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Diffusion of hydrogen and its isotopes in BCC-metals

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Quantum states and potential configurational relief of hydrogen atom in BCC-metals is considered. On the basis of the quantum state data, two regimes of hydrogen and its isotopes incoherent transport through model BCC-systems, pure metals and dilute solid solutions are considered. Local lattice deformation near impurity centre and phonons dispersion was taken into account under diffusion coefficient derivation.

The type of a crystal lattice determines the mechanism of the hydrogen atom diffusion elementary act in metals. Difference of diffusion mechanisms is caused by different located AB state in different crystal lattices. In particular, in BCC-metals it is formed due to deformation effects and self-trapping of hydrogen atom, instead of Coulomb forces.

Tunnel transitions of hydrogen atom in metals may take place not only in the field of zero temperature (coherent transitions), they also may occur at the high temperatures considerably exceeding Debye temperature; and in this range of temperatures phonon-induced (incoherent) tunneling takes place.

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