_r and the velocity of sound v_s decrease with increasing temperature under orthobaric conditions. A more detailed analysis of the data according to (4) has to take into account the temperature dependence of the binding energy E_b .

The present measurements could not be extended above 280 K. The hole mobility decreases further with temperature due to the dramatic increase of $b(T)$ resulting in a decrease of the transfer integral. $J(b(T))$ becomes the dominating factor in (4). At the same time, the mobility of positive impurity ions becomes comparable to the hole mobility. Due to the simultaneous presence of holes and positive ions in the liquid sample, no definite breaks in the temporal dependence of the ionization current could be detected. It was not possible any longer to distinguish between the ionic part and the hole part of the drift signal.

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