

Al-Moatasem El-Sayed
University College London
Gower Street, London, WC1E 6BT
United Kingdom
☎ +44 (0) 7983 577077
☎ +44 (0)20 7679 7875
🌐 <http://www.cmmmp.ucl.ac.uk/kpm/people/tasem.htm>

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Dear Editor,

In this manuscript we address the important question of the interaction of atomic and molecular hydrogen with amorphous silica network. Atomic hydrogen is produced by photolysis or radiolysis of silica glass, during anneal and hole injection in CMOS devices, and plays an important role in tectosilicate minerals. It is usually assumed that atomic hydrogen interacts weakly with non-defective silica networks, instead reacting solely with structural defects.

We show that the interaction of atomic hydrogen with strained Si–O bonds in defect-free a-SiO₂ networks results in the formation of two distinct defect structures referred to as the [SiO₄/H]⁰ and the hydroxyl E' center. We study the distribution of each defect's properties and demonstrate that the hydroxyl E' center can be thermodynamically stable in the neutral charge state. We describe in detail the interaction of H with a single oxygen vacancy in a-SiO₂. In order to understand the origins and reactions of these defects, different mechanisms of formation, passivation and de-passivation have been investigated.

These results provide a better understanding of how atomic and molecular hydrogen can both passivate existing defects and create new electrically active defects in amorphous silica matrices. Better understanding of the reactivity of atomic hydrogen may have significant implications for our understanding of processes in silica glass and nano-scaled silica, e.g. in porous low-permittivity insulators, and strained variants of a-SiO₂, and therefore should be of interest to a wide community of chemists, mineralogists, physicists and engineers, which comprise the PRB readership.

Yours faithfully,

Al-Moatasem El-Sayed