

van den Hoven *et al.* Reply: In his Comment [1], Weyer raises two issues about our Letter [2] to which we would like to respond.

(i) "Previous ^{119}Sn Mössbauer data for *a*-Si are in conflict . . ."

As work in the author's group has shown [3], Sn-vacancy complexes are difficult to observe even in heavily (α particle) damaged crystal Si (*c*-Si), and it would be unlikely that Sn-defect complexes could be observed in amorphous Si (*a*-Si) where the concentration of point defects has been estimated to be ~ 1 at.% [4]. In our Letter, we referred to a number of studies of ^{119}Sn in *a*-Si (Refs. [13–16], including work by Weyer *et al.*) to make the same point. These references, and the references in the preceding Comment by Weyer, show that Sn does not trap vacancies in *c*-Si, and so Sn is not an appropriate Mössbauer probe for observing point defects in either crystal or amorphous Si. This is precisely why we instead chose to use ^{119}Sb (which decays to ^{119}Sn) as our probe nucleus. References [12] and [17–19] in our original paper (including work by Weyer *et al.*) clearly demonstrate that Sb is very efficient at trapping vacancies in *c*-Si, and furthermore that the Sb-vacancy complex in *c*-Si is readily distinguishable using Mössbauer spectroscopy.

A second issue is that the *a*-Si layers used in previous Mössbauer studies were neither pure nor well characterized. These *a*-Si layers generally contained high concentrations (~ 1 at.%) of Mössbauer atoms or other impurities. Furthermore, any amorphizing implants did not produce continuous amorphous material from the surface to a depth significantly deeper than the range of implanted Mössbauer probe atoms. In many cases no prior amorphizing implant was even performed. In contrast, the *a*-Si layers in our study were created by implanting Si into *c*-Si, resulting in a continuous, well-characterized amorphous layer from the surface to a depth of ≈ 750 nm [2,5], much deeper than the Sb implant profile. This is the first experiment in which the Mössbauer signal is unambiguously from the *a*-Si.

(ii) "This interpretation of the main results from their experiment is not sound. . ."

Our translation of Weyer's lengthy arguments is as follows: *Sb-defect complexes are formed in the collision cascade during implantation, so the same complexes are found in both c-Si and a-Si. Therefore, the observation of Sb-vacancy complexes in a-Si provides no information about point defects in the a-Si itself.*

The primary conclusion from the experimental data in our paper is that "Mössbauer spectroscopy of ^{119}Sb in *a*-Si demonstrates that Sb occupies two distinct sites in the *a*-Si network. These sites are identified by close analogy with *c*-Si data as substitutional fourfold coordinated Sb and an Sb-vacancy complex" [2]. We then suggest that these data indicate the existence of point defects in *a*-Si. The sites we identify are indeed associated with the Sb, since that is our probe atom.

The emphasis in the Comment is on the impurity

defining its own surroundings during the final phase of the collision cascade. However, this ignores the constraint that the Sb site must *also* be acceptable to the covalently bonded Si. In the *c*-Si lattice, Sb fits either on a substitutional lattice site or as an Sb-vacancy complex. This limited choice of sites is forced by the surrounding lattice. In *a*-Si, one could picture the random network deforming to give an Sb atom whatever environment it wanted, without any constraints. Instead, two distinct sites for Sb in *a*-Si are observed experimentally, with Mössbauer parameters that conform closely to Sb sites in the crystal. This requires the bonding constraints imposed by the *a*-Si network to correspond closely to those in *c*-Si. Of course, if the network imposes bonding constraints on Sb, the network also imposes constraints on itself. Since such constraints lead to vacancies in *c*-Si, the proposal that vacancies may exist in *a*-Si is reasonable.

Furthermore, if processes in the collision cascade would completely determine the final site of the Sb atom, without influence of the surrounding matrix, one would not expect differences in the Mössbauer spectra after low-dose implantations of ^{119}Sb into crystal or amorphous silicon. However, the relative intensity of the Mössbauer line associated with Sb-vacancy complexes is larger for *a*-Si than for *c*-Si. This implies that in addition to vacancies trapped in their own damage cascade, a fraction of the Sb atoms in vacancy complexes must have trapped vacancies from the *a*-Si network.

Our data are the first Mössbauer experiment carried out on pure, well-characterized *a*-Si with very low probe concentrations contained completely within a well-characterized *a*-Si layer, and is thus the first to unambiguously probe *a*-Si properties. The *a*-Si network constrains the Sb to occupy sites that closely correspond to sites in *c*-Si. Our Letter is "the first local structural evidence indicating the existence of point defects in *a*-Si."

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