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HYDROGEN DIFFUSION IN CRYSTALLINE SILICON

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Abstract : The high temperature H^+ diffusion in c-Si is studied by means of ab-initio molecular dynamics. The simulation shows the importance of dynamical effects on hydrogen motion. The computed diffusion coefficient is in very good agreement with the available experimental data. We suggest that scattering experiments may distinguish between different diffusion mechanisms.

In view of the great technological importance, the behaviour of hydrogen in crystalline Silicon (c-Si) has been the object of extensive experimental and theoretical investigations. However a detailed microscopic understanding of a basic phenomenon like the hydrogen diffusion process is still lacking.

A first principles molecular dynamics [1] to simulate the diffusion process of a proton in c-Si has recently been performed [2]. Within this scheme the interatomic potential is obtained from accurate local density functional calculations, and dynamical finite temperature effects are completely taken into account.

The main results are: (i) The diffusion process is jump like between highly symmetric interstitial sites. (ii) The computed diffusion coefficient D is in good agreement with the experimental data of ref. [3], thus confirming the high mobility of hydrogen in c-Si. (iii) The inclusion of dynamical effects substantially modifies the picture inferred by T=0 total energy calculations [4].

In fig. 1 we report the computed diffusion data at different temperatures together with some of the available experimental data. Our data agree with the experimental results of ref [3], obtained in the same range of temperature.

Our simulation has detected as the most favourable the path that alternates sites situated in regions of high electronic charge density (Bond Center and M sites), with sites situated in the low electronic density region (Hexagonal and Tetrahedral). Another path completely lying in the low density region and not requiring any distortion in the host lattice has also been observed. At present we are not able to give precise estimation of the relative occurrence of the two paths. However the computed hydrogen related phonon spectra of these two paths show significative differences [2], suggesting

the possibility of using scattering experiments to establish the nature of the diffusive path.

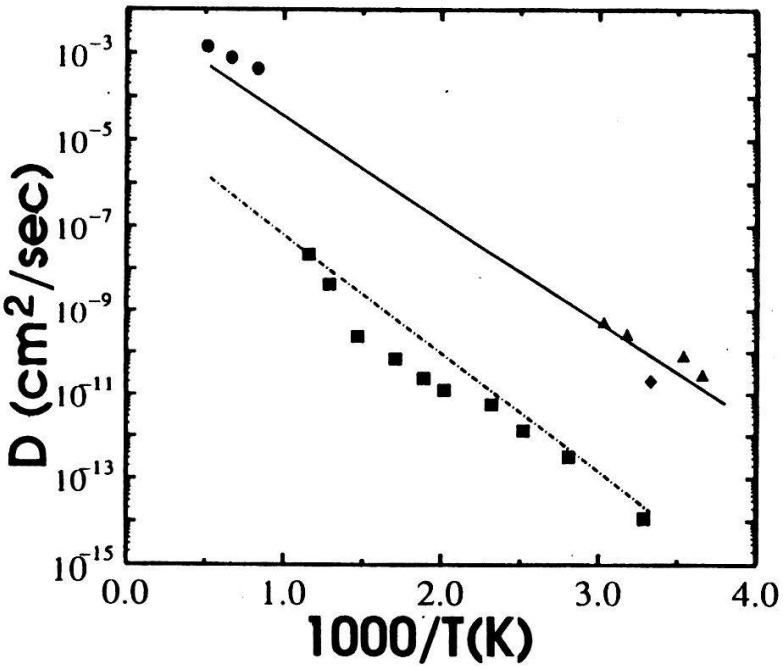

Fig. 1: Diffusion coefficient for hydrogen in c-Si as a function of inverse temperature. Circles: present calculation for H^+. Solid line: experimental results from ref. [3]. Dash dotted line: ref. [5] Squares: ref. [6]. Diamond: experimental measurement at room temperature from ref.[7]. Triangles: experimental determined diffusivity values in Au Schottky barrier sample [8].

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