

New Microscopic Model of the Staebler-Wronski Effect in Hydrogenated Amorphous Silicon

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New Microscopic Model of the Staebler-Wronski Effect in Hydrogenated Amorphous Silicon

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Abstract. A new microscopic and kinetic model of light-induced metastability in hydrogenated amorphous silicon (a-Si:H) was recently proposed. Carrier recombination excites H from deep Si-H bonds into a mobile configuration, leaving a threefold-coordinated Si dangling bond (DB) defect at the site of excitation – a process long suspected to be an element of metastable DB production. Normally, mobile H are recaptured at DB defects and neither metastability nor net DB production results. However, when two mobile H collide, they form a metastable two-hydrogen complex and leave two spatially-uncorrelated Staebler-Wronski DBs. The model leads to differential equations describing the evolution of the mobile H and DB densities and a variety of new predictions. New directions for improving the stability of a-Si:H are discussed.

INTRODUCTION

Over 20 years ago, Staebler and Wronski (SW) discovered light-induced metastability in hydrogenated amorphous silicon (a-Si:H) (1). The density of neutral threefold-coordinated dangling bond (DB) defects increases by one to two orders of magnitude as a result of illumination or carrier injection (2). These DBs are metastable; they can be annealed away by about 2 hours heating at 150°C (1). Because DBs act as carrier recombination centers and traps in a-Si:H, the metastable DBs cause significant performance degradation of photovoltaic and other devices made from a-Si:H. Numerous microscopic and kinetic models of the SW effect have been proposed and are reviewed elsewhere (3-5). However, all of these models appear to be incompatible with certain experiments (5-7).

I have recently developed a new "H collision" model of the SW effect (5-7). The microscopic model leads to differential equations describing the evolution of the mobile H and DB densities and to a variety of new predictions. This microscopic and kinetic model is consistent with the main experimental SW results, predicting 1) isolated SW DB defects uncorrelated with H or other DBs, 2) an intrinsic creation mechanism, 3) $N_{db} \sim G^{2/3} t^{1/3}$ DB creation kinetics at room temperature, 4) light-induced annealing of DBs resulting in saturation at $N_{sat} \sim G^{1/3}$, 5) $N_{db} \sim t^{1/3}$ DB creation kinetics at 4.2 K, and 6) $N_{db} \sim t^{1/2}$ laser-pulse DB creation kinetics. In this paper, I present an abbreviated

description of the microscopic model and outline possible directions for improving the stabilized properties of a-Si:H. Rigorous derivations of the main results and predictions are found elsewhere (5-7).

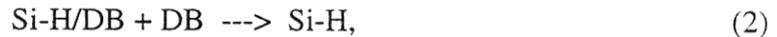
H COLLISION MODEL

In the H collision model (5-7) of the SW effect, DBs are created when light-induced carriers stimulate emission of mobile H from Si-H bonds (normally about 10 at.%), according to:



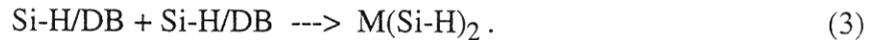
The mobile H is labelled here by Si-H/DB because calculations by Biswas et al. (8) show that mobile H break Si-Si bonds and form Si-H bonds as they hop between Si-Si sites. Each broken Si-Si bond reforms as the mobile H hops away. Mobile H is weakly bound compared to H in normal Si-H bonds; mobile H diffuses rapidly through a-Si:H (9).

Mobile H reverts to immobile Si-H through one of two mechanisms. Most often, it retraps to an immobile DB:

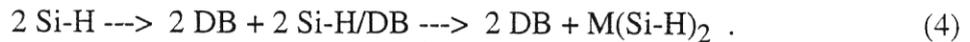


the inverse process to Eqn. (1). Taken together, Eqns. (1) and (2) neither create nor destroy DBs.

Infrequently, H retraps by associating with another mobile H in a metastable complex containing two Si-H bonds in close proximity:



Eqn. (3) is the key step of SW defect creation. The reaction annihilates two mobile DBs and forms no DBs, consistent with bond-counting constraints. Combining Eqns. (1) and (3), the net reaction leaves DB defects at the sites of the original H excitation according to:



The created SW DBs appear on the rightmost side of Eqn. (4). The H atoms are slightly less stable in $\text{M}(\text{Si-H})_2$ than in Si-H, and the created DBs are therefore metastable.

NEW DIRECTIONS FOR BETTER STABILITY

The H collision model provides new perspective and therefore suggests new directions that may be taken to improve the stability of a-Si:H materials and devices. Certainly, reduction of H content could reduce the metastability; perhaps this was already observed in the improved stability of hot-wire a-Si:H containing about 1 at.% H (10). However, stabilized defect density increases only as the two-thirds power of H content (5-7), and some H is needed to relieve strain, so this tactic may not yield further dramatic improvements.

A more subtle approach would be to increase the diffusion rate of mobile H. This may increase the retrapping rate of Eqn. (2) and thereby reduce the mobile H concentration. Improved ordering may be a key to this approach. Finally, it may be helpful to grow a-Si:H with "benign" H stored in excess $M(\text{Si-H})_2$, but without an increase of the DB or isolated Si-H densities. This H would form a reservoir of H that light could liberate (5-7) by the reverse reaction of Eqn. (3). Light-induced annealing of defects by the reverse of Eqn. (4) should then improve stabilized properties.

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