HYDROGEN INTERACTIONS WITH SEMICONDUCTORS AND OXIDES

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Hydrogen displays a range of complex behaviors when introduced as an impurity in solids. Interstitial hydrogen is a fast diffuser. It can bind to native defects or to other impurities, often eliminating their electrical activity – a phenomenon known as passivation. But hydrogen can also *induce* electrically active defects. Various technological developments are lending new urgency to a fuller understanding of the behavior of hydrogen in solids: the search for improved hydrogen storage systems and proton exchange membranes for fuel cells; the pursuit of novel dielectrics for integrated circuits (in which hydrogen may play an equally important role as it does at the Si/SiO_2 interface); and efforts to take advantage of the passivation of dopant impurities during growth to enhance doping levels (codoping). It turns out that many aspects of hydrogen's interactions with materials can be understood on the basis of the behavior of hydrogen as an *isolated* interstitial impurity. In most semiconductors and oxides hydrogen is *amphoteric*: H acts as a donor (H^+) in *p*-type material, and as an acceptor (H^-) in *n*-type material, always *counteracting* the prevailing conductivity. It therefore came as a surprise when calculations showed that hydrogen behaves exclusively as a *donor* in ZnO [1]. Only the positive charge state is stable in ZnO, and therefore hydrogen can act as a *source* of doping, rather than merely reducing the conductivity introduced by other dopants. The donor character of hydrogen in ZnO has a number of practical consequences that will be addressed in the talk. However, maybe the most interesting issue is: what is the fundamental reason for hydrogen to behave differently in ZnO? In the course of investigating this question we have been able to predict that hydrogen will act as a source of doping in a number of other materials as well, including InN [2] and InGaAsN alloys [3], where first-principles calculations have already confirmed the behavior. A general model for predicting the behavior of H in semiconductors and oxides will be discussed.

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