RESONANT DIFFUSION OF BERYLLIUM MOLECULE

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The report represents the calculation of the probabilities for resonant tunneling [1] of realistic beryllium molecule comprising a continuous spectrum through the potential barriers of the Gaussian type. The parameters of the barrier potential correspond to the potential surface of copper crystal (001) for the hydrogen atom.

Based on the derived probability we calculated the diffusion of beryllium molecule. The quantum coefficient of diffusion in solids can be written in the form $D_{qua} = D_0 F(T)$, and transforms to the coefficient of classical diffusion $D_c = D_0 e^{-E_{max}/T}$ at high temperature.

Comparison of different types of diffusion is illustrated in Figure 1. The quantum diffusion of the molecule is shown by the solid line. For comparison, we calculated the classical diffusion of the molecule (dot-dashed line), quantum diffusion of the atom (dotted line) and of rigid molecule (dashed line).

It can be seen that at the temperatures below 80 K the molecular diffusion is much higher than atomic. The differences reach 8 orders.

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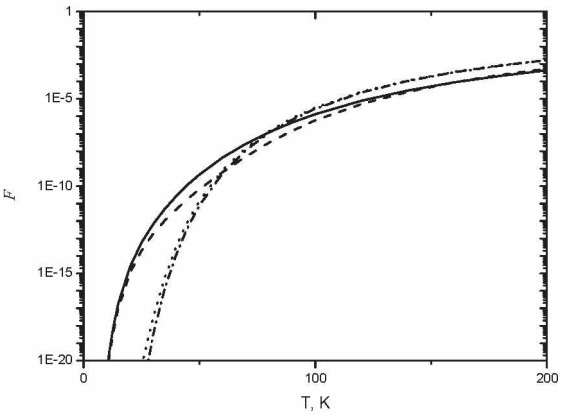

Fig. 1. Comparison of different types of diffusion for beryllium molecule.

1. F.M.Pen'kov. // Phys. Rev. A. 2000. V.62. 044701-1,4.